Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 12:31 PM EDT

PDB ID	:	3C2W
Title	:	Crystal structure of the photosensory core domain of P. aeruginosa bacteriophytochrome PaBphP in the Pfr state
Authors	:	Yang, X.; Kuk, J.; Moffat, K.
Deposited on	:	2008-01-25
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

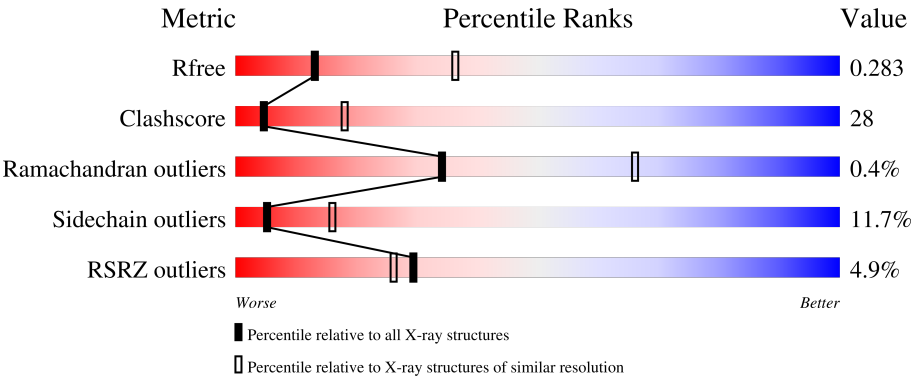
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	.% 48% 41% 6% 5%
1	B	505	6% 46% 41% 6% 7%
1	C	505	.% 48% 41% 7% 5%
1	D	505	5% 49% 41% 5% 5%
1	E	505	6% 47% 41% 6% 7%

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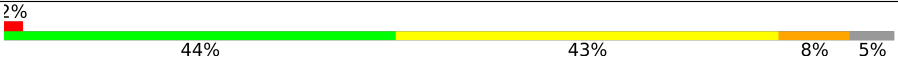
Mol	Chain	Length	Quality of chain
1	F	505	
1	G	505	
1	H	505	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30494 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3782	2382	681	700	19			
1	B	468	Total	C	N	O	S	0	0	0
			3693	2322	663	689	19			
1	C	482	Total	C	N	O	S	0	0	0
			3812	2398	688	707	19			
1	D	478	Total	C	N	O	S	0	0	0
			3788	2383	683	703	19			
1	E	471	Total	C	N	O	S	0	0	0
			3725	2344	673	689	19			
1	F	469	Total	C	N	O	S	0	0	0
			3704	2331	664	690	19			
1	G	482	Total	C	N	O	S	0	1	0
			3816	2401	688	707	20			
1	H	480	Total	C	N	O	S	0	0	0
			3800	2392	686	703	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP Q9HWR3
A	499	GLU	-	expression tag	UNP Q9HWR3
A	500	HIS	-	expression tag	UNP Q9HWR3
A	501	HIS	-	expression tag	UNP Q9HWR3
A	502	HIS	-	expression tag	UNP Q9HWR3
A	503	HIS	-	expression tag	UNP Q9HWR3
A	504	HIS	-	expression tag	UNP Q9HWR3
A	505	HIS	-	expression tag	UNP Q9HWR3
B	498	LEU	-	expression tag	UNP Q9HWR3
B	499	GLU	-	expression tag	UNP Q9HWR3
B	500	HIS	-	expression tag	UNP Q9HWR3
B	501	HIS	-	expression tag	UNP Q9HWR3
B	502	HIS	-	expression tag	UNP Q9HWR3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3
C	498	LEU	-	expression tag	UNP Q9HWR3
C	499	GLU	-	expression tag	UNP Q9HWR3
C	500	HIS	-	expression tag	UNP Q9HWR3
C	501	HIS	-	expression tag	UNP Q9HWR3
C	502	HIS	-	expression tag	UNP Q9HWR3
C	503	HIS	-	expression tag	UNP Q9HWR3
C	504	HIS	-	expression tag	UNP Q9HWR3
C	505	HIS	-	expression tag	UNP Q9HWR3
D	498	LEU	-	expression tag	UNP Q9HWR3
D	499	GLU	-	expression tag	UNP Q9HWR3
D	500	HIS	-	expression tag	UNP Q9HWR3
D	501	HIS	-	expression tag	UNP Q9HWR3
D	502	HIS	-	expression tag	UNP Q9HWR3
D	503	HIS	-	expression tag	UNP Q9HWR3
D	504	HIS	-	expression tag	UNP Q9HWR3
D	505	HIS	-	expression tag	UNP Q9HWR3
E	498	LEU	-	expression tag	UNP Q9HWR3
E	499	GLU	-	expression tag	UNP Q9HWR3
E	500	HIS	-	expression tag	UNP Q9HWR3
E	501	HIS	-	expression tag	UNP Q9HWR3
E	502	HIS	-	expression tag	UNP Q9HWR3
E	503	HIS	-	expression tag	UNP Q9HWR3
E	504	HIS	-	expression tag	UNP Q9HWR3
E	505	HIS	-	expression tag	UNP Q9HWR3
F	498	LEU	-	expression tag	UNP Q9HWR3
F	499	GLU	-	expression tag	UNP Q9HWR3
F	500	HIS	-	expression tag	UNP Q9HWR3
F	501	HIS	-	expression tag	UNP Q9HWR3
F	502	HIS	-	expression tag	UNP Q9HWR3
F	503	HIS	-	expression tag	UNP Q9HWR3
F	504	HIS	-	expression tag	UNP Q9HWR3
F	505	HIS	-	expression tag	UNP Q9HWR3
G	498	LEU	-	expression tag	UNP Q9HWR3
G	499	GLU	-	expression tag	UNP Q9HWR3
G	500	HIS	-	expression tag	UNP Q9HWR3
G	501	HIS	-	expression tag	UNP Q9HWR3
G	502	HIS	-	expression tag	UNP Q9HWR3
G	503	HIS	-	expression tag	UNP Q9HWR3
G	504	HIS	-	expression tag	UNP Q9HWR3

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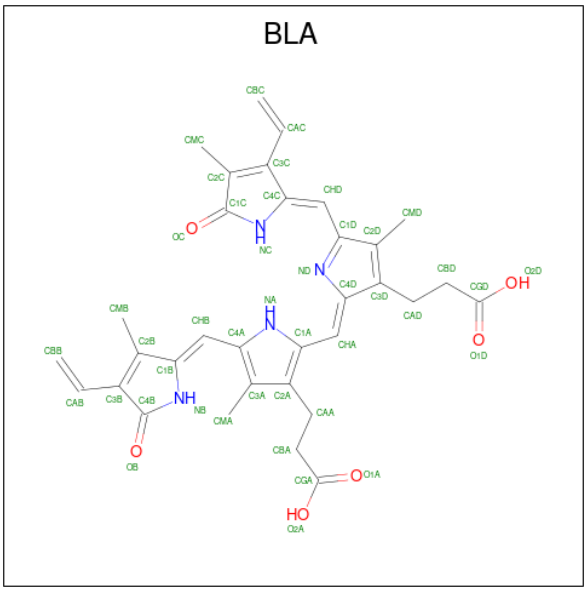
Chain	Residue	Modelled	Actual	Comment	Reference
G	505	HIS	-	expression tag	UNP Q9HWR3
H	498	LEU	-	expression tag	UNP Q9HWR3
H	499	GLU	-	expression tag	UNP Q9HWR3
H	500	HIS	-	expression tag	UNP Q9HWR3
H	501	HIS	-	expression tag	UNP Q9HWR3
H	502	HIS	-	expression tag	UNP Q9HWR3
H	503	HIS	-	expression tag	UNP Q9HWR3
H	504	HIS	-	expression tag	UNP Q9HWR3
H	505	HIS	-	expression tag	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		
2	E	1	Total	C	N	O	0	0
			43	33	4	6		
2	F	1	Total	C	N	O	0	0
			43	33	4	6		
2	G	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 3 is water.

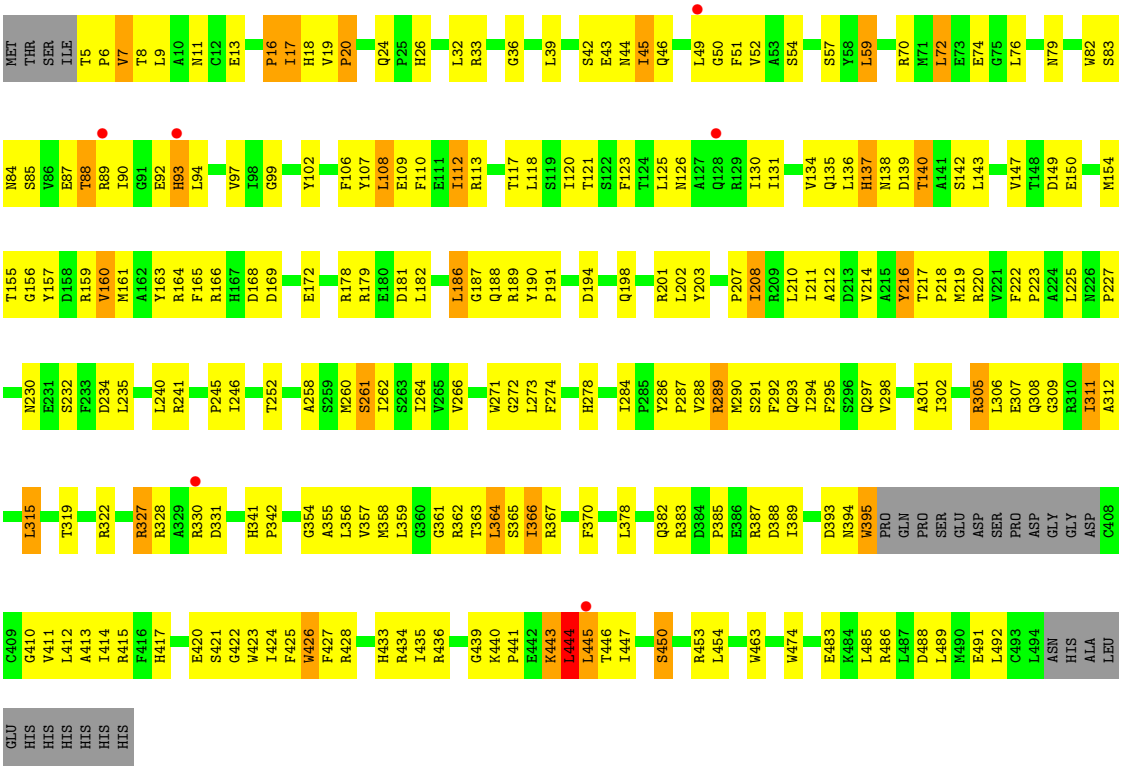
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	2	Total	O	0	0
			2	2		
3	C	6	Total	O	0	0
			6	6		
3	D	3	Total	O	0	0
			3	3		
3	E	1	Total	O	0	0
			1	1		
3	F	2	Total	O	0	0
			2	2		
3	G	7	Total	O	0	0
			7	7		
3	H	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

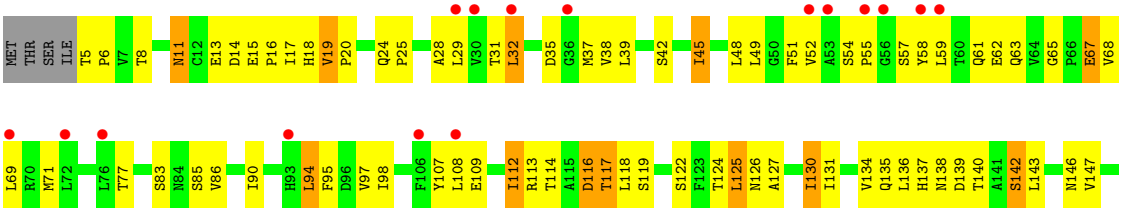
• Molecule 1: Bacteriophytochrome

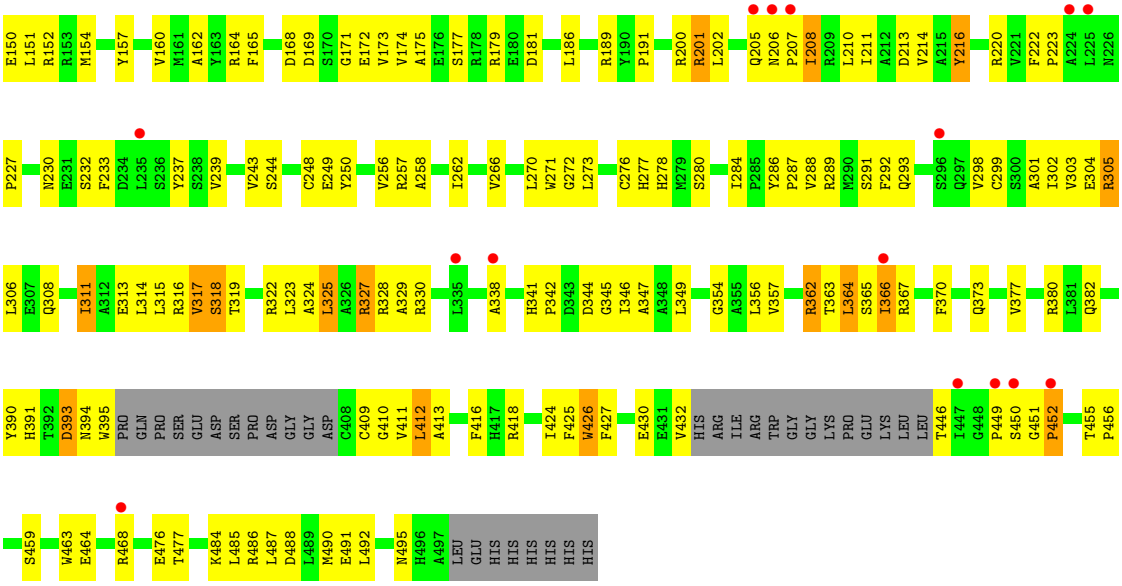
Chain A:



• Molecule 1: Bacteriophytochrome

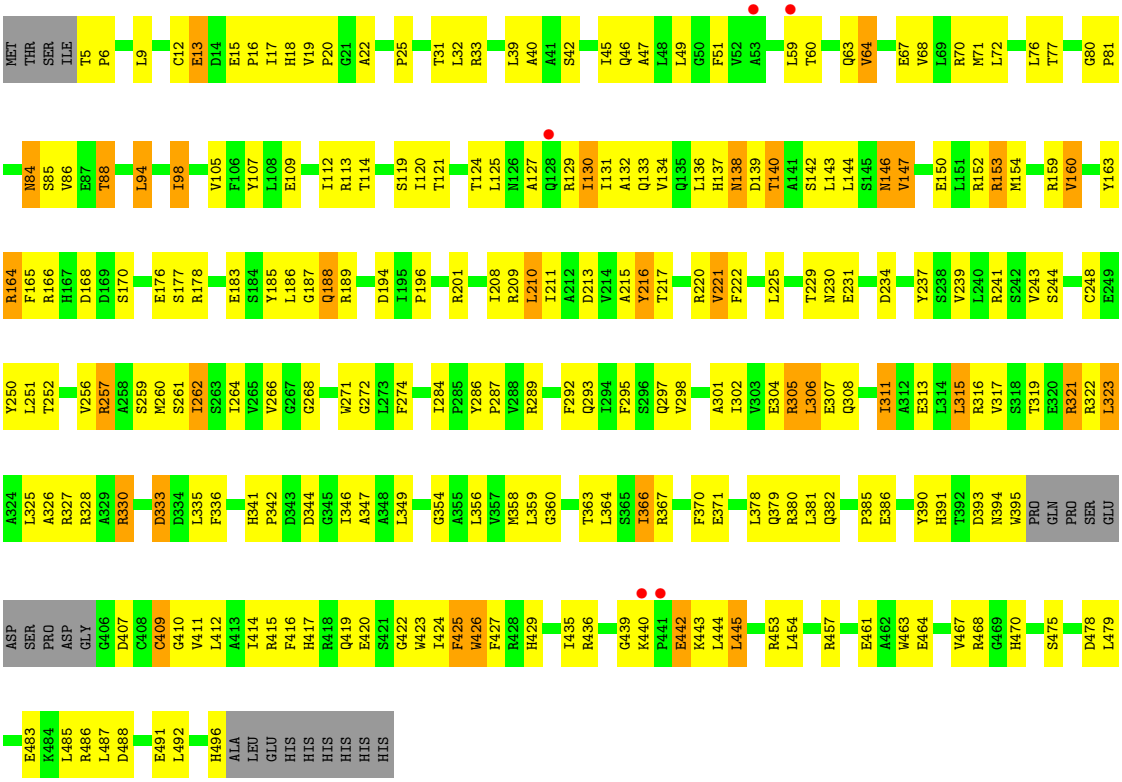
Chain B:





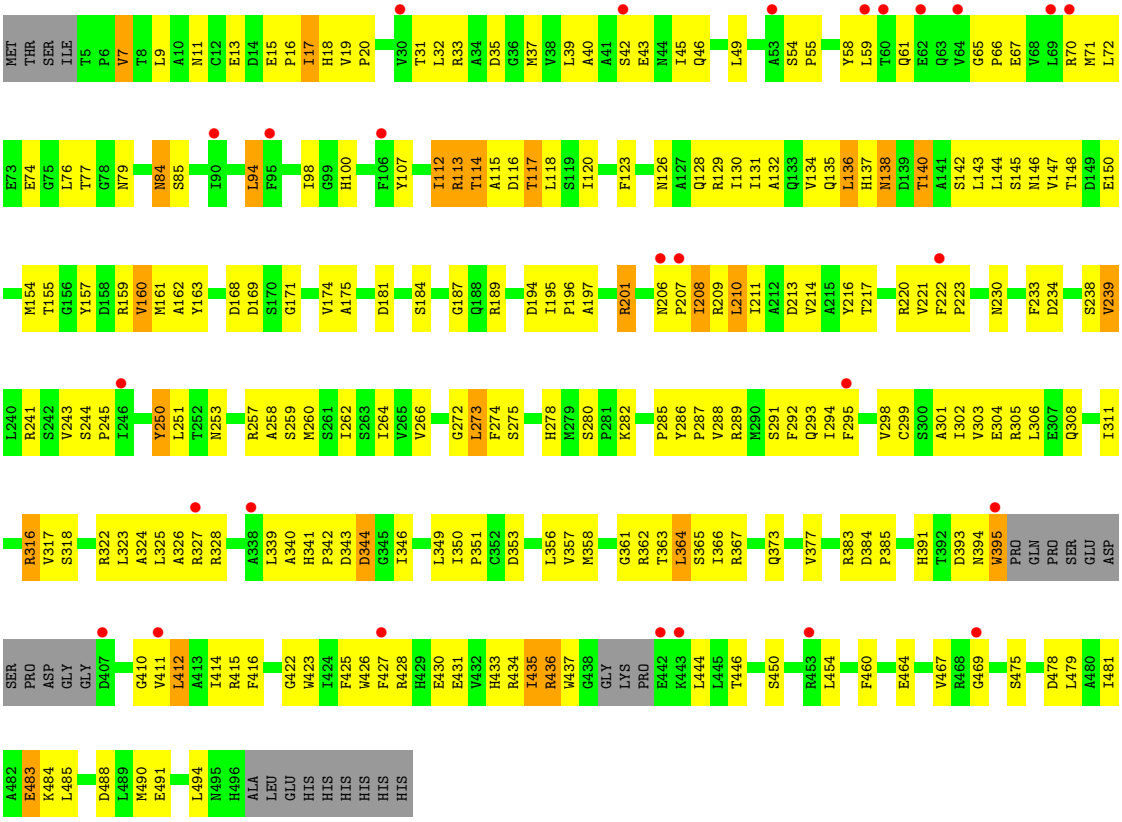
• Molecule 1: Bacteriophytochrome

Chain C:



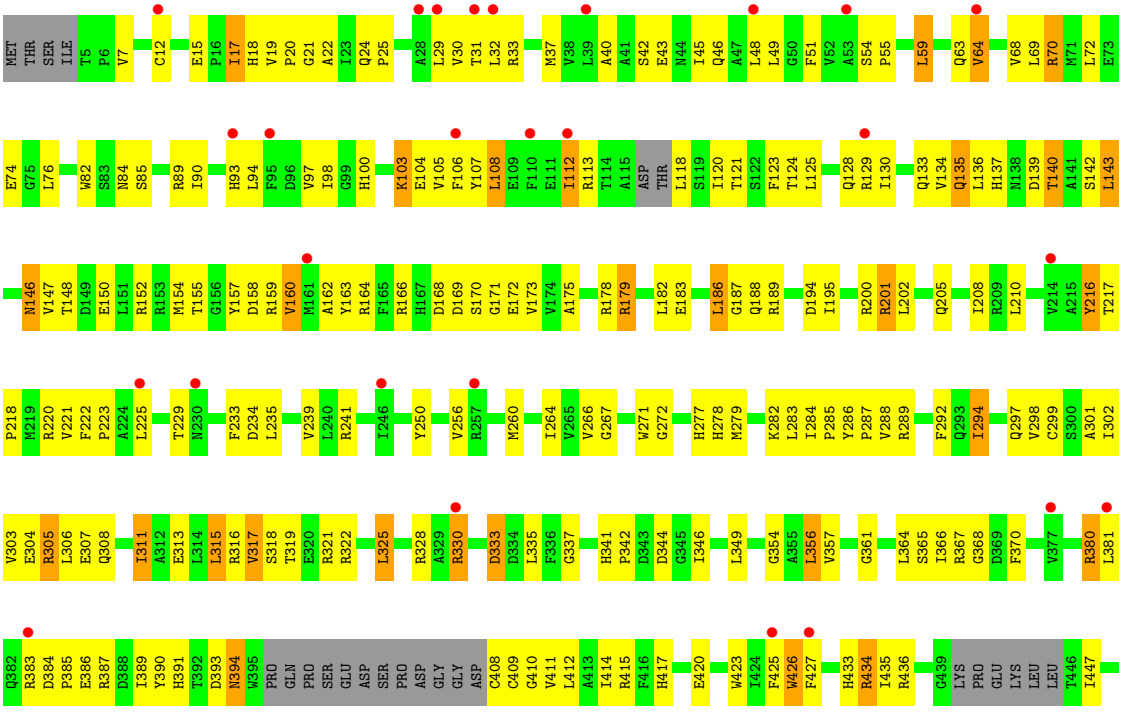
• Molecule 1: Bacteriophytochrome

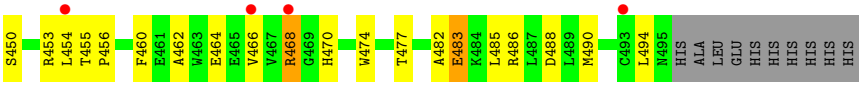
Chain D:



• Molecule 1: Bacteriophytochrome

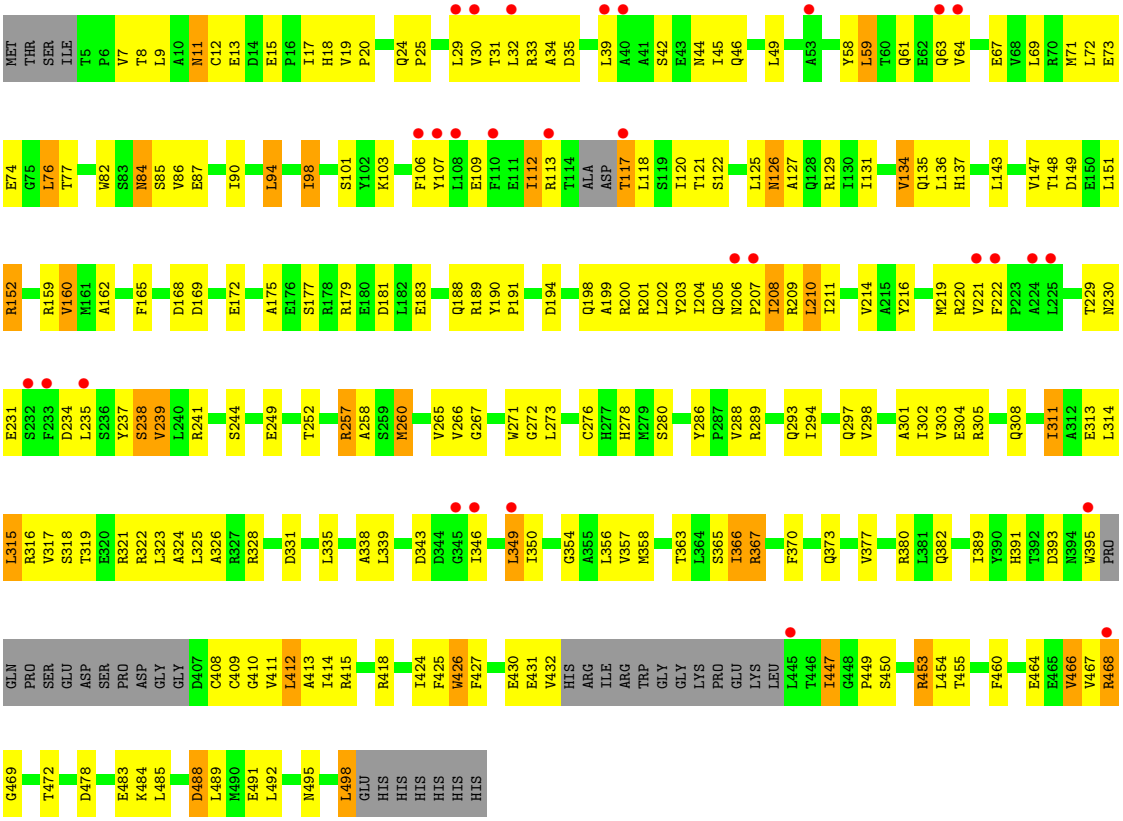
Chain E:





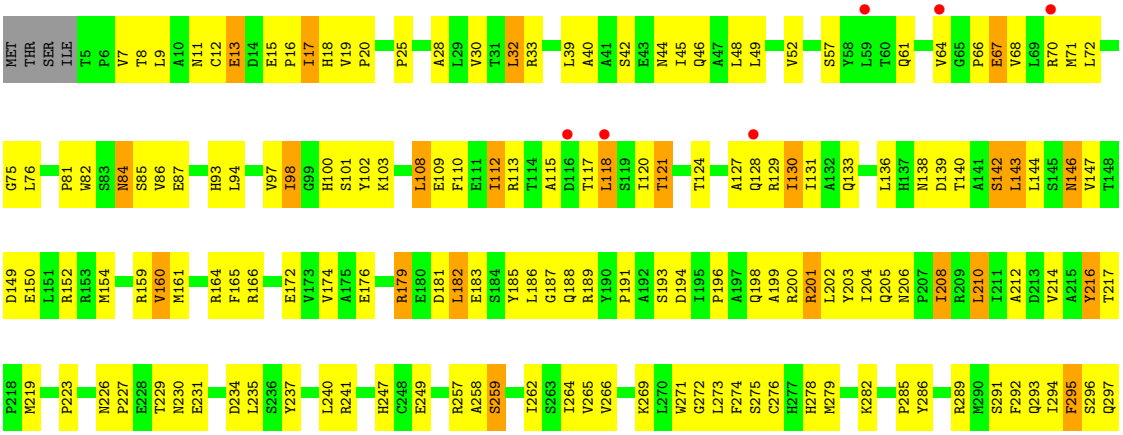
• Molecule 1: Bacteriophytochrome

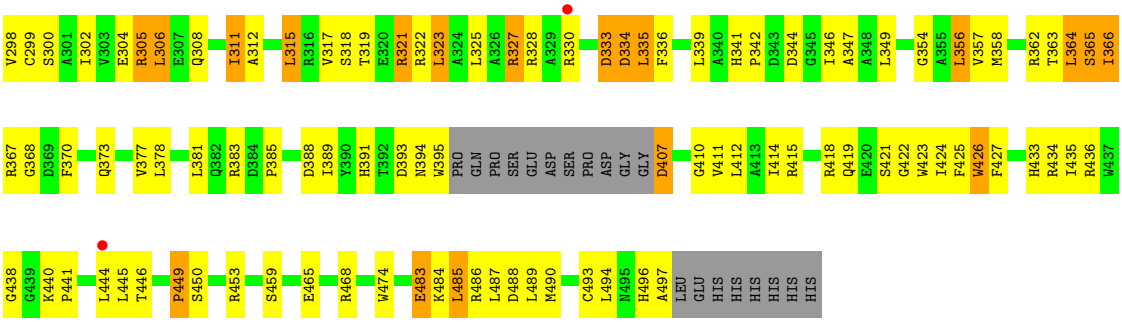
Chain F:



• Molecule 1: Bacteriophytochrome

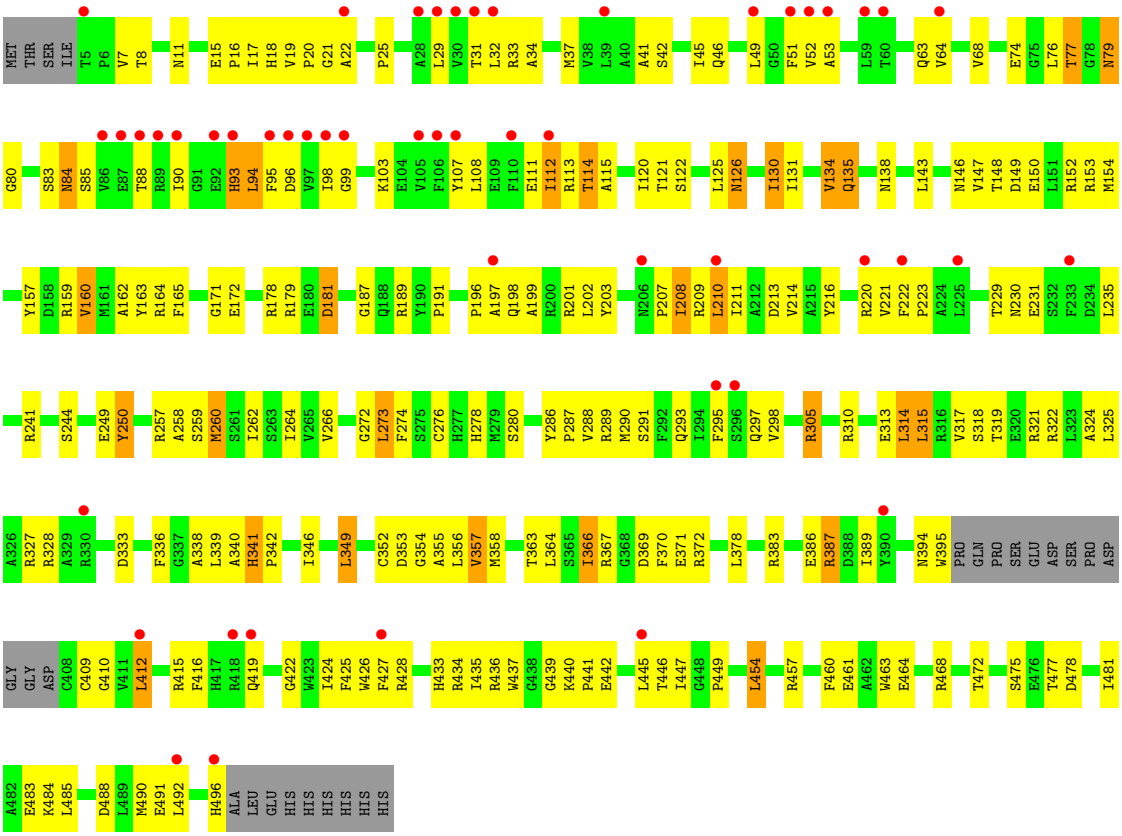
Chain G:





- Molecule 1: Bacteriophytochrome

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	154.42Å 164.25Å 434.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 49.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	72.1 (15.00-2.90) 60.1 (49.96-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.283 0.216 , 0.283	Depositor DCC
R_{free} test set	4546 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	30494	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/3866	0.59	4/5247 (0.1%)
1	B	0.26	0/3773	0.50	0/5122
1	C	0.33	1/3897 (0.0%)	0.58	2/5289 (0.0%)
1	D	0.26	0/3871	0.49	0/5253
1	E	0.26	0/3806	0.49	0/5163
1	F	0.26	0/3783	0.52	1/5134 (0.0%)
1	G	0.36	2/3904 (0.1%)	0.57	3/5299 (0.1%)
1	H	0.26	0/3885	0.49	0/5273
All	All	0.29	3/30785 (0.0%)	0.53	10/41780 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	G	0	1
All	All	1	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	333	ASP	CB-CG	5.53	1.63	1.51
1	C	442	GLU	CB-CG	5.28	1.62	1.52
1	G	334	ASP	CA-CB	5.21	1.65	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	498	LEU	CB-CG-CD2	-12.96	88.97	111.00
1	A	444	LEU	CB-CA-C	10.35	129.87	110.20
1	G	333	ASP	CB-CG-OD2	7.60	125.14	118.30
1	C	153	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	G	333	ASP	N-CA-C	7.13	130.25	111.00
1	C	333	ASP	N-CA-C	6.83	129.44	111.00
1	A	444	LEU	N-CA-CB	6.70	123.79	110.40
1	A	445	LEU	N-CA-CB	6.18	122.76	110.40
1	A	445	LEU	CA-CB-CG	5.63	128.24	115.30
1	G	333	ASP	CA-C-N	5.28	128.81	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	444	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	443	LYS	Peptide
1	A	444	LEU	Mainchain,Peptide
1	G	333	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3782	0	3730	236	1
1	B	3693	0	3626	211	0
1	C	3812	0	3750	209	1
1	D	3788	0	3723	219	0
1	E	3725	0	3662	231	0
1	F	3704	0	3642	215	0
1	G	3816	0	3757	247	0
1	H	3800	0	3743	201	0
2	A	43	0	31	6	0
2	B	43	0	31	6	0
2	C	43	0	30	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	11	0
2	E	43	0	31	8	0
2	F	43	0	31	7	0
2	G	43	0	31	10	0
2	H	43	0	30	10	0
3	A	7	0	0	0	0
3	B	2	0	0	0	0
3	C	6	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	7	0	0	2	0
3	H	2	0	0	0	0
All	All	30494	0	29878	1694	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ARG:CD	1:F:498:LEU:HD21	1.25	1.57
1:C:153:ARG:HD3	1:F:498:LEU:CD2	1.13	1.56
1:C:153:ARG:NH1	1:F:498:LEU:HD11	1.41	1.35
1:C:257:ARG:HG2	1:C:257:ARG:HH11	1.04	1.13
1:E:48:LEU:HD11	1:E:93:HIS:HD2	1.16	1.05
1:A:444:LEU:CD1	1:A:447:ILE:HD11	1.88	1.03
1:D:42:SER:HB3	1:D:221:VAL:HG12	1.40	1.02
1:A:444:LEU:HD12	1:A:447:ILE:CD1	1.90	1.02
1:C:153:ARG:NH1	1:F:498:LEU:CD1	2.23	1.02
2:G:900:BLA:HMC1	2:G:900:BLA:HBC1	1.41	1.02
1:A:444:LEU:HD12	1:A:447:ILE:HD11	1.06	1.02
1:G:347:ALA:HB2	1:G:366:ILE:HD11	1.42	0.99
1:D:412:LEU:HB3	1:D:426:TRP:HD1	1.28	0.99
1:E:305:ARG:HA	1:E:308:GLN:HG2	1.46	0.98
1:F:87:GLU:HB3	1:F:113:ARG:NH1	1.79	0.97
1:G:179:ARG:HG2	1:G:179:ARG:HH11	1.26	0.96
1:A:364:LEU:HD21	1:G:435:ILE:HG22	1.45	0.94
1:E:140:THR:HG22	1:E:306:LEU:HB3	1.50	0.94
1:A:417:HIS:CD2	1:A:420:GLU:HB2	2.02	0.94
1:A:417:HIS:HD2	1:A:420:GLU:HB2	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:ASN:HD21	1:E:470:HIS:CD2	1.86	0.94
1:A:125:LEU:HD11	1:B:83:SER:HB3	1.49	0.93
1:D:356:LEU:HD21	1:D:363:THR:HG23	1.51	0.92
1:A:415:ARG:HD3	1:A:423:TRP:CZ2	2.03	0.92
1:B:356:LEU:HD23	1:B:365:SER:HB3	1.52	0.91
1:B:327:ARG:HG3	1:B:327:ARG:HH11	1.35	0.91
1:C:45:ILE:HD12	1:C:46:GLN:H	1.34	0.91
1:A:130:ILE:HD11	1:A:150:GLU:HG2	1.53	0.91
1:F:266:VAL:HG22	1:F:271:TRP:HB2	1.51	0.91
1:H:79:ASN:HD22	1:H:80:GLY:H	1.19	0.91
1:C:264:ILE:HB	1:C:272:GLY:O	1.70	0.91
1:B:210:LEU:HD12	1:B:289:ARG:HD3	1.50	0.91
1:A:327:ARG:HA	1:B:330:ARG:NH1	1.85	0.91
1:G:112:ILE:HD13	1:G:112:ILE:H	1.35	0.90
1:H:220:ARG:HE	1:H:222:PHE:HZ	1.13	0.89
1:H:21:GLY:O	1:H:221:VAL:HG22	1.72	0.89
1:C:257:ARG:HH11	1:C:257:ARG:CG	1.86	0.89
1:D:210:LEU:HD12	1:D:289:ARG:HD3	1.53	0.88
1:B:130:ILE:HD13	1:B:130:ILE:H	1.35	0.88
1:E:48:LEU:HD11	1:E:93:HIS:CD2	2.06	0.88
1:H:220:ARG:NE	1:H:222:PHE:HZ	1.70	0.87
1:G:20:PRO:HD2	1:G:235:LEU:HD12	1.57	0.87
1:G:165:PHE:HD1	1:G:272:GLY:HA2	1.37	0.87
1:C:305:ARG:HA	1:C:308:GLN:HG2	1.57	0.87
1:D:19:VAL:HG12	1:D:234:ASP:HA	1.55	0.87
1:C:257:ARG:HG2	1:C:257:ARG:NH1	1.83	0.86
1:C:304:GLU:HG2	1:D:135:GLN:HE22	1.39	0.86
1:G:33:ARG:HB3	1:G:39:LEU:HD11	1.57	0.86
1:C:153:ARG:NE	1:F:498:LEU:HD21	1.91	0.86
1:A:220:ARG:HG3	1:A:220:ARG:HH11	1.41	0.85
1:C:153:ARG:HH12	1:F:498:LEU:HD11	1.42	0.85
1:C:215:ALA:HB3	1:C:257:ARG:HH12	1.41	0.85
1:A:45:ILE:HD12	1:A:46:GLN:H	1.42	0.85
1:E:306:LEU:HD11	1:F:305:ARG:NH2	1.92	0.84
1:A:252:THR:O	1:A:445:LEU:HD21	1.78	0.84
1:G:139:ASP:HB2	1:G:142:SER:HB2	1.60	0.83
1:A:436:ARG:O	1:G:364:LEU:HA	1.78	0.83
1:G:336:PHE:HB3	1:G:364:LEU:HD21	1.58	0.83
1:D:112:ILE:HD13	1:D:112:ILE:H	1.42	0.83
1:E:380:ARG:HB2	1:E:380:ARG:HH11	1.44	0.83
1:E:453:ARG:O	1:E:453:ARG:HD3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:VAL:HG21	1:D:143:LEU:HD23	1.62	0.82
2:H:900:BLA:HBC1	2:H:900:BLA:HMC1	1.62	0.82
1:E:319:THR:HG22	1:E:322:ARG:HH21	1.44	0.82
1:C:153:ARG:CD	1:F:498:LEU:CD2	2.10	0.81
1:F:220:ARG:HG3	1:F:220:ARG:HH11	1.43	0.81
1:C:153:ARG:HH11	1:F:498:LEU:CD1	1.93	0.81
1:G:266:VAL:HG22	1:G:271:TRP:HB2	1.62	0.81
1:D:258:ALA:HB3	1:D:278:HIS:HB3	1.60	0.81
1:A:20:PRO:HD2	1:A:235:LEU:HD12	1.61	0.81
1:C:323:LEU:HA	1:D:323:LEU:HD12	1.63	0.80
1:D:147:VAL:HG11	1:D:295:PHE:CZ	2.16	0.80
1:C:330:ARG:HH21	1:C:496:HIS:HB3	1.44	0.80
1:B:305:ARG:HA	1:B:308:GLN:HG2	1.62	0.80
1:G:356:LEU:HB3	1:G:425:PHE:HB2	1.62	0.80
1:G:8:THR:H	1:G:11:ASN:HB2	1.46	0.79
1:H:112:ILE:H	1:H:112:ILE:HD13	1.47	0.79
1:F:33:ARG:HB3	1:F:39:LEU:HD11	1.65	0.79
1:F:117:THR:O	1:F:118:LEU:HD23	1.81	0.79
1:A:434:ARG:HG2	1:A:435:ILE:HG23	1.61	0.79
1:A:441:PRO:HB3	1:A:443:LYS:CE	2.12	0.79
1:E:21:GLY:HA2	1:E:233:PHE:CZ	2.18	0.79
1:B:327:ARG:HH11	1:B:327:ARG:CG	1.96	0.79
1:B:162:ALA:HB3	1:B:175:ALA:HB3	1.64	0.79
1:C:153:ARG:HH11	1:F:498:LEU:HD11	1.43	0.79
1:C:196:PRO:HG3	2:C:900:BLA:HAC	1.63	0.79
1:A:341:HIS:CD2	1:A:342:PRO:HD2	2.17	0.78
1:C:124:THR:HA	1:D:294:ILE:HD11	1.65	0.78
1:D:412:LEU:HB3	1:D:426:TRP:CD1	2.17	0.78
1:H:42:SER:O	1:H:45:ILE:HG13	1.84	0.78
1:B:418:ARG:HB3	1:H:201:ARG:HH22	1.49	0.78
1:F:339:LEU:HD13	1:F:357:VAL:HG21	1.65	0.77
1:H:20:PRO:HD2	1:H:235:LEU:HD12	1.64	0.77
1:A:308:GLN:HA	1:A:311:ILE:HD12	1.67	0.77
1:F:94:LEU:HD23	1:F:113:ARG:NH1	2.00	0.77
1:G:196:PRO:HD2	1:G:199:ALA:HB3	1.66	0.77
1:G:201:ARG:HG2	1:G:201:ARG:HH11	1.50	0.77
1:D:9:LEU:HD21	1:D:450:SER:HB2	1.66	0.77
2:E:900:BLA:HMC1	2:E:900:BLA:HBC1	1.67	0.76
1:B:61:GLN:HA	1:B:69:LEU:CD1	2.15	0.76
1:G:264:ILE:HD11	1:G:274:PHE:CE1	2.21	0.76
2:C:900:BLA:HMB3	2:C:900:BLA:CMA	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:VAL:HG11	1:D:295:PHE:HZ	1.50	0.76
1:G:434:ARG:CZ	1:G:435:ILE:HD11	2.15	0.76
1:F:86:VAL:HG12	1:F:87:GLU:H	1.49	0.76
1:E:162:ALA:HB3	1:E:175:ALA:HB3	1.68	0.75
1:G:336:PHE:HD2	1:G:364:LEU:CD2	1.99	0.75
1:C:153:ARG:HD3	1:F:498:LEU:HD22	1.59	0.75
1:E:139:ASP:OD1	1:E:142:SER:HB2	1.85	0.75
1:H:7:VAL:HA	1:H:11:ASN:HD22	1.52	0.75
1:A:363:THR:HB	1:G:438:GLY:HA3	1.68	0.74
1:C:72:LEU:O	1:C:76:LEU:HD13	1.86	0.74
1:H:394:ASN:O	1:H:395:TRP:HB2	1.88	0.74
2:B:900:BLA:HMB3	2:B:900:BLA:CMA	2.16	0.74
1:H:286:TYR:HB3	1:H:287:PRO:HD3	1.69	0.74
1:D:214:VAL:HB	1:D:257:ARG:HA	1.69	0.74
2:H:900:BLA:HMB3	2:H:900:BLA:CMA	2.17	0.74
1:H:258:ALA:HB3	1:H:278:HIS:HB3	1.70	0.74
1:G:165:PHE:CD1	1:G:272:GLY:HA2	2.21	0.73
1:G:434:ARG:NE	1:G:435:ILE:HD11	2.02	0.73
1:B:208:ILE:HD13	1:B:208:ILE:H	1.53	0.73
1:D:45:ILE:HD12	1:D:46:GLN:H	1.53	0.73
1:B:324:ALA:HA	1:B:327:ARG:HD2	1.71	0.73
1:C:51:PHE:CG	1:C:63:GLN:HB2	2.24	0.73
1:A:72:LEU:O	1:A:76:LEU:HD13	1.89	0.73
1:C:215:ALA:HB3	1:C:257:ARG:HH22	1.53	0.73
1:C:391:HIS:HA	1:C:411:VAL:O	1.87	0.73
1:E:164:ARG:O	1:E:171:GLY:HA2	1.88	0.73
2:A:900:BLA:HMB3	2:A:900:BLA:CMA	2.18	0.72
1:C:443:LYS:O	1:C:444:LEU:C	2.24	0.72
1:F:210:LEU:HD12	1:F:289:ARG:HD3	1.71	0.72
1:A:284:ILE:HG22	1:A:289:ARG:HG3	1.71	0.72
1:C:215:ALA:CB	1:C:257:ARG:HH12	2.01	0.72
1:D:148:THR:HG23	1:D:160:VAL:HG22	1.72	0.72
1:E:328:ARG:HH12	1:E:344:ASP:HB2	1.54	0.72
1:F:29:LEU:HD12	1:F:109:GLU:HG2	1.71	0.72
2:G:900:BLA:HMB3	2:G:900:BLA:CMA	2.19	0.72
1:G:194:ASP:HB3	2:G:900:BLA:HHB	1.70	0.72
1:E:45:ILE:O	1:E:49:LEU:HB2	1.88	0.72
1:B:208:ILE:HD12	1:B:293:GLN:HG3	1.72	0.72
2:C:900:BLA:HMB3	2:C:900:BLA:HMA2	1.71	0.72
1:H:214:VAL:HB	1:H:257:ARG:HA	1.72	0.72
1:C:45:ILE:HD12	1:C:46:GLN:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:ALA:HB3	1:F:278:HIS:HB3	1.71	0.71
1:F:468:ARG:CZ	1:F:468:ARG:HA	2.21	0.71
1:F:325:LEU:HD12	1:F:326:ALA:N	2.05	0.71
1:C:152:ARG:HD2	1:C:177:SER:OG	1.91	0.71
2:F:900:BLA:CMA	2:F:900:BLA:HMB3	2.21	0.71
1:F:162:ALA:HB3	1:F:175:ALA:HB3	1.73	0.71
1:D:113:ARG:NH2	1:D:117:THR:HG23	2.05	0.70
1:G:45:ILE:HD12	1:G:46:GLN:N	2.06	0.70
1:G:336:PHE:HD2	1:G:364:LEU:HD23	1.56	0.70
1:A:264:ILE:HD11	1:A:274:PHE:CE1	2.25	0.70
1:F:380:ARG:HH11	1:F:380:ARG:HB2	1.56	0.70
1:F:24:GLN:HE22	1:F:211:ILE:HA	1.57	0.70
1:E:20:PRO:HD2	1:E:235:LEU:HD12	1.72	0.70
1:H:484:LYS:O	1:H:488:ASP:HB2	1.91	0.70
1:A:7:VAL:HG21	1:A:245:PRO:HG2	1.73	0.70
1:A:208:ILE:HD12	1:A:293:GLN:HE21	1.57	0.70
1:A:210:LEU:HD23	1:A:211:ILE:N	2.05	0.70
1:D:33:ARG:HB3	1:D:39:LEU:HD11	1.72	0.70
1:F:45:ILE:HD12	1:F:46:GLN:N	2.05	0.70
1:C:153:ARG:HD3	1:F:498:LEU:HD23	1.57	0.70
1:C:187:GLY:HA3	1:C:435:ILE:HD12	1.72	0.70
1:G:179:ARG:HH11	1:G:179:ARG:CG	2.03	0.70
1:G:383:ARG:O	1:G:385:PRO:HD3	1.90	0.70
1:B:200:ARG:HD3	1:H:386:GLU:OE2	1.91	0.70
1:G:414:ILE:HD12	1:G:486:ARG:HB2	1.74	0.70
1:B:346:ILE:O	1:B:426:TRP:HZ3	1.75	0.69
1:D:394:ASN:O	1:D:395:TRP:HB3	1.92	0.69
1:F:380:ARG:HB2	1:F:380:ARG:NH1	2.06	0.69
1:A:17:ILE:H	1:A:17:ILE:HD12	1.57	0.69
1:D:346:ILE:O	1:D:426:TRP:HZ3	1.75	0.69
1:A:159:ARG:HD3	1:A:161:MET:SD	2.32	0.69
1:B:220:ARG:HE	1:B:222:PHE:HZ	1.41	0.69
1:A:305:ARG:HA	1:A:308:GLN:HG2	1.75	0.69
1:G:67:GLU:HA	1:G:70:ARG:HD2	1.74	0.69
1:B:249:GLU:OE2	1:B:450:SER:HB2	1.92	0.69
1:G:327:ARG:HH11	1:H:491:GLU:HG2	1.57	0.69
1:B:258:ALA:HB3	1:B:278:HIS:HB3	1.74	0.69
1:F:220:ARG:CZ	1:F:222:PHE:HZ	2.05	0.68
1:F:366:ILE:HD13	1:F:366:ILE:H	1.58	0.68
1:C:335:LEU:HD21	1:C:492:LEU:HD23	1.75	0.68
1:E:260:MET:HE3	1:E:289:ARG:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:491:GLU:O	1:F:495:ASN:HB2	1.93	0.68
1:A:130:ILE:CD1	1:A:150:GLU:HG2	2.23	0.68
1:A:414:ILE:HD12	1:A:486:ARG:HB2	1.76	0.68
1:E:89:ARG:HH21	1:E:94:LEU:HG	1.58	0.68
1:F:408:CYS:SG	1:F:427:PHE:HB3	2.34	0.68
1:G:46:GLN:HG2	1:G:52:VAL:HG22	1.75	0.68
1:B:410:GLY:O	1:B:427:PHE:HA	1.94	0.68
2:H:900:BLA:HMB3	2:H:900:BLA:HMA2	1.75	0.68
2:D:900:BLA:HMB3	2:D:900:BLA:CMA	2.24	0.67
1:F:134:VAL:HG23	1:F:143:LEU:HD11	1.76	0.67
1:D:373:GLN:NE2	1:D:395:TRP:HE1	1.93	0.67
1:H:49:LEU:HB3	1:H:63:GLN:NE2	2.09	0.67
1:A:415:ARG:HB2	1:A:423:TRP:CZ3	2.30	0.67
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.28	0.67
1:C:134:VAL:CG1	1:C:302:ILE:HG12	2.24	0.67
1:C:215:ALA:HB3	1:C:257:ARG:NH1	2.09	0.67
1:C:317:VAL:O	1:C:321:ARG:HG2	1.94	0.67
1:B:8:THR:H	1:B:11:ASN:HB3	1.60	0.67
1:A:87:GLU:HG2	1:A:113:ARG:HH22	1.60	0.67
1:E:260:MET:CE	1:E:289:ARG:HG2	2.24	0.67
1:F:15:GLU:HG2	1:F:17:ILE:HG23	1.75	0.67
1:F:424:ILE:HD11	1:F:489:LEU:HD12	1.77	0.67
1:G:18:HIS:C	1:G:20:PRO:HD3	2.15	0.67
1:G:201:ARG:HH11	1:G:201:ARG:CG	2.08	0.67
1:G:327:ARG:NH1	1:H:491:GLU:HG2	2.10	0.66
1:A:439:GLY:O	1:A:441:PRO:HD3	1.95	0.66
1:B:39:LEU:HD22	1:B:227:PRO:HG2	1.75	0.66
1:E:152:ARG:HH21	1:E:179:ARG:HG2	1.59	0.66
1:H:84:ASN:ND2	1:H:85:SER:H	1.92	0.66
1:H:208:ILE:HD13	1:H:208:ILE:H	1.60	0.66
2:A:900:BLA:HMB3	2:A:900:BLA:HMA2	1.77	0.66
1:B:328:ARG:HB3	1:B:338:ALA:HB2	1.76	0.66
1:G:118:LEU:HD23	1:G:118:LEU:H	1.60	0.66
1:D:213:ASP:O	1:D:216:TYR:HB3	1.95	0.66
1:F:87:GLU:HB3	1:F:113:ARG:CZ	2.25	0.66
1:D:98:ILE:HG21	1:D:286:TYR:CD1	2.31	0.66
1:D:113:ARG:HH22	1:D:117:THR:HG23	1.60	0.66
1:F:214:VAL:HB	1:F:257:ARG:HA	1.78	0.66
1:E:194:ASP:HB3	2:E:900:BLA:HHB	1.77	0.66
1:A:150:GLU:O	1:A:154:MET:HG3	1.95	0.66
1:C:208:ILE:HD12	1:C:289:ARG:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:O	1:C:330:ARG:HD3	1.96	0.66
1:C:266:VAL:HG22	1:C:271:TRP:HB2	1.78	0.65
1:C:394:ASN:O	1:C:395:TRP:HB2	1.95	0.65
1:G:322:ARG:HD2	1:G:488:ASP:OD2	1.96	0.65
1:D:366:ILE:O	1:D:367:ARG:HB2	1.96	0.65
1:G:305:ARG:HA	1:G:308:GLN:HG2	1.78	0.65
1:G:394:ASN:O	1:G:395:TRP:HB2	1.96	0.65
1:A:117:THR:HG22	1:A:118:LEU:N	2.10	0.65
2:G:900:BLA:HMB3	2:G:900:BLA:HMA2	1.78	0.65
1:B:139:ASP:HB2	1:B:142:SER:HB2	1.78	0.65
1:E:308:GLN:HA	1:E:311:ILE:HD12	1.79	0.65
1:A:443:LYS:CB	1:A:444:LEU:HD22	2.27	0.65
1:B:147:VAL:O	1:B:151:LEU:HG	1.96	0.65
1:A:220:ARG:HG3	1:A:220:ARG:NH1	2.11	0.65
1:F:7:VAL:HA	1:F:11:ASN:HD22	1.62	0.65
1:H:387:ARG:HB3	1:H:387:ARG:HH11	1.61	0.65
1:E:21:GLY:HA2	1:E:233:PHE:HZ	1.59	0.64
1:A:45:ILE:CD1	1:A:46:GLN:H	2.10	0.64
1:D:299:CYS:O	1:D:303:VAL:HB	1.96	0.64
1:D:391:HIS:HB3	1:D:412:LEU:HD23	1.79	0.64
1:F:121:THR:O	1:F:125:LEU:HB2	1.96	0.64
1:G:139:ASP:HB2	1:G:142:SER:H	1.62	0.64
1:H:328:ARG:HD3	1:H:341:HIS:CE1	2.32	0.64
1:A:383:ARG:O	1:A:385:PRO:HD3	1.96	0.64
1:A:426:TRP:N	1:A:426:TRP:CD1	2.65	0.64
1:E:135:GLN:HE22	1:F:305:ARG:NH1	1.95	0.64
1:A:441:PRO:HB3	1:A:443:LYS:NZ	2.13	0.64
1:D:184:SER:HB3	1:D:437:TRP:CZ2	2.33	0.64
1:B:327:ARG:HG3	1:B:327:ARG:NH1	2.03	0.64
1:H:412:LEU:HB3	1:H:426:TRP:HD1	1.61	0.64
1:B:214:VAL:HB	1:B:257:ARG:HA	1.80	0.64
1:H:49:LEU:HB3	1:H:63:GLN:HE22	1.61	0.64
1:E:134:VAL:HG21	1:E:143:LEU:CB	2.28	0.64
1:F:112:ILE:HD13	1:F:112:ILE:H	1.62	0.64
1:C:381:LEU:HD21	1:C:390:TYR:CD1	2.33	0.64
1:F:94:LEU:CD2	1:F:113:ARG:HD3	2.28	0.64
1:F:94:LEU:HD22	1:F:113:ARG:HD3	1.80	0.64
1:F:172:GLU:HG3	1:F:189:ARG:HD3	1.80	0.64
1:G:318:SER:O	1:G:322:ARG:HB2	1.97	0.64
1:D:434:ARG:NH2	1:H:340:ALA:O	2.31	0.64
1:E:143:LEU:O	1:E:147:VAL:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:LEU:HD13	1:E:357:VAL:N	2.13	0.64
1:F:45:ILE:HD12	1:F:46:GLN:H	1.62	0.64
1:D:147:VAL:HG21	1:D:295:PHE:CZ	2.32	0.64
1:E:410:GLY:O	1:E:427:PHE:HA	1.97	0.64
1:H:8:THR:H	1:H:11:ASN:HB3	1.62	0.64
1:H:79:ASN:HD22	1:H:80:GLY:N	1.95	0.64
1:B:380:ARG:HB2	1:B:380:ARG:HH11	1.63	0.63
1:C:304:GLU:HG2	1:D:135:GLN:NE2	2.11	0.63
1:C:319:THR:HA	1:C:322:ARG:HB2	1.80	0.63
1:E:305:ARG:HB3	1:E:308:GLN:HE21	1.62	0.63
1:G:265:VAL:O	1:G:300:SER:HB3	1.98	0.63
1:H:94:LEU:HD21	1:H:113:ARG:HG2	1.80	0.63
1:F:220:ARG:HH11	1:F:220:ARG:CG	2.12	0.63
1:F:389:ILE:HD11	1:F:483:GLU:OE2	1.99	0.63
1:G:262:ILE:HD12	1:G:292:PHE:HB3	1.80	0.63
1:B:137:HIS:CD2	1:B:146:ASN:HD22	2.16	0.63
1:C:84:ASN:ND2	1:C:85:SER:H	1.97	0.63
1:F:201:ARG:HG3	1:F:205:GLN:HE21	1.64	0.63
1:F:319:THR:HG22	1:F:322:ARG:HH21	1.64	0.63
1:H:394:ASN:O	1:H:395:TRP:CB	2.47	0.63
1:H:412:LEU:HB3	1:H:426:TRP:CD1	2.34	0.63
1:C:60:THR:H	1:C:63:GLN:HE21	1.46	0.63
1:G:311:ILE:O	1:G:315:LEU:HB2	1.99	0.63
1:B:143:LEU:O	1:B:147:VAL:HG22	1.98	0.63
1:C:176:GLU:OE1	1:C:178:ARG:HD3	1.99	0.63
1:G:143:LEU:O	1:G:147:VAL:HG13	1.99	0.63
1:C:152:ARG:HB2	1:C:160:VAL:CG1	2.29	0.62
1:E:317:VAL:O	1:E:321:ARG:HD2	1.99	0.62
1:A:319:THR:HG22	1:A:322:ARG:HH21	1.64	0.62
1:F:168:ASP:O	1:F:169:ASP:HB2	1.98	0.62
1:G:138:ASN:HA	1:H:305:ARG:HH22	1.64	0.62
1:A:59:LEU:H	1:A:59:LEU:HD22	1.64	0.62
1:A:355:ALA:HB3	1:A:366:ILE:HG13	1.81	0.62
1:E:143:LEU:C	1:E:143:LEU:HD12	2.18	0.62
1:E:417:HIS:HD2	1:E:420:GLU:HB2	1.65	0.62
1:H:366:ILE:O	1:H:367:ARG:HB2	1.99	0.62
2:B:900:BLA:HMB3	2:B:900:BLA:HMA2	1.79	0.62
1:C:440:LYS:HG2	1:E:361:GLY:HA3	1.81	0.62
1:G:229:THR:HG23	1:G:231:GLU:H	1.63	0.62
1:E:164:ARG:HH12	1:E:166:ARG:HE	1.48	0.62
1:E:464:GLU:O	1:E:468:ARG:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:ILE:HD11	1:H:297:GLN:HB2	1.82	0.62
1:A:294:ILE:O	1:A:298:VAL:HG23	1.99	0.62
1:A:415:ARG:HB2	1:A:423:TRP:CH2	2.35	0.62
1:B:61:GLN:HA	1:B:69:LEU:HD11	1.80	0.62
1:G:247:HIS:CD2	2:G:900:BLA:HBD1	2.35	0.62
1:C:17:ILE:HD12	1:C:244:SER:HB2	1.82	0.61
1:E:380:ARG:HB2	1:E:380:ARG:NH1	2.15	0.61
1:C:359:LEU:HD12	1:C:360:GLY:H	1.65	0.61
1:H:31:THR:HG22	1:H:107:TYR:CD1	2.35	0.61
1:A:130:ILE:HD11	1:A:150:GLU:CG	2.28	0.61
1:A:138:ASN:HD22	1:A:138:ASN:N	1.99	0.61
1:A:164:ARG:NH1	1:A:166:ARG:HH21	1.98	0.61
1:E:322:ARG:HD2	1:E:488:ASP:OD1	2.00	0.61
1:G:410:GLY:O	1:G:427:PHE:HA	2.00	0.61
1:D:301:ALA:O	1:D:305:ARG:HG2	2.01	0.61
1:G:295:PHE:CE1	1:G:299[B]:CYS:SG	2.94	0.61
1:D:16:PRO:HB3	1:D:18:HIS:CE1	2.35	0.61
1:F:468:ARG:HA	1:F:468:ARG:NH1	2.15	0.61
1:G:336:PHE:CD2	1:G:364:LEU:CD2	2.83	0.61
1:H:324:ALA:O	1:H:328:ARG:HB2	2.01	0.61
1:E:433:HIS:HD2	1:E:436:ARG:HG2	1.64	0.61
1:G:445:LEU:O	1:G:446:THR:HG22	2.00	0.61
1:H:333:ASP:HB2	1:H:496:HIS:CD2	2.36	0.61
1:H:433:HIS:HD2	1:H:436:ARG:HG2	1.65	0.61
1:A:356:LEU:HD13	1:A:357:VAL:N	2.15	0.61
1:C:196:PRO:CG	2:C:900:BLA:HAC	2.29	0.61
1:E:19:VAL:HG12	1:E:233:PHE:O	2.00	0.61
1:G:33:ARG:HB3	1:G:39:LEU:CD1	2.31	0.61
1:A:383:ARG:C	1:A:385:PRO:HD3	2.21	0.61
1:C:220:ARG:HE	1:C:222:PHE:HZ	1.47	0.61
1:C:354:GLY:HA3	1:C:370:PHE:CE1	2.36	0.61
1:F:117:THR:O	1:F:117:THR:CG2	2.48	0.61
1:G:16:PRO:HB3	1:G:18:HIS:HE1	1.65	0.61
1:C:426:TRP:N	1:C:426:TRP:CD1	2.68	0.61
1:G:179:ARG:HG2	1:G:179:ARG:NH1	2.07	0.61
1:H:210:LEU:HD12	1:H:289:ARG:HE	1.64	0.61
1:A:17:ILE:O	1:A:241:ARG:HD2	1.99	0.61
1:B:51:PHE:HB2	1:B:63:GLN:OE1	2.00	0.61
1:C:328:ARG:HH12	1:C:344:ASP:HB2	1.64	0.61
1:A:322:ARG:HD2	1:A:488:ASP:OD1	2.01	0.60
1:D:7:VAL:HG12	1:D:11:ASN:HD22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:ARG:HH12	1:G:344:ASP:HB2	1.66	0.60
1:G:335:LEU:HD11	1:G:489:LEU:HD22	1.82	0.60
1:G:425:PHE:HB3	1:G:427:PHE:CE1	2.36	0.60
1:E:307:GLU:O	1:E:311:ILE:HG23	2.01	0.60
1:F:179:ARG:NH1	1:F:181:ASP:HB3	2.17	0.60
1:H:172:GLU:HB2	1:H:189:ARG:HD3	1.83	0.60
1:A:208:ILE:H	1:A:208:ILE:HD13	1.66	0.60
1:A:42:SER:O	1:A:45:ILE:HG13	2.01	0.60
1:D:434:ARG:NH1	1:D:435:ILE:HD13	2.17	0.60
1:A:298:VAL:HG13	1:B:298:VAL:HG13	1.83	0.60
1:G:493:CYS:HA	1:G:496:HIS:HD2	1.65	0.60
1:H:264:ILE:HD11	1:H:274:PHE:CE1	2.37	0.60
1:B:24:GLN:HE22	1:B:211:ILE:HA	1.65	0.60
1:D:145:SER:HA	1:D:175:ALA:HB1	1.84	0.60
1:E:85:SER:HB2	1:E:98:ILE:HG22	1.82	0.60
1:B:31:THR:HG22	1:B:107:TYR:HD1	1.66	0.60
1:B:418:ARG:HB3	1:H:201:ARG:NH2	2.15	0.60
1:C:51:PHE:CD2	1:C:63:GLN:HB2	2.36	0.60
1:G:113:ARG:HG2	1:G:115:ALA:O	2.01	0.60
1:A:364:LEU:HD21	1:G:435:ILE:CG2	2.26	0.59
1:D:350:ILE:HG23	1:D:351:PRO:HD2	1.84	0.59
1:G:258:ALA:HB1	3:G:903:HOH:O	2.02	0.59
1:B:412:LEU:HB3	1:B:426:TRP:HD1	1.67	0.59
1:E:19:VAL:HG23	1:E:19:VAL:O	2.01	0.59
1:E:112:ILE:H	1:E:112:ILE:HD13	1.66	0.59
1:G:191:PRO:HB2	1:G:193:SER:H	1.67	0.59
1:H:220:ARG:HB2	1:H:222:PHE:CZ	2.36	0.59
1:D:322:ARG:NH2	1:D:484:LYS:HB3	2.17	0.59
1:E:356:LEU:HB3	1:E:425:PHE:HB2	1.84	0.59
1:G:72:LEU:O	1:G:72:LEU:HD13	2.02	0.59
1:A:134:VAL:HG21	1:A:143:LEU:HD13	1.83	0.59
1:C:209:ARG:NH1	2:C:900:BLA:O1D	2.36	0.59
1:F:321:ARG:HG3	1:F:349:LEU:HD22	1.84	0.59
2:F:900:BLA:HMB3	2:F:900:BLA:HMA2	1.84	0.59
1:A:59:LEU:HD22	1:A:59:LEU:N	2.16	0.59
1:B:311:ILE:O	1:B:315:LEU:HG	2.02	0.59
1:C:215:ALA:HB3	1:C:257:ARG:NH2	2.17	0.59
1:D:274:PHE:CE1	1:D:295:PHE:CE2	2.91	0.59
1:F:19:VAL:N	1:F:20:PRO:HD3	2.16	0.59
1:F:324:ALA:HB1	1:F:328:ARG:HH22	1.66	0.59
1:H:416:PHE:HE1	1:H:424:ILE:HG13	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HG3	1:A:189:ARG:N	2.18	0.59
1:G:264:ILE:HB	1:G:272:GLY:O	2.03	0.59
1:A:443:LYS:HB2	1:A:444:LEU:HD22	1.85	0.59
1:E:412:LEU:O	1:E:426:TRP:HD1	1.84	0.59
1:F:59:LEU:HD13	1:F:59:LEU:H	1.68	0.59
1:G:275:SER:OG	2:G:900:BLA:O2A	2.21	0.59
1:G:295:PHE:CZ	1:G:299[B]:CYS:SG	2.95	0.59
1:B:354:GLY:HA3	1:B:370:PHE:CZ	2.38	0.59
1:G:302:ILE:HG13	1:H:305:ARG:HG3	1.84	0.59
1:A:262:ILE:CD1	1:A:292:PHE:HB3	2.33	0.59
1:D:410:GLY:O	1:D:427:PHE:HA	2.03	0.59
1:G:108:LEU:HD12	1:G:110:PHE:CZ	2.39	0.58
1:C:127:ALA:O	1:C:131:ILE:HG12	2.03	0.58
1:G:71:MET:SD	1:G:86:VAL:HG23	2.43	0.58
1:H:79:ASN:ND2	1:H:80:GLY:H	1.96	0.58
1:F:136:LEU:O	1:F:136:LEU:HD23	2.03	0.58
1:H:346:ILE:O	1:H:426:TRP:HZ3	1.86	0.58
1:B:495:ASN:O	1:B:495:ASN:OD1	2.21	0.58
1:C:129:ARG:HE	1:C:154:MET:HG2	1.68	0.58
1:D:266:VAL:HG23	1:D:266:VAL:O	2.04	0.58
1:E:18:HIS:C	1:E:20:PRO:HD3	2.24	0.58
1:F:346:ILE:HD11	1:F:366:ILE:HD11	1.85	0.58
1:H:18:HIS:C	1:H:20:PRO:HD3	2.23	0.58
1:H:134:VAL:HG13	1:H:143:LEU:HB2	1.85	0.58
1:A:82:TRP:HE3	1:A:83:SER:O	1.86	0.58
1:A:131:ILE:O	1:A:135:GLN:HB2	2.04	0.58
1:A:143:LEU:O	1:A:147:VAL:HG13	2.04	0.58
1:D:286:TYR:HB3	1:D:287:PRO:HD3	1.84	0.58
1:E:48:LEU:HD12	1:E:48:LEU:O	2.03	0.58
1:F:239:VAL:HG11	1:F:289:ARG:NH2	2.19	0.58
1:G:201:ARG:HG2	1:G:205:GLN:NE2	2.18	0.58
1:H:138:ASN:HD22	1:H:138:ASN:N	2.02	0.58
1:H:220:ARG:NE	1:H:222:PHE:CZ	2.62	0.58
1:A:359:LEU:HA	1:A:421:SER:O	2.04	0.58
2:B:900:BLA:HBB1	2:B:900:BLA:OB	2.03	0.58
1:C:185:TYR:O	1:C:188:GLN:HB2	2.04	0.58
1:A:446:THR:CG2	1:A:446:THR:O	2.51	0.58
1:B:19:VAL:H	1:B:20:PRO:HD3	1.69	0.58
1:B:116:ASP:O	1:B:116:ASP:OD2	2.22	0.58
1:B:266:VAL:HG23	1:B:266:VAL:O	2.02	0.58
1:B:299:CYS:O	1:B:303:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:HIS:CD2	1:E:436:ARG:HG2	2.38	0.58
1:G:131:ILE:HG22	1:G:295:PHE:HB2	1.84	0.58
1:H:51:PHE:CG	1:H:52:VAL:N	2.72	0.58
1:B:391:HIS:HA	1:B:411:VAL:O	2.03	0.58
1:C:80:GLY:O	1:C:81:PRO:C	2.42	0.58
1:D:430:GLU:HG2	1:D:431:GLU:N	2.19	0.58
1:E:385:PRO:O	1:E:386:GLU:HB2	2.04	0.58
1:G:336:PHE:CD2	1:G:364:LEU:HD23	2.39	0.58
1:D:339:LEU:CD1	1:D:357:VAL:HG21	2.34	0.57
1:D:373:GLN:HE22	1:D:395:TRP:HE1	1.53	0.57
1:F:373:GLN:O	1:F:377:VAL:HG23	2.05	0.57
1:H:488:ASP:O	1:H:492:LEU:HD13	2.04	0.57
1:D:43:GLU:HA	1:D:45:ILE:HG13	1.86	0.57
1:E:415:ARG:HD3	1:E:423:TRP:CZ2	2.39	0.57
1:B:45:ILE:HD13	1:B:52:VAL:HA	1.85	0.57
1:C:420:GLU:OE2	1:G:81:PRO:HG3	2.05	0.57
1:E:134:VAL:HG22	1:E:134:VAL:O	2.04	0.57
1:F:206:ASN:HD21	1:F:237:TYR:HA	1.68	0.57
1:A:117:THR:HG23	1:A:287:PRO:HG2	1.87	0.57
1:B:323:LEU:HD23	1:B:323:LEU:C	2.24	0.57
1:D:138:ASN:HD22	1:D:138:ASN:N	2.01	0.57
1:D:433:HIS:CE1	1:D:460:PHE:HE1	2.23	0.57
1:C:201:ARG:HD3	1:G:385:PRO:HB3	1.85	0.57
1:C:378:LEU:HD11	1:C:423:TRP:CE2	2.39	0.57
1:B:17:ILE:HG21	1:B:244:SER:HB2	1.87	0.57
1:B:19:VAL:N	1:B:20:PRO:HD3	2.19	0.57
1:B:94:LEU:O	1:B:113:ARG:HB3	2.04	0.57
1:B:256:VAL:HG11	1:B:277:HIS:CD2	2.40	0.57
1:D:17:ILE:O	1:D:241:ARG:HD2	2.05	0.57
1:D:46:GLN:HA	1:D:49:LEU:O	2.05	0.57
1:D:358:MET:CE	1:D:423:TRP:HB2	2.35	0.57
1:H:84:ASN:HD22	1:H:85:SER:H	1.52	0.57
1:G:356:LEU:HD13	1:G:357:VAL:N	2.20	0.57
1:B:28:ALA:HB2	1:B:48:LEU:HD22	1.86	0.57
1:B:122:SER:O	1:B:126:ASN:HB2	2.04	0.57
1:C:327:ARG:HH11	1:D:491:GLU:HG2	1.70	0.57
1:E:135:GLN:NE2	1:F:305:ARG:NH1	2.53	0.57
1:B:347:ALA:HB1	1:B:367:ARG:HH21	1.70	0.57
1:D:126:ASN:O	1:D:130:ILE:HG23	2.05	0.57
1:D:250:TYR:CZ	1:D:454:LEU:O	2.58	0.57
1:D:373:GLN:O	1:D:377:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ILE:HG21	1:F:244:SER:HB2	1.86	0.57
1:G:164:ARG:HG3	1:G:174:VAL:HG21	1.87	0.57
1:A:356:LEU:HB3	1:A:425:PHE:HB2	1.87	0.57
1:A:361:GLY:O	1:G:440:LYS:HB2	2.05	0.57
1:C:98:ILE:HG12	1:C:109:GLU:HB2	1.86	0.57
2:D:900:BLA:HMB3	2:D:900:BLA:HMA2	1.85	0.57
1:E:48:LEU:CD1	1:E:93:HIS:HD2	2.03	0.57
1:E:490:MET:O	1:E:494:LEU:HD23	2.05	0.57
1:F:305:ARG:HD2	1:F:305:ARG:N	2.20	0.56
1:H:213:ASP:O	1:H:216:TYR:HB3	2.05	0.56
1:A:441:PRO:HB3	1:A:443:LYS:HE3	1.85	0.56
1:D:294:ILE:O	1:D:298:VAL:HG23	2.05	0.56
1:E:135:GLN:NE2	1:E:135:GLN:HA	2.16	0.56
1:E:202:LEU:HD13	1:E:241:ARG:NH2	2.20	0.56
1:F:301:ALA:O	1:F:304:GLU:HB3	2.05	0.56
1:F:366:ILE:HD13	1:F:366:ILE:N	2.20	0.56
1:H:321:ARG:HD3	1:H:349:LEU:HD22	1.85	0.56
1:A:305:ARG:HB3	1:A:308:GLN:NE2	2.20	0.56
1:B:364:LEU:O	1:B:364:LEU:HD23	2.05	0.56
1:C:262:ILE:HD12	1:C:292:PHE:HB3	1.87	0.56
1:D:341:HIS:CG	1:D:342:PRO:HD2	2.40	0.56
1:E:48:LEU:CD1	1:E:93:HIS:CD2	2.85	0.56
1:F:339:LEU:HD22	1:F:346:ILE:HG23	1.86	0.56
1:F:425:PHE:HB3	1:F:427:PHE:CE1	2.40	0.56
1:A:33:ARG:HB3	1:A:39:LEU:HD11	1.88	0.56
1:A:70:ARG:O	1:A:74:GLU:HG2	2.06	0.56
1:D:19:VAL:HG23	1:D:19:VAL:O	2.06	0.56
1:F:18:HIS:C	1:F:20:PRO:HD3	2.25	0.56
1:G:118:LEU:O	1:G:121:THR:HG22	2.04	0.56
1:C:186:LEU:HD23	1:C:187:GLY:N	2.20	0.56
1:G:98:ILE:HG21	1:G:286:TYR:CE1	2.40	0.56
1:H:114:THR:HG22	1:H:115:ALA:H	1.70	0.56
1:E:134:VAL:HG21	1:E:143:LEU:HB3	1.85	0.56
1:A:8:THR:H	1:A:11:ASN:HB3	1.69	0.56
1:A:354:GLY:HA3	1:A:370:PHE:CZ	2.41	0.56
1:D:356:LEU:HB3	1:D:425:PHE:HB2	1.87	0.56
1:D:358:MET:HE3	1:D:423:TRP:HB2	1.88	0.56
1:E:330:ARG:NH1	1:E:333:ASP:OD1	2.39	0.56
1:E:414:ILE:HD12	1:E:486:ARG:HB2	1.87	0.56
1:D:238:SER:HB3	1:D:241:ARG:HB2	1.88	0.56
1:E:408:CYS:SG	1:E:427:PHE:HB3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:ILE:HG12	1:H:112:ILE:O	2.06	0.56
1:C:134:VAL:HG13	1:C:302:ILE:HG21	1.87	0.56
1:B:302:ILE:O	1:B:306:LEU:HB2	2.06	0.56
1:D:250:TYR:O	1:D:253:ASN:HB2	2.05	0.56
1:G:336:PHE:HD2	1:G:364:LEU:HD21	1.71	0.56
1:H:52:VAL:HG22	1:H:53:ALA:H	1.71	0.56
1:H:159:ARG:HG2	1:H:160:VAL:N	2.20	0.56
1:B:85:SER:HB2	1:B:98:ILE:HG22	1.87	0.55
1:E:434:ARG:HD2	1:E:435:ILE:HG23	1.89	0.55
1:F:260:MET:O	1:F:276:CYS:HB2	2.06	0.55
1:H:325:LEU:HD21	1:H:339:LEU:HD23	1.87	0.55
1:B:213:ASP:O	1:B:216:TYR:HB3	2.05	0.55
1:G:258:ALA:HB3	1:G:278:HIS:HB3	1.87	0.55
1:G:426:TRP:N	1:G:426:TRP:CD1	2.74	0.55
1:A:123:PHE:CZ	1:A:291:SER:HB2	2.41	0.55
1:D:494:LEU:HD23	1:E:133:GLN:HG2	1.88	0.55
2:D:900:BLA:HMA2	2:D:900:BLA:O2A	2.06	0.55
1:G:378:LEU:HD11	1:G:425:PHE:HZ	1.72	0.55
1:A:54:SER:O	1:A:57:SER:HB3	2.06	0.55
1:B:29:LEU:HD12	1:B:108:LEU:O	2.06	0.55
1:E:318:SER:O	1:E:322:ARG:HB2	2.07	0.55
1:E:394:ASN:ND2	1:E:470:HIS:CD2	2.68	0.55
1:E:17:ILE:H	1:E:17:ILE:HD12	1.71	0.55
1:E:120:ILE:CG1	1:F:120:ILE:HD13	2.36	0.55
1:E:133:GLN:HB3	1:E:146:ASN:OD1	2.06	0.55
1:F:208:ILE:H	1:F:208:ILE:HD13	1.70	0.55
1:H:51:PHE:CE2	1:H:52:VAL:HG12	2.42	0.55
1:H:295:PHE:HA	1:H:298:VAL:HG12	1.88	0.55
1:A:311:ILE:O	1:A:315:LEU:HB2	2.06	0.55
1:A:378:LEU:O	1:A:382:GLN:HG2	2.07	0.55
1:E:30:VAL:HG12	1:E:32:LEU:CD1	2.36	0.55
1:F:8:THR:H	1:F:11:ASN:ND2	2.03	0.55
1:G:82:TRP:O	1:G:100:HIS:HA	2.07	0.55
1:H:130:ILE:HG12	1:H:147:VAL:HG13	1.87	0.55
1:H:339:LEU:HD13	1:H:357:VAL:HG21	1.89	0.55
2:H:900:BLA:HMC1	2:H:900:BLA:CBC	2.35	0.55
1:E:256:VAL:CG1	1:E:277:HIS:HB3	2.37	0.55
1:E:389:ILE:HD11	1:E:483:GLU:HG2	1.89	0.55
1:A:447:ILE:HD13	1:A:447:ILE:N	2.21	0.55
1:C:131:ILE:HG22	1:C:295:PHE:HD1	1.70	0.55
1:C:133:GLN:O	1:C:137:HIS:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:PHE:HE1	1:C:424:ILE:HG13	1.72	0.55
1:D:325:LEU:HD12	1:D:326:ALA:N	2.21	0.55
1:F:356:LEU:HD23	1:F:365:SER:HB3	1.87	0.55
1:G:423:TRP:HB3	1:G:425:PHE:CE1	2.42	0.55
1:A:290:MET:HB3	1:B:124:THR:OG1	2.05	0.55
1:G:17:ILE:H	1:G:17:ILE:HD12	1.72	0.55
2:G:900:BLA:HBB1	2:G:900:BLA:OB	2.07	0.55
1:B:61:GLN:HA	1:B:69:LEU:HD13	1.88	0.54
1:D:340:ALA:O	1:H:434:ARG:NH2	2.39	0.54
1:E:159:ARG:HG2	1:E:160:VAL:N	2.22	0.54
1:F:31:THR:HG22	1:F:107:TYR:CD1	2.41	0.54
1:F:266:VAL:O	1:F:266:VAL:HG23	2.07	0.54
1:G:64:VAL:CG1	1:G:68:VAL:HG11	2.37	0.54
1:G:412:LEU:HB3	1:G:426:TRP:CD1	2.42	0.54
1:H:266:VAL:HG23	1:H:266:VAL:O	2.08	0.54
1:D:322:ARG:HD3	1:D:488:ASP:OD1	2.08	0.54
1:G:40:ALA:HB2	1:G:223:PRO:HD2	1.88	0.54
1:G:285:PRO:HG3	3:G:907:HOH:O	2.06	0.54
1:G:493:CYS:HA	1:G:496:HIS:CD2	2.42	0.54
1:A:46:GLN:HB2	1:A:52:VAL:HG22	1.88	0.54
1:C:488:ASP:O	1:C:491:GLU:HB3	2.07	0.54
1:E:325:LEU:O	1:E:325:LEU:HD22	2.07	0.54
1:G:179:ARG:HH12	1:G:181:ASP:HB2	1.72	0.54
1:A:121:THR:CG2	1:B:85:SER:OG	2.54	0.54
1:C:40:ALA:HB1	1:C:222:PHE:O	2.07	0.54
1:C:475:SER:HB2	1:C:478:ASP:H	1.73	0.54
1:D:208:ILE:H	1:D:208:ILE:HD13	1.73	0.54
1:F:148:THR:HG23	1:F:160:VAL:HG22	1.89	0.54
1:G:198:GLN:O	1:G:198:GLN:HG3	2.08	0.54
1:B:51:PHE:HD2	1:B:63:GLN:HG3	1.71	0.54
1:D:351:PRO:HB2	1:D:428:ARG:HH21	1.72	0.54
1:E:113:ARG:HH12	1:E:285:PRO:HB3	1.72	0.54
1:E:330:ARG:HD2	1:F:331:ASP:OD2	2.07	0.54
1:G:201:ARG:CG	1:G:201:ARG:NH1	2.70	0.54
1:G:311:ILE:HD13	1:G:312:ALA:N	2.22	0.54
1:A:354:GLY:HA3	1:A:370:PHE:CE1	2.42	0.54
1:B:19:VAL:N	1:B:20:PRO:CD	2.70	0.54
1:B:313:GLU:O	1:B:317:VAL:HG13	2.08	0.54
1:D:411:VAL:HG13	1:D:427:PHE:CE2	2.43	0.54
1:F:323:LEU:O	1:F:323:LEU:HD23	2.07	0.54
1:G:133:GLN:HB3	1:G:147:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLY:HA2	1:G:418:ARG:NH2	2.23	0.54
1:D:460:PHE:HE2	1:D:464:GLU:OE1	1.91	0.54
1:E:316:ARG:HH21	1:E:317:VAL:HG12	1.73	0.54
1:H:286:TYR:O	1:H:290:MET:HG2	2.07	0.54
1:A:491:GLU:HG3	1:A:492:LEU:N	2.22	0.54
1:E:40:ALA:HB2	1:E:223:PRO:HD2	1.90	0.54
1:E:173:VAL:O	1:E:186:LEU:HD23	2.08	0.54
1:A:165:PHE:CD1	1:A:272:GLY:HA2	2.42	0.54
1:A:364:LEU:HD23	1:G:436:ARG:O	2.07	0.54
1:B:54:SER:O	1:B:57:SER:HB3	2.08	0.54
1:B:346:ILE:O	1:B:426:TRP:CZ3	2.59	0.54
1:E:134:VAL:HG21	1:E:143:LEU:HB2	1.89	0.54
1:F:118:LEU:O	1:F:122:SER:CB	2.56	0.54
1:G:423:TRP:HB3	1:G:425:PHE:HE1	1.72	0.54
2:H:900:BLA:HMA2	2:H:900:BLA:O2A	2.08	0.54
1:A:330:ARG:HH21	1:B:327:ARG:HB2	1.73	0.54
1:C:125:LEU:O	1:C:125:LEU:HD23	2.08	0.54
1:F:391:HIS:HB3	1:F:412:LEU:HD23	1.88	0.54
1:C:139:ASP:HB3	1:C:142:SER:HB2	1.89	0.53
1:D:288:VAL:O	1:D:291:SER:HB2	2.08	0.53
1:G:327:ARG:O	1:G:327:ARG:HG2	2.08	0.53
1:G:412:LEU:HD12	1:G:474:TRP:CE3	2.43	0.53
1:C:341:HIS:ND1	1:C:342:PRO:HD2	2.23	0.53
1:D:434:ARG:HH12	1:D:435:ILE:HD13	1.73	0.53
1:A:19:VAL:HG23	1:A:19:VAL:O	2.08	0.53
1:A:50:GLY:O	1:A:51:PHE:HB3	2.09	0.53
1:A:82:TRP:CE3	1:A:83:SER:O	2.62	0.53
1:A:208:ILE:HA	1:A:261:SER:O	2.08	0.53
1:C:194:ASP:HB3	2:C:900:BLA:HHB	1.90	0.53
1:D:415:ARG:HB2	1:D:423:TRP:CE2	2.43	0.53
1:E:172:GLU:HG2	1:E:173:VAL:N	2.22	0.53
1:E:260:MET:HE1	1:E:289:ARG:CG	2.38	0.53
1:F:72:LEU:O	1:F:76:LEU:HD13	2.08	0.53
2:F:900:BLA:HBC1	2:F:900:BLA:HMC1	1.91	0.53
1:G:202:LEU:O	1:G:206:ASN:HB2	2.08	0.53
1:H:229:THR:HG23	1:H:231:GLU:H	1.74	0.53
1:A:32:LEU:CD2	1:A:72:LEU:HD11	2.38	0.53
1:A:302:ILE:HD12	1:B:302:ILE:HD11	1.90	0.53
1:C:114:THR:HG22	1:C:114:THR:O	2.09	0.53
1:D:143:LEU:HD12	1:D:144:LEU:N	2.23	0.53
1:E:105:VAL:HG12	1:E:106:PHE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:VAL:O	1:F:321:ARG:HD2	2.07	0.53
1:F:412:LEU:HB3	1:F:426:TRP:CD1	2.43	0.53
1:H:135:GLN:N	1:H:135:GLN:HE21	2.06	0.53
1:A:72:LEU:HD13	1:A:76:LEU:HD13	1.89	0.53
1:C:94:LEU:CD1	1:C:94:LEU:H	2.21	0.53
1:D:222:PHE:HA	1:D:223:PRO:C	2.27	0.53
1:F:188:GLN:NE2	1:F:460:PHE:HB2	2.23	0.53
1:F:412:LEU:O	1:F:426:TRP:HD1	1.92	0.53
1:G:297:GLN:HB3	1:H:131:ILE:HD11	1.91	0.53
1:H:46:GLN:HG2	1:H:52:VAL:HA	1.90	0.53
1:A:18:HIS:C	1:A:20:PRO:HD3	2.29	0.53
1:A:382:GLN:NE2	1:A:382:GLN:HA	2.24	0.53
1:A:414:ILE:HG12	1:A:424:ILE:HB	1.91	0.53
1:C:415:ARG:HD3	1:C:423:TRP:CZ2	2.43	0.53
1:E:354:GLY:HA3	1:E:370:PHE:CE1	2.44	0.53
1:F:314:LEU:O	1:F:317:VAL:HG22	2.09	0.53
1:H:410:GLY:O	1:H:427:PHE:HA	2.08	0.53
1:D:40:ALA:CB	1:D:223:PRO:HD2	2.39	0.53
1:D:84:ASN:HD22	1:D:85:SER:H	1.55	0.53
1:E:120:ILE:HD11	1:F:120:ILE:HD13	1.90	0.53
1:E:294:ILE:HD11	1:F:127:ALA:HB3	1.91	0.53
1:F:239:VAL:HG11	1:F:289:ARG:HH21	1.74	0.53
1:H:149:ASP:HB3	1:H:153:ARG:HH22	1.74	0.53
1:B:205:GLN:NE2	1:B:237:TYR:HE2	2.07	0.53
1:E:301:ALA:HB2	1:F:135:GLN:HG2	1.90	0.53
1:G:117:THR:O	1:G:118:LEU:C	2.46	0.53
1:H:358:MET:HG3	1:H:363:THR:CG2	2.39	0.53
1:A:327:ARG:HA	1:B:330:ARG:HH12	1.72	0.52
1:B:63:GLN:O	1:B:63:GLN:HG2	2.09	0.52
1:B:315:LEU:O	1:B:319:THR:HG23	2.08	0.52
1:C:385:PRO:HB3	1:G:201:ARG:HG3	1.90	0.52
1:D:243:VAL:HG12	1:D:244:SER:N	2.25	0.52
1:D:250:TYR:CE1	1:D:454:LEU:O	2.62	0.52
1:D:416:PHE:O	1:D:490:MET:HG2	2.09	0.52
1:E:365:SER:HB2	1:E:368:GLY:O	2.09	0.52
1:G:138:ASN:HA	1:H:305:ARG:NH2	2.22	0.52
1:C:25:PRO:HD3	1:C:216:TYR:HD2	1.74	0.52
1:D:194:ASP:O	1:D:196:PRO:HD3	2.08	0.52
1:F:322:ARG:NH1	1:F:484:LYS:HB3	2.23	0.52
1:F:356:LEU:HB3	1:F:425:PHE:HB2	1.91	0.52
1:H:315:LEU:O	1:H:318:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:THR:HG23	1:A:90:ILE:HG13	1.90	0.52
1:C:213:ASP:O	1:C:216:TYR:HB3	2.09	0.52
1:E:148:THR:HG23	1:E:160:VAL:HG22	1.92	0.52
1:G:143:LEU:C	1:G:143:LEU:HD12	2.30	0.52
1:G:377:VAL:HG21	1:G:411:VAL:HG11	1.90	0.52
1:H:138:ASN:N	1:H:138:ASN:ND2	2.58	0.52
1:H:191:PRO:HG3	1:H:463:TRP:HB2	1.91	0.52
1:D:162:ALA:O	1:D:174:VAL:HG22	2.10	0.52
1:E:31:THR:HG22	1:E:107:TYR:CD1	2.44	0.52
1:E:31:THR:HG22	1:E:107:TYR:HD1	1.74	0.52
2:E:900:BLA:HMB3	2:E:900:BLA:CMA	2.40	0.52
1:F:134:VAL:HG22	1:F:302:ILE:HG21	1.91	0.52
1:F:278:HIS:HD2	1:F:280:SER:O	1.93	0.52
1:G:72:LEU:HD13	1:G:76:LEU:HD13	1.90	0.52
1:G:389:ILE:HD11	1:G:483:GLU:HG2	1.90	0.52
1:A:258:ALA:HB3	1:A:278:HIS:HB3	1.92	0.52
1:B:94:LEU:O	1:B:94:LEU:HD13	2.09	0.52
1:C:31:THR:O	1:C:32:LEU:HD12	2.09	0.52
1:C:140:THR:HG21	1:C:307:GLU:OE2	2.09	0.52
1:E:140:THR:CA	1:E:306:LEU:HD23	2.40	0.52
1:E:304:GLU:HG2	1:E:305:ARG:NH1	2.25	0.52
1:F:149:ASP:OD1	1:F:177:SER:HB3	2.10	0.52
1:F:266:VAL:CG2	1:F:271:TRP:HB2	2.31	0.52
1:B:412:LEU:HB3	1:B:426:TRP:CD1	2.44	0.52
1:D:142:SER:O	1:D:146:ASN:HB2	2.10	0.52
2:E:900:BLA:HBD2	2:E:900:BLA:HMD1	1.92	0.52
1:G:64:VAL:HG12	1:G:68:VAL:HG11	1.91	0.52
1:G:294:ILE:O	1:G:298:VAL:HG23	2.10	0.52
1:D:325:LEU:HD22	1:D:339:LEU:HD23	1.91	0.52
1:D:394:ASN:O	1:D:395:TRP:CB	2.57	0.52
1:F:94:LEU:HD22	1:F:113:ARG:HB2	1.91	0.52
1:F:391:HIS:HA	1:F:411:VAL:O	2.09	0.52
1:H:29:LEU:HD12	1:H:108:LEU:O	2.10	0.52
1:H:353:ASP:O	1:H:367:ARG:HD2	2.09	0.52
1:B:325:LEU:O	1:B:325:LEU:HD22	2.09	0.52
1:F:447:ILE:HD13	1:F:447:ILE:N	2.25	0.52
1:G:325:LEU:O	1:G:325:LEU:HD22	2.09	0.52
1:H:31:THR:C	1:H:32:LEU:HD12	2.30	0.52
1:H:310:ARG:O	1:H:314:LEU:HD23	2.09	0.52
1:H:346:ILE:O	1:H:426:TRP:CZ3	2.62	0.52
1:H:358:MET:HG3	1:H:363:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:HB2	1:A:286:TYR:CE2	2.45	0.52
1:B:202:LEU:O	1:B:206:ASN:HB2	2.10	0.52
2:B:900:BLA:HMA2	2:B:900:BLA:O2A	2.10	0.52
1:B:125:LEU:O	1:B:125:LEU:HD12	2.10	0.52
1:C:239:VAL:HG11	1:C:289:ARG:NH2	2.25	0.52
1:C:457:ARG:O	1:C:461:GLU:HG3	2.10	0.52
1:G:16:PRO:HB3	1:G:18:HIS:CE1	2.44	0.52
1:G:124:THR:HG21	1:H:291:SER:HA	1.91	0.52
1:H:152:ARG:HB2	1:H:160:VAL:CG1	2.40	0.52
1:A:18:HIS:O	1:A:20:PRO:HD3	2.09	0.51
1:B:130:ILE:H	1:B:130:ILE:CD1	2.14	0.51
1:C:19:VAL:HG12	1:C:234:ASP:HA	1.91	0.51
1:C:366:ILE:O	1:C:367:ARG:HB2	2.09	0.51
1:C:439:GLY:HA3	1:E:361:GLY:O	2.09	0.51
1:D:13:GLU:OE1	1:D:196:PRO:HB3	2.10	0.51
1:E:384:ASP:HB3	1:E:387:ARG:HB2	1.92	0.51
1:C:323:LEU:CA	1:D:323:LEU:HD12	2.38	0.51
1:D:356:LEU:HD21	1:D:363:THR:CG2	2.34	0.51
1:D:434:ARG:O	1:H:366:ILE:HA	2.10	0.51
1:E:105:VAL:HG12	1:E:106:PHE:H	1.74	0.51
1:F:86:VAL:HG12	1:F:87:GLU:N	2.23	0.51
1:G:42:SER:O	1:G:45:ILE:HG13	2.11	0.51
1:H:18:HIS:ND1	1:H:198:GLN:HG2	2.25	0.51
1:D:214:VAL:HB	1:D:257:ARG:CA	2.40	0.51
2:D:900:BLA:OB	2:D:900:BLA:HBB1	2.10	0.51
1:E:32:LEU:HD23	1:E:72:LEU:HD21	1.93	0.51
1:H:371:GLU:HG3	1:H:372:ARG:N	2.25	0.51
1:H:416:PHE:O	1:H:490:MET:HG2	2.11	0.51
1:C:425:PHE:CD1	1:C:425:PHE:N	2.78	0.51
1:D:32:LEU:HD21	1:D:59:LEU:CD2	2.40	0.51
1:D:162:ALA:HB3	1:D:175:ALA:HB3	1.92	0.51
1:E:98:ILE:HD11	1:E:239:VAL:HG21	1.92	0.51
1:G:259:SER:HA	1:G:276:CYS:O	2.10	0.51
1:A:443:LYS:HB2	1:A:444:LEU:CD2	2.41	0.51
1:B:16:PRO:O	1:B:20:PRO:HD3	2.10	0.51
1:B:127:ALA:HA	1:B:130:ILE:HD11	1.92	0.51
1:C:71:MET:SD	1:C:86:VAL:HG23	2.51	0.51
1:C:147:VAL:HA	1:C:150:GLU:HB3	1.92	0.51
1:C:435:ILE:HG22	1:E:364:LEU:CD2	2.41	0.51
1:F:202:LEU:O	1:F:206:ASN:HB2	2.11	0.51
1:G:319:THR:HG22	1:G:322:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:445:LEU:O	1:G:446:THR:CG2	2.59	0.51
1:A:159:ARG:HG2	1:A:160:VAL:N	2.25	0.51
1:A:387:ARG:HD2	1:A:389:ILE:O	2.11	0.51
1:B:205:GLN:NE2	1:B:237:TYR:CE2	2.78	0.51
1:B:301:ALA:O	1:B:305:ARG:HD2	2.10	0.51
1:E:412:LEU:O	1:E:426:TRP:CD1	2.63	0.51
1:D:94:LEU:HD22	1:D:113:ARG:HB3	1.93	0.51
1:E:46:GLN:HA	1:E:49:LEU:O	2.11	0.51
1:F:94:LEU:HD23	1:F:113:ARG:HH11	1.76	0.51
1:A:121:THR:HG21	1:B:85:SER:N	2.26	0.51
1:B:464:GLU:O	1:B:468:ARG:HG3	2.11	0.51
1:C:150:GLU:O	1:C:153:ARG:HB2	2.10	0.51
1:E:195:ILE:HG22	1:E:200:ARG:HB2	1.92	0.51
1:G:336:PHE:CD2	1:G:364:LEU:HD21	2.45	0.51
1:G:358:MET:O	1:G:422:GLY:HA2	2.11	0.51
1:H:51:PHE:CZ	1:H:52:VAL:HG12	2.46	0.51
1:A:139:ASP:HB2	1:A:142:SER:HB2	1.93	0.51
1:B:416:PHE:O	1:B:490:MET:HG2	2.11	0.51
2:C:900:BLA:CBC	2:C:900:BLA:HMC1	2.40	0.51
1:F:18:HIS:CD2	1:F:19:VAL:HG13	2.46	0.51
1:A:130:ILE:HD12	1:A:295:PHE:CZ	2.45	0.51
1:A:210:LEU:HD12	1:A:289:ARG:HD3	1.92	0.51
1:A:366:ILE:HG22	1:G:435:ILE:HD13	1.93	0.51
1:A:443:LYS:HB3	1:A:444:LEU:HD22	1.92	0.51
1:B:328:ARG:CB	1:B:338:ALA:HB2	2.40	0.51
1:C:164:ARG:HB3	1:C:164:ARG:HH11	1.76	0.51
1:D:415:ARG:HB2	1:D:423:TRP:CZ2	2.46	0.51
1:D:430:GLU:HG3	1:D:469:GLY:H	1.74	0.51
1:E:70:ARG:O	1:E:74:GLU:HG3	2.11	0.51
1:H:22:ALA:HA	1:H:220:ARG:HA	1.92	0.51
1:A:117:THR:HG22	1:A:118:LEU:H	1.74	0.50
1:B:117:THR:O	1:B:118:LEU:HD23	2.10	0.50
1:A:9:LEU:HD21	1:A:450:SER:HB3	1.93	0.50
1:D:45:ILE:HD12	1:D:46:GLN:N	2.22	0.50
1:E:256:VAL:HG11	1:E:277:HIS:HB3	1.92	0.50
1:G:249:GLU:OE1	1:G:449:PRO:HD2	2.11	0.50
1:H:222:PHE:HA	1:H:223:PRO:C	2.30	0.50
1:A:7:VAL:HA	1:A:11:ASN:HD22	1.77	0.50
1:A:356:LEU:CD2	1:A:365:SER:HB2	2.42	0.50
1:C:153:ARG:CZ	1:F:498:LEU:HD21	2.41	0.50
1:E:25:PRO:HD3	1:E:216:TYR:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:ARG:CZ	1:F:484:LYS:HB3	2.42	0.50
1:H:17:ILE:CG2	1:H:244:SER:HB2	2.41	0.50
1:A:97:VAL:HG22	1:A:110:PHE:CD2	2.45	0.50
1:B:14:ASP:HA	1:H:383:ARG:HH12	1.77	0.50
1:B:68:VAL:HG13	1:B:97:VAL:HG11	1.93	0.50
1:B:191:PRO:HD3	1:B:459:SER:O	2.12	0.50
1:C:130:ILE:HG23	1:C:295:PHE:CD1	2.47	0.50
1:C:301:ALA:O	1:C:304:GLU:HB3	2.12	0.50
1:C:336:PHE:CE1	1:C:359:LEU:HB3	2.47	0.50
1:D:214:VAL:CB	1:D:257:ARG:HA	2.41	0.50
1:E:264:ILE:HB	1:E:272:GLY:O	2.11	0.50
1:G:30:VAL:HG12	1:G:32:LEU:CD1	2.42	0.50
1:G:75:GLY:HA2	1:G:82:TRP:CD1	2.45	0.50
1:G:212:ALA:HA	1:G:282:LYS:O	2.11	0.50
1:H:121:THR:O	1:H:125:LEU:HD13	2.12	0.50
1:A:203:TYR:OH	2:A:900:BLA:HAA1	2.12	0.50
1:B:51:PHE:CD2	1:B:63:GLN:HG3	2.47	0.50
1:D:211:ILE:HB	1:D:259:SER:HB3	1.93	0.50
1:D:391:HIS:HA	1:D:411:VAL:O	2.11	0.50
1:E:426:TRP:CD1	1:E:426:TRP:N	2.79	0.50
1:F:147:VAL:O	1:F:151:LEU:HG	2.11	0.50
1:G:394:ASN:O	1:G:395:TRP:CB	2.58	0.50
1:H:209:ARG:HH12	2:H:900:BLA:CGD	2.24	0.50
1:B:380:ARG:HB2	1:B:380:ARG:NH1	2.26	0.50
1:C:464:GLU:O	1:C:468:ARG:HG2	2.12	0.50
1:D:84:ASN:HD22	1:D:85:SER:N	2.09	0.50
1:D:274:PHE:CE1	1:D:295:PHE:HE2	2.27	0.50
1:D:351:PRO:HB2	1:D:428:ARG:NH2	2.26	0.50
1:E:283:LEU:HD23	1:E:284:ILE:N	2.27	0.50
1:G:388:ASP:HB3	1:G:486:ARG:HE	1.77	0.50
1:A:87:GLU:CG	1:A:113:ARG:HH22	2.23	0.50
1:A:165:PHE:CE1	1:A:272:GLY:HA2	2.46	0.50
1:B:19:VAL:HB	1:B:232:SER:HB3	1.94	0.50
1:B:382:GLN:O	1:H:197:ALA:HB1	2.11	0.50
1:C:313:GLU:OE1	1:C:316:ARG:NH1	2.45	0.50
1:C:326:ALA:HB2	1:D:327:ARG:NH2	2.27	0.50
1:C:346:ILE:O	1:C:426:TRP:HZ3	1.94	0.50
1:F:120:ILE:O	1:F:120:ILE:HG22	2.12	0.50
1:H:454:LEU:N	1:H:454:LEU:HD23	2.26	0.50
1:B:98:ILE:HG21	1:B:286:TYR:CE1	2.47	0.50
1:D:264:ILE:HB	1:D:272:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:O	1:D:385:PRO:HD3	2.12	0.50
1:E:140:THR:HA	1:E:306:LEU:HD23	1.93	0.50
1:E:187:GLY:HA3	1:E:435:ILE:HG13	1.93	0.50
1:E:304:GLU:HG2	1:E:305:ARG:CZ	2.41	0.50
2:E:900:BLA:HBB1	2:E:900:BLA:OB	2.10	0.50
1:F:98:ILE:HG21	1:F:286:TYR:CD1	2.47	0.50
1:G:336:PHE:CD1	1:G:336:PHE:N	2.79	0.50
1:H:457:ARG:O	1:H:461:GLU:HG2	2.11	0.50
1:D:72:LEU:O	1:D:76:LEU:HD13	2.12	0.49
1:D:220:ARG:HE	1:D:222:PHE:HZ	1.59	0.49
1:E:163:TYR:HA	1:E:172:GLU:O	2.12	0.49
1:E:164:ARG:NH1	1:E:166:ARG:HE	2.10	0.49
1:A:210:LEU:CD1	1:A:289:ARG:HD3	2.42	0.49
1:A:315:LEU:HD12	1:B:316:ARG:HD2	1.92	0.49
1:C:423:TRP:HB3	1:C:425:PHE:CE1	2.47	0.49
1:F:414:ILE:HD11	1:F:424:ILE:HD12	1.92	0.49
1:G:330:ARG:NH1	1:H:327:ARG:HB3	2.26	0.49
1:H:112:ILE:H	1:H:112:ILE:CD1	2.22	0.49
2:H:900:BLA:HBD2	2:H:900:BLA:HMD1	1.94	0.49
1:C:142:SER:O	1:C:146:ASN:HB2	2.13	0.49
1:D:302:ILE:O	1:D:306:LEU:HB2	2.12	0.49
1:E:113:ARG:NH1	1:E:285:PRO:HB3	2.27	0.49
1:E:394:ASN:HA	1:E:409:CYS:HB2	1.93	0.49
1:F:58:TYR:CZ	1:F:59:LEU:HD11	2.47	0.49
1:G:118:LEU:HD23	1:G:118:LEU:N	2.27	0.49
1:A:147:VAL:HG22	1:A:274:PHE:CE2	2.47	0.49
1:B:94:LEU:HD21	1:B:113:ARG:HG2	1.93	0.49
1:C:284:ILE:HG22	1:C:289:ARG:HG3	1.94	0.49
1:D:59:LEU:HD22	1:D:59:LEU:N	2.26	0.49
1:E:260:MET:CE	1:E:289:ARG:CG	2.91	0.49
2:E:900:BLA:HMC1	2:E:900:BLA:CBC	2.39	0.49
1:F:34:ALA:O	1:F:76:LEU:HG	2.12	0.49
1:H:90:ILE:HD12	1:H:95:PHE:HB2	1.94	0.49
1:C:144:LEU:HD11	1:C:271:TRP:CZ3	2.47	0.49
1:D:94:LEU:CD2	1:D:113:ARG:HB3	2.42	0.49
1:D:187:GLY:HA3	1:D:435:ILE:HG13	1.94	0.49
1:F:315:LEU:O	1:F:319:THR:HG23	2.13	0.49
1:H:262:ILE:O	1:H:273:LEU:HB2	2.11	0.49
1:A:305:ARG:HH21	1:B:138:ASN:HD22	1.61	0.49
1:B:37:MET:HB2	1:B:58:TYR:CZ	2.48	0.49
1:B:172:GLU:HG3	1:B:189:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:LEU:HD22	1:C:113:ARG:HB3	1.95	0.49
1:C:133:GLN:O	1:C:137:HIS:CD2	2.65	0.49
1:C:327:ARG:NH1	1:D:491:GLU:HG2	2.28	0.49
1:E:366:ILE:O	1:E:367:ARG:HB2	2.13	0.49
1:C:330:ARG:HH21	1:C:496:HIS:CB	2.21	0.49
1:E:22:ALA:HA	1:E:220:ARG:HA	1.94	0.49
1:G:354:GLY:HA3	1:G:370:PHE:CE1	2.47	0.49
1:A:92:GLU:OE1	1:A:93:HIS:CD2	2.65	0.49
1:A:262:ILE:HD11	1:A:292:PHE:HB3	1.95	0.49
1:C:239:VAL:O	1:C:239:VAL:HG12	2.13	0.49
1:G:46:GLN:HE21	1:G:52:VAL:HG21	1.77	0.49
1:H:20:PRO:HG2	1:H:241:ARG:HG3	1.95	0.49
1:A:137:HIS:C	1:A:138:ASN:HD22	2.16	0.49
1:A:157:TYR:HD2	1:A:278:HIS:HB2	1.78	0.49
1:A:485:LEU:O	1:A:489:LEU:HG	2.12	0.49
1:B:67:GLU:CD	1:B:67:GLU:H	2.16	0.49
1:C:379:GLN:HA	1:C:382:GLN:HG2	1.94	0.49
1:D:304:GLU:O	1:D:308:GLN:HG2	2.12	0.49
1:E:29:LEU:HD23	1:E:221:VAL:HG11	1.95	0.49
1:C:136:LEU:HB2	1:C:137:HIS:CD2	2.47	0.49
1:E:42:SER:HA	1:E:221:VAL:HA	1.95	0.49
1:E:222:PHE:HA	1:E:223:PRO:C	2.32	0.49
1:E:260:MET:HE1	1:E:289:ARG:HG3	1.95	0.49
1:G:389:ILE:CD1	1:G:483:GLU:HG2	2.42	0.49
1:A:140:THR:HA	1:A:306:LEU:HD23	1.94	0.48
1:A:168:ASP:O	1:A:169:ASP:HB2	2.12	0.48
1:B:31:THR:HG22	1:B:107:TYR:CD1	2.47	0.48
1:B:430:GLU:O	1:B:432:VAL:HG23	2.13	0.48
1:E:136:LEU:HB2	1:E:137:HIS:CD2	2.48	0.48
1:E:341:HIS:ND1	1:E:342:PRO:HD2	2.29	0.48
1:H:439:GLY:O	1:H:440:LYS:C	2.50	0.48
1:A:252:THR:O	1:A:445:LEU:CD2	2.57	0.48
1:A:446:THR:O	1:A:446:THR:HG23	2.12	0.48
1:F:31:THR:HG22	1:F:107:TYR:HD1	1.78	0.48
1:F:229:THR:HG23	1:F:231:GLU:H	1.78	0.48
1:G:120:ILE:HA	1:H:120:ILE:HD11	1.94	0.48
1:B:143:LEU:O	1:B:143:LEU:HD12	2.14	0.48
1:B:318:SER:O	1:B:322:ARG:HB2	2.13	0.48
1:B:325:LEU:HD13	1:B:325:LEU:C	2.33	0.48
1:B:329:ALA:HB3	1:B:492:LEU:HD21	1.96	0.48
1:C:152:ARG:HB2	1:C:160:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ASP:O	1:D:169:ASP:HB2	2.12	0.48
1:E:128:GLN:HG2	1:F:297:GLN:CD	2.34	0.48
1:A:302:ILE:O	1:A:306:LEU:HB2	2.13	0.48
1:B:98:ILE:HG21	1:B:286:TYR:CD1	2.48	0.48
1:B:324:ALA:HA	1:B:327:ARG:CD	2.43	0.48
1:B:362:ARG:H	1:B:362:ARG:HD2	1.77	0.48
1:C:221:VAL:CG2	1:C:221:VAL:O	2.61	0.48
1:C:321:ARG:O	1:C:325:LEU:HB2	2.14	0.48
1:C:358:MET:O	1:C:422:GLY:HA2	2.13	0.48
1:C:410:GLY:O	1:C:427:PHE:HA	2.13	0.48
1:D:294:ILE:O	1:D:294:ILE:HG22	2.14	0.48
1:E:121:THR:O	1:E:125:LEU:HB2	2.12	0.48
1:E:335:LEU:C	1:E:337:GLY:N	2.66	0.48
1:G:25:PRO:HD3	1:G:216:TYR:HD2	1.78	0.48
1:G:139:ASP:CB	1:G:142:SER:HB2	2.37	0.48
1:H:349:LEU:HD12	1:H:481:ILE:HG21	1.95	0.48
1:A:366:ILE:O	1:A:367:ARG:HB2	2.14	0.48
1:C:208:ILE:CD1	1:C:289:ARG:O	2.62	0.48
2:C:900:BLA:OB	2:C:900:BLA:HBB1	2.14	0.48
1:B:157:TYR:CD2	1:B:276:CYS:HB3	2.49	0.48
1:B:390:TYR:O	1:B:412:LEU:HD23	2.13	0.48
2:B:900:BLA:HMA1	2:B:900:BLA:C2B	2.43	0.48
1:C:163:TYR:CE1	2:C:900:BLA:HMA3	2.49	0.48
1:E:299:CYS:O	1:E:303:VAL:HB	2.14	0.48
1:E:315:LEU:O	1:E:319:THR:HG23	2.14	0.48
1:G:140:THR:HB	1:G:306:LEU:HB3	1.95	0.48
1:H:41:ALA:HB1	1:H:45:ILE:HG21	1.96	0.48
1:H:74:GLU:HA	1:H:77:THR:HB	1.94	0.48
1:A:72:LEU:HD13	1:A:76:LEU:CD1	2.43	0.48
1:D:305:ARG:N	1:D:305:ARG:HD2	2.28	0.48
1:E:266:VAL:HG22	1:E:271:TRP:HB2	1.95	0.48
1:E:455:THR:HB	1:E:456:PRO:HD2	1.95	0.48
1:G:172:GLU:HG3	1:G:189:ARG:HD2	1.96	0.48
1:H:42:SER:HA	1:H:221:VAL:HA	1.95	0.48
1:A:20:PRO:HG2	1:A:241:ARG:HG3	1.94	0.48
2:A:900:BLA:OB	2:A:900:BLA:HBB1	2.13	0.48
1:B:31:THR:C	1:B:32:LEU:HD12	2.33	0.48
1:C:264:ILE:HD11	1:C:274:PHE:CE1	2.49	0.48
1:D:325:LEU:HA	1:D:328:ARG:HB3	1.95	0.48
1:G:273:LEU:C	1:G:273:LEU:HD12	2.34	0.48
1:A:117:THR:CG2	1:A:118:LEU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	1:C:147:VAL:HG13	2.14	0.48
1:C:407:ASP:N	1:C:407:ASP:OD1	2.47	0.48
1:D:123:PHE:O	1:D:123:PHE:CG	2.67	0.48
1:E:178:ARG:HD2	1:E:183:GLU:O	2.14	0.48
1:F:98:ILE:HG13	1:F:109:GLU:HB2	1.96	0.48
1:F:346:ILE:HD13	1:F:357:VAL:HG23	1.94	0.48
1:F:468:ARG:HA	1:F:468:ARG:NE	2.26	0.48
2:F:900:BLA:OB	2:F:900:BLA:HBB1	2.13	0.48
1:G:112:ILE:HD13	1:G:112:ILE:N	2.17	0.48
1:G:124:THR:O	1:G:128:GLN:HG3	2.14	0.48
1:G:317:VAL:O	1:G:321:ARG:HB3	2.14	0.48
1:B:286:TYR:HB3	1:B:287:PRO:HD3	1.95	0.48
1:C:211:ILE:HD13	1:C:243:VAL:HG21	1.95	0.48
1:G:82:TRP:H	1:G:101:SER:HB3	1.78	0.48
1:A:159:ARG:CG	1:A:160:VAL:N	2.77	0.47
1:B:126:ASN:HD22	1:B:288:VAL:HG22	1.79	0.47
1:C:347:ALA:CB	1:C:366:ILE:HD11	2.44	0.47
1:D:17:ILE:H	1:D:17:ILE:HD12	1.79	0.47
1:E:412:LEU:HB3	1:E:426:TRP:CD1	2.49	0.47
2:F:900:BLA:C2B	2:F:900:BLA:HMA1	2.44	0.47
1:G:319:THR:O	1:G:323:LEU:HB2	2.14	0.47
1:A:106:PHE:HE2	1:A:108:LEU:HD23	1.79	0.47
1:A:330:ARG:NH2	1:B:327:ARG:HB2	2.28	0.47
1:B:207:PRO:HB2	1:B:293:GLN:HG3	1.96	0.47
1:E:308:GLN:HA	1:E:311:ILE:CD1	2.43	0.47
1:G:377:VAL:O	1:G:381:LEU:HG	2.13	0.47
1:H:52:VAL:HG22	1:H:53:ALA:N	2.29	0.47
1:A:139:ASP:HB2	1:A:142:SER:CB	2.44	0.47
1:A:157:TYR:CD2	1:A:278:HIS:HB2	2.49	0.47
1:B:15:GLU:HA	1:B:16:PRO:HD3	1.76	0.47
1:B:127:ALA:HB2	1:B:291:SER:OG	2.15	0.47
1:B:134:VAL:HG13	1:B:302:ILE:HG12	1.96	0.47
1:D:114:THR:HG22	1:D:115:ALA:H	1.79	0.47
1:E:42:SER:O	1:E:45:ILE:HG13	2.14	0.47
1:G:129:ARG:HH21	1:G:154:MET:HG2	1.78	0.47
1:H:152:ARG:HB2	1:H:160:VAL:HG12	1.96	0.47
1:C:46:GLN:HA	1:C:51:PHE:O	2.14	0.47
1:D:273:LEU:HD12	1:D:273:LEU:O	2.13	0.47
1:E:250:TYR:N	1:E:454:LEU:HD21	2.29	0.47
1:G:85:SER:HB2	1:G:98:ILE:HG22	1.96	0.47
1:G:179:ARG:CG	1:G:179:ARG:NH1	2.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:313:GLU:O	1:H:317:VAL:HG22	2.14	0.47
1:H:336:PHE:CD2	1:H:364:LEU:HD22	2.48	0.47
1:H:352:CYS:O	1:H:367:ARG:NH2	2.48	0.47
1:D:159:ARG:HG2	1:D:160:VAL:N	2.29	0.47
1:D:244:SER:HB3	2:D:900:BLA:HMD2	1.96	0.47
1:H:211:ILE:HD12	1:H:259:SER:HB3	1.96	0.47
1:H:353:ASP:HA	1:H:367:ARG:NH1	2.30	0.47
1:H:442:GLU:O	1:H:442:GLU:HG3	2.13	0.47
1:A:266:VAL:HG21	1:A:271:TRP:CD1	2.50	0.47
1:B:32:LEU:HD12	1:B:32:LEU:N	2.30	0.47
1:B:319:THR:HG22	1:B:322:ARG:NH2	2.30	0.47
1:D:37:MET:HB2	1:D:58:TYR:CZ	2.49	0.47
2:D:900:BLA:C2B	2:D:900:BLA:HMA1	2.45	0.47
1:E:278:HIS:CE1	1:E:282:LYS:HD2	2.50	0.47
1:E:462:ALA:O	1:E:466:VAL:HG23	2.14	0.47
1:F:131:ILE:C	1:F:131:ILE:HD12	2.35	0.47
1:G:335:LEU:HD12	1:G:339:LEU:HD11	1.95	0.47
1:H:7:VAL:HA	1:H:11:ASN:ND2	2.24	0.47
1:H:415:ARG:HA	1:H:422:GLY:O	2.15	0.47
1:H:433:HIS:CD2	1:H:436:ARG:HG2	2.46	0.47
2:A:900:BLA:HMB3	2:A:900:BLA:C3A	2.45	0.47
1:B:324:ALA:HB1	1:B:328:ARG:NH2	2.30	0.47
1:B:394:ASN:O	1:B:395:TRP:HB2	2.14	0.47
1:B:455:THR:HB	1:B:456:PRO:HD2	1.97	0.47
1:C:414:ILE:HD12	1:C:486:ARG:HB2	1.96	0.47
2:C:900:BLA:HMB3	2:C:900:BLA:C3A	2.43	0.47
1:D:61:GLN:NE2	1:D:66:PRO:HG3	2.28	0.47
1:D:100:HIS:CD2	1:D:107:TYR:HB2	2.50	0.47
1:D:207:PRO:HG2	1:D:293:GLN:NE2	2.29	0.47
1:D:289:ARG:O	1:D:292:PHE:HD2	1.97	0.47
1:D:436:ARG:HG3	1:H:369:ASP:OD1	2.14	0.47
1:E:59:LEU:HD23	1:E:59:LEU:H	1.79	0.47
1:E:189:ARG:HH21	1:E:189:ARG:HB3	1.79	0.47
1:F:118:LEU:O	1:F:122:SER:HB2	2.15	0.47
1:G:490:MET:HB2	1:G:490:MET:HE2	1.65	0.47
1:H:355:ALA:HB3	1:H:366:ILE:HG13	1.96	0.47
1:A:26:HIS:O	1:A:112:ILE:HG12	2.15	0.47
1:B:266:VAL:HG22	1:B:271:TRP:HB2	1.97	0.47
1:B:393:ASP:HA	1:B:409:CYS:O	2.15	0.47
1:E:356:LEU:CD2	1:E:365:SER:HB3	2.45	0.47
1:G:103:LYS:HD3	1:G:103:LYS:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HG22	1:B:286:TYR:OH	2.15	0.47
1:A:410:GLY:O	1:A:427:PHE:HA	2.15	0.47
1:A:445:LEU:HG	1:A:446:THR:H	1.80	0.47
1:E:40:ALA:CB	1:E:223:PRO:HD2	2.44	0.47
1:E:128:GLN:HG2	1:F:297:GLN:OE1	2.14	0.47
1:E:283:LEU:HD23	1:E:283:LEU:C	2.35	0.47
1:E:335:LEU:C	1:E:337:GLY:H	2.17	0.47
2:F:900:BLA:HMC1	2:F:900:BLA:CBC	2.45	0.47
1:G:315:LEU:O	1:G:318:SER:HB2	2.15	0.47
1:G:378:LEU:CD1	1:G:425:PHE:HZ	2.27	0.47
1:H:94:LEU:O	1:H:94:LEU:HD13	2.14	0.47
1:H:149:ASP:HB3	1:H:153:ARG:NH2	2.30	0.47
1:C:208:ILE:HD11	1:C:293:GLN:N	2.30	0.47
1:D:79:ASN:H	1:D:79:ASN:HD22	1.62	0.47
1:F:430:GLU:HB3	1:F:468:ARG:NH1	2.30	0.47
1:G:322:ARG:NH2	1:G:484:LYS:HD3	2.30	0.47
1:D:19:VAL:HG12	1:D:233:PHE:O	2.15	0.46
1:D:339:LEU:HD13	1:D:357:VAL:HG21	1.97	0.46
1:E:315:LEU:HD22	1:E:315:LEU:HA	1.72	0.46
1:F:350:ILE:HD13	1:F:478:ASP:HB3	1.96	0.46
1:F:412:LEU:HB3	1:F:426:TRP:HD1	1.80	0.46
1:G:412:LEU:HB3	1:G:426:TRP:HD1	1.78	0.46
1:A:307:GLU:C	1:A:309:GLY:H	2.17	0.46
1:C:130:ILE:O	1:C:130:ILE:HD13	2.14	0.46
1:C:417:HIS:HD2	1:C:420:GLU:HB2	1.80	0.46
1:G:262:ILE:CG2	1:G:296:SER:HB2	2.45	0.46
1:H:319:THR:HA	1:H:322:ARG:HB2	1.98	0.46
1:D:356:LEU:HD23	1:D:365:SER:HA	1.96	0.46
1:E:64:VAL:HG12	1:E:68:VAL:HG11	1.98	0.46
1:G:48:LEU:HD11	1:G:112:ILE:HD12	1.97	0.46
1:G:68:VAL:HG13	1:G:97:VAL:HG11	1.96	0.46
1:G:109:GLU:HG2	1:G:240:LEU:HD12	1.98	0.46
1:A:102:TYR:HE2	1:A:234:ASP:OD2	1.98	0.46
1:B:237:TYR:OH	1:H:419:GLN:HG2	2.15	0.46
1:C:138:ASN:ND2	1:D:305:ARG:HH22	2.14	0.46
1:D:134:VAL:CG2	1:D:143:LEU:HD23	2.41	0.46
1:E:305:ARG:CA	1:E:308:GLN:HG2	2.32	0.46
1:F:118:LEU:O	1:F:122:SER:HB3	2.15	0.46
1:F:354:GLY:HA3	1:F:370:PHE:CZ	2.50	0.46
2:G:900:BLA:HMC1	2:G:900:BLA:CBC	2.27	0.46
1:A:178:ARG:NH2	1:G:334:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ARG:O	1:G:364:LEU:CA	2.55	0.46
1:B:18:HIS:CD2	1:B:19:VAL:HG13	2.50	0.46
1:B:168:ASP:O	1:B:169:ASP:HB2	2.16	0.46
1:D:362:ARG:HH12	1:H:178:ARG:HH22	1.61	0.46
1:F:29:LEU:CD1	1:F:109:GLU:HG2	2.44	0.46
1:G:336:PHE:H	1:G:336:PHE:HD1	1.58	0.46
1:H:278:HIS:HD2	1:H:280:SER:O	1.97	0.46
1:A:16:PRO:HB2	1:A:19:VAL:HG22	1.97	0.46
1:C:121:THR:HG23	1:D:287:PRO:HB3	1.98	0.46
1:D:391:HIS:HB3	1:D:412:LEU:CD2	2.46	0.46
1:E:278:HIS:ND1	1:E:282:LYS:HD2	2.30	0.46
1:F:71:MET:HG2	1:F:82:TRP:CZ2	2.51	0.46
1:F:159:ARG:NH1	1:F:183:GLU:O	2.48	0.46
1:F:207:PRO:HG2	1:F:293:GLN:HG3	1.97	0.46
1:F:466:VAL:HG12	1:F:467:VAL:HG13	1.98	0.46
1:G:143:LEU:HD12	1:G:144:LEU:N	2.31	0.46
1:A:108:LEU:HD22	1:A:108:LEU:HA	1.70	0.46
1:A:214:VAL:O	1:A:214:VAL:HG12	2.16	0.46
1:A:319:THR:HG22	1:A:322:ARG:NH2	2.31	0.46
1:D:339:LEU:O	1:D:346:ILE:HG12	2.16	0.46
1:E:103:LYS:HD2	1:E:103:LYS:HA	1.63	0.46
1:H:33:ARG:HG2	1:H:37:MET:HB3	1.97	0.46
1:H:130:ILE:HG12	1:H:147:VAL:CG1	2.45	0.46
1:D:71:MET:O	1:D:74:GLU:HG2	2.15	0.46
1:E:172:GLU:HB2	1:E:189:ARG:HD3	1.98	0.46
1:F:44:ASN:OD1	1:F:219:MET:HG2	2.16	0.46
1:A:109:GLU:HG2	1:A:240:LEU:HD12	1.98	0.46
2:B:900:BLA:CBC	2:B:900:BLA:HMC1	2.46	0.46
1:C:94:LEU:H	1:C:94:LEU:HD13	1.80	0.46
1:C:119:SER:O	1:D:120:ILE:HD11	2.15	0.46
1:G:129:ARG:NH2	1:G:154:MET:HG2	2.31	0.46
1:G:154:MET:HE2	1:G:292:PHE:CE1	2.51	0.46
1:G:465:GLU:HG2	1:G:468:ARG:HH21	1.80	0.46
1:H:103:LYS:HD2	1:H:103:LYS:HA	1.76	0.46
1:A:89:ARG:HG3	1:A:94:LEU:HA	1.98	0.46
1:A:140:THR:HG21	1:A:307:GLU:OE2	2.16	0.46
1:B:11:ASN:O	1:B:11:ASN:ND2	2.49	0.46
1:C:262:ILE:CD1	1:C:292:PHE:HB3	2.46	0.46
1:D:339:LEU:HD12	1:D:357:VAL:HG21	1.98	0.46
1:D:358:MET:O	1:D:422:GLY:HA2	2.16	0.46
1:E:82:TRP:O	1:E:100:HIS:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ILE:HG13	1:F:120:ILE:HD13	1.98	0.46
1:E:130:ILE:HG23	1:E:147:VAL:HG12	1.98	0.46
1:E:142:SER:O	1:E:146:ASN:HB2	2.16	0.46
1:E:260:MET:HE1	1:E:289:ARG:HG2	1.99	0.46
1:E:294:ILE:O	1:E:298:VAL:HG23	2.16	0.46
1:E:389:ILE:HG22	1:E:390:TYR:N	2.31	0.46
1:F:101:SER:HB2	1:F:106:PHE:CE2	2.51	0.46
1:F:485:LEU:HD13	1:F:485:LEU:O	2.15	0.46
1:G:199:ALA:O	1:G:203:TYR:CD1	2.69	0.46
1:A:108:LEU:HD12	1:A:110:PHE:CZ	2.52	0.45
1:B:38:VAL:O	1:B:55:PRO:HA	2.16	0.45
1:E:7:VAL:HG11	1:E:15:GLU:HG3	1.97	0.45
1:E:383:ARG:C	1:E:385:PRO:HD3	2.36	0.45
1:E:384:ASP:CG	1:E:387:ARG:HG3	2.37	0.45
1:G:98:ILE:HG21	1:G:286:TYR:CZ	2.51	0.45
1:G:308:GLN:HA	1:G:311:ILE:HD12	1.98	0.45
1:G:485:LEU:HD23	1:G:485:LEU:HA	1.79	0.45
1:H:464:GLU:O	1:H:468:ARG:HB2	2.16	0.45
1:A:32:LEU:HD23	1:A:72:LEU:HD11	1.99	0.45
1:B:140:THR:CG2	1:B:306:LEU:HB3	2.46	0.45
1:D:273:LEU:HD12	1:D:273:LEU:C	2.37	0.45
1:F:126:ASN:OD1	1:F:288:VAL:HG13	2.16	0.45
1:G:13:GLU:H	1:G:13:GLU:HG3	1.49	0.45
1:H:354:GLY:HA3	1:H:370:PHE:CE2	2.51	0.45
1:C:286:TYR:N	1:C:287:PRO:CD	2.79	0.45
1:D:364:LEU:HD23	1:D:364:LEU:HA	1.72	0.45
1:F:235:LEU:O	1:F:238:SER:HB3	2.17	0.45
1:G:102:TYR:HE2	1:G:234:ASP:CG	2.19	0.45
1:C:165:PHE:HD1	1:C:272:GLY:HA2	1.82	0.45
1:E:146:ASN:HD22	1:E:146:ASN:C	2.20	0.45
1:F:271:TRP:CE3	1:F:303:VAL:HG11	2.52	0.45
1:A:217:THR:HA	1:A:218:PRO:HD3	1.72	0.45
1:C:60:THR:N	1:C:63:GLN:HE21	2.14	0.45
1:F:19:VAL:HG12	1:F:234:ASP:HA	1.97	0.45
1:F:179:ARG:HH11	1:F:181:ASP:HB3	1.82	0.45
2:F:900:BLA:HBD2	2:F:900:BLA:HMD1	1.99	0.45
1:G:133:GLN:CB	1:G:147:VAL:HG12	2.47	0.45
1:G:186:LEU:HD23	1:G:187:GLY:N	2.31	0.45
1:H:410:GLY:HA3	1:H:428:ARG:HB2	1.98	0.45
1:A:417:HIS:NE2	1:A:420:GLU:OE1	2.49	0.45
1:B:201:ARG:HA	1:B:201:ARG:HD3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:ILE:H	1:F:366:ILE:CD1	2.23	0.45
1:G:159:ARG:NH1	1:G:183:GLU:O	2.49	0.45
1:G:266:VAL:HG23	1:G:266:VAL:O	2.16	0.45
1:H:288:VAL:O	1:H:291:SER:HB3	2.15	0.45
1:A:45:ILE:HD12	1:A:46:GLN:N	2.22	0.45
1:B:24:GLN:NE2	1:B:211:ILE:HG23	2.31	0.45
1:B:173:VAL:HG12	1:B:186:LEU:HD23	1.99	0.45
1:B:315:LEU:HD21	1:B:477:THR:HG23	1.99	0.45
1:C:31:THR:C	1:C:32:LEU:HD12	2.37	0.45
1:C:237:TYR:OH	1:G:419:GLN:HG2	2.16	0.45
1:E:43:GLU:HB3	1:E:222:PHE:HE2	1.80	0.45
1:E:140:THR:CG2	1:E:306:LEU:HB3	2.35	0.45
1:G:249:GLU:OE2	1:G:450:SER:HB2	2.17	0.45
1:H:152:ARG:HG3	1:H:157:TYR:O	2.16	0.45
1:C:25:PRO:HD3	1:C:216:TYR:CD2	2.52	0.45
1:C:336:PHE:HE1	1:C:359:LEU:HB3	1.81	0.45
1:C:443:LYS:O	1:C:445:LEU:N	2.49	0.45
1:D:66:PRO:O	1:D:70:ARG:HB2	2.16	0.45
1:D:181:ASP:OD1	1:D:181:ASP:N	2.41	0.45
1:E:135:GLN:OE1	1:F:305:ARG:CZ	2.65	0.45
1:F:204:ILE:HG23	1:F:265:VAL:HG21	1.98	0.45
1:G:179:ARG:NH1	1:G:181:ASP:HB2	2.32	0.45
1:G:187:GLY:O	1:G:433:HIS:HE1	1.99	0.45
1:H:416:PHE:CE1	1:H:424:ILE:HG13	2.48	0.45
1:H:475:SER:HB3	1:H:478:ASP:H	1.81	0.45
1:B:164:ARG:HG3	1:B:174:VAL:HG21	1.98	0.45
1:C:183:GLU:HG2	1:C:443:LYS:HE3	1.99	0.45
1:D:251:LEU:HD23	1:D:251:LEU:HA	1.81	0.45
1:F:214:VAL:CG1	1:F:252:THR:HG23	2.47	0.45
1:G:391:HIS:HA	1:G:411:VAL:O	2.17	0.45
1:G:424:ILE:HD11	1:G:489:LEU:HD11	1.98	0.45
1:H:278:HIS:CD2	1:H:280:SER:O	2.69	0.45
1:H:336:PHE:HD2	1:H:364:LEU:HD22	1.82	0.45
1:H:356:LEU:HD12	1:H:425:PHE:CD1	2.52	0.45
1:A:84:ASN:HB2	1:A:99:GLY:O	2.16	0.45
1:A:327:ARG:HH11	1:A:328:ARG:HE	1.65	0.45
1:B:68:VAL:CG1	1:B:97:VAL:HG11	2.46	0.45
1:C:435:ILE:HG22	1:E:364:LEU:HD22	1.98	0.45
1:D:43:GLU:C	1:D:45:ILE:H	2.20	0.45
1:D:197:ALA:HB1	1:F:382:GLN:O	2.16	0.45
1:F:415:ARG:CZ	1:F:418:ARG:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:426:TRP:CD1	1:F:426:TRP:N	2.85	0.45
1:G:493:CYS:O	1:G:496:HIS:CD2	2.70	0.45
1:A:155:THR:OG1	1:A:156:GLY:N	2.50	0.44
1:B:341:HIS:O	1:B:345:GLY:HA3	2.17	0.44
1:C:64:VAL:CG1	1:C:68:VAL:HB	2.47	0.44
1:C:134:VAL:HG12	1:C:302:ILE:HG12	1.99	0.44
1:F:200:ARG:O	1:F:204:ILE:HG13	2.17	0.44
1:F:424:ILE:HD11	1:F:489:LEU:CD1	2.44	0.44
2:H:900:BLA:HBB1	2:H:900:BLA:OB	2.16	0.44
1:A:24:GLN:HE22	1:A:212:ALA:H	1.64	0.44
1:A:363:THR:HB	1:G:438:GLY:CA	2.45	0.44
1:B:150:GLU:O	1:B:154:MET:HG3	2.17	0.44
1:C:20:PRO:HG2	1:C:241:ARG:HG3	1.98	0.44
1:C:243:VAL:HB	1:C:248:CYS:SG	2.57	0.44
1:E:135:GLN:NE2	1:E:135:GLN:CA	2.80	0.44
1:E:159:ARG:CG	1:E:160:VAL:N	2.80	0.44
1:E:292:PHE:C	1:E:294:ILE:N	2.70	0.44
1:F:328:ARG:HD2	1:F:338:ALA:HA	1.99	0.44
1:H:162:ALA:HA	1:H:273:LEU:O	2.18	0.44
1:H:328:ARG:HD3	1:H:341:HIS:ND1	2.32	0.44
1:A:331:ASP:OD2	1:B:495:ASN:ND2	2.50	0.44
1:B:164:ARG:HB3	1:B:164:ARG:NH1	2.32	0.44
1:B:327:ARG:HH11	1:B:327:ARG:CB	2.30	0.44
1:D:98:ILE:HG21	1:D:286:TYR:CE1	2.52	0.44
1:D:346:ILE:O	1:D:426:TRP:CZ3	2.63	0.44
1:H:319:THR:HG22	1:H:322:ARG:HH21	1.83	0.44
1:H:356:LEU:HB3	1:H:425:PHE:HB2	1.99	0.44
1:A:138:ASN:N	1:A:138:ASN:ND2	2.64	0.44
1:A:202:LEU:HD13	1:A:241:ARG:NH2	2.32	0.44
1:A:246:ILE:HG23	1:A:454:LEU:HD21	2.00	0.44
1:B:164:ARG:O	1:B:171:GLY:HA2	2.17	0.44
1:B:373:GLN:O	1:B:377:VAL:HG23	2.18	0.44
1:B:411:VAL:HG22	1:B:427:PHE:CE2	2.52	0.44
1:C:302:ILE:HG23	1:C:306:LEU:HD22	1.98	0.44
2:C:900:BLA:HMA2	2:C:900:BLA:O2A	2.18	0.44
1:G:161:MET:HG2	1:G:176:GLU:HG3	2.00	0.44
1:A:434:ARG:O	1:G:366:ILE:HA	2.18	0.44
1:C:215:ALA:HB3	1:C:257:ARG:CZ	2.47	0.44
1:E:286:TYR:HB3	1:E:287:PRO:HD3	1.99	0.44
1:F:305:ARG:HA	1:F:308:GLN:HG2	2.00	0.44
1:G:127:ALA:HB2	1:G:291:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLN:CG	1:H:52:VAL:HA	2.47	0.44
1:A:24:GLN:HG2	1:A:216:TYR:HE2	1.81	0.44
1:A:394:ASN:O	1:A:395:TRP:CD1	2.71	0.44
1:C:153:ARG:HD3	1:F:498:LEU:HD21	0.45	0.44
1:D:98:ILE:HG21	1:D:286:TYR:CG	2.52	0.44
1:D:208:ILE:HG22	1:D:262:ILE:CD1	2.48	0.44
1:E:59:LEU:HD12	1:E:69:LEU:HD13	1.98	0.44
1:E:140:THR:HG22	1:E:306:LEU:CB	2.34	0.44
1:E:195:ILE:CG2	1:E:200:ARG:HB2	2.47	0.44
1:F:24:GLN:NE2	1:F:211:ILE:HA	2.27	0.44
1:G:17:ILE:O	1:G:241:ARG:HD2	2.18	0.44
1:G:201:ARG:HG2	1:G:205:GLN:HE21	1.83	0.44
2:H:900:BLA:HBC1	2:H:900:BLA:CMC	2.41	0.44
1:A:164:ARG:HH12	1:A:166:ARG:HH21	1.64	0.44
1:A:225:LEU:O	1:A:227:PRO:HD3	2.18	0.44
1:A:301:ALA:HB2	1:B:135:GLN:HG2	2.00	0.44
1:B:136:LEU:HB2	1:B:137:HIS:ND1	2.33	0.44
1:B:451:GLY:HA2	1:B:452:PRO:HD3	1.65	0.44
1:C:189:ARG:NH2	1:C:463:TRP:HE1	2.15	0.44
1:D:206:ASN:HA	1:D:207:PRO:HD3	1.76	0.44
1:D:324:ALA:O	1:D:328:ARG:HB2	2.18	0.44
1:D:366:ILE:HG23	1:H:435:ILE:HG22	2.00	0.44
1:E:120:ILE:CD1	1:F:120:ILE:HD13	2.48	0.44
1:E:130:ILE:HD11	1:E:150:GLU:HB2	1.99	0.44
1:H:314:LEU:O	1:H:318:SER:HB2	2.18	0.44
1:A:297:GLN:HA	1:B:135:GLN:NE2	2.32	0.44
1:A:305:ARG:HB3	1:A:308:GLN:HE21	1.82	0.44
1:B:305:ARG:HE	1:B:305:ARG:HB3	1.67	0.44
1:C:13:GLU:H	1:C:13:GLU:HG3	1.44	0.44
1:C:19:VAL:HG23	1:C:19:VAL:O	2.18	0.44
1:C:297:GLN:NE2	1:D:128:GLN:NE2	2.66	0.44
1:D:129:ARG:NH2	1:G:497:ALA:CB	2.80	0.44
1:D:195:ILE:HA	1:D:196:PRO:HD3	1.74	0.44
1:E:188:GLN:HE22	1:E:460:PHE:HB2	1.83	0.44
1:E:225:LEU:HD22	1:E:225:LEU:N	2.32	0.44
1:E:292:PHE:C	1:E:294:ILE:H	2.21	0.44
1:E:311:ILE:HB	1:E:477:THR:HG21	1.99	0.44
1:G:306:LEU:HD12	1:G:306:LEU:HA	1.71	0.44
1:C:18:HIS:C	1:C:20:PRO:HD3	2.37	0.44
1:C:210:LEU:HD12	1:C:289:ARG:HD3	2.00	0.44
1:D:42:SER:O	1:D:45:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ILE:CD1	1:E:239:VAL:HG21	2.48	0.44
1:E:306:LEU:HD11	1:F:305:ARG:CZ	2.47	0.44
1:F:199:ALA:O	1:F:203:TYR:HD1	2.01	0.44
1:F:201:ARG:CG	1:F:205:GLN:HE21	2.30	0.44
1:F:313:GLU:O	1:F:317:VAL:HG13	2.18	0.44
1:G:45:ILE:O	1:G:49:LEU:HB2	2.17	0.44
1:G:131:ILE:HD11	1:H:297:GLN:CB	2.46	0.44
1:G:273:LEU:HD12	1:G:273:LEU:O	2.18	0.44
1:H:93:HIS:CD2	1:H:93:HIS:H	2.35	0.44
1:C:315:LEU:O	1:C:319:THR:HG23	2.17	0.43
1:F:117:THR:O	1:F:117:THR:HG22	2.18	0.43
1:F:413:ALA:HB2	1:F:425:PHE:CE2	2.53	0.43
1:H:34:ALA:O	1:H:76:LEU:HD23	2.18	0.43
1:H:121:THR:O	1:H:121:THR:HG22	2.18	0.43
1:A:298:VAL:HG12	1:A:302:ILE:HD13	2.00	0.43
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.79	0.43
1:B:210:LEU:HD23	1:B:211:ILE:N	2.33	0.43
1:C:306:LEU:HA	1:C:306:LEU:HD12	1.54	0.43
1:C:419:GLN:HG3	1:G:237:TYR:CZ	2.53	0.43
1:D:131:ILE:O	1:D:134:VAL:HG12	2.18	0.43
2:D:900:BLA:HMB3	2:D:900:BLA:C3A	2.47	0.43
1:E:140:THR:N	1:E:306:LEU:HD23	2.33	0.43
1:E:182:LEU:HD13	1:E:279:MET:CE	2.49	0.43
1:E:297:GLN:HB2	1:F:131:ILE:HD11	2.00	0.43
1:F:69:LEU:O	1:F:73:GLU:HB2	2.19	0.43
1:A:44:ASN:CG	1:A:219:MET:HG2	2.39	0.43
1:A:358:MET:O	1:A:422:GLY:HA2	2.18	0.43
1:E:128:GLN:HE21	1:F:297:GLN:CG	2.31	0.43
1:E:325:LEU:HD13	1:E:325:LEU:C	2.39	0.43
1:F:220:ARG:NE	1:F:222:PHE:HZ	2.17	0.43
1:G:19:VAL:N	1:G:20:PRO:HD3	2.33	0.43
1:H:85:SER:HB2	1:H:98:ILE:HG22	2.00	0.43
1:C:5:THR:HA	1:C:6:PRO:HD3	1.81	0.43
1:C:22:ALA:HA	1:C:221:VAL:HG13	1.99	0.43
1:C:488:ASP:HB3	1:D:327:ARG:NH2	2.33	0.43
1:D:414:ILE:HG13	1:D:414:ILE:O	2.18	0.43
1:E:394:ASN:HD21	1:E:470:HIS:CG	2.33	0.43
1:E:412:LEU:HD12	1:E:474:TRP:CE3	2.53	0.43
1:A:163:TYR:CG	1:A:190:TYR:OH	2.68	0.43
1:A:222:PHE:HA	1:A:223:PRO:C	2.39	0.43
1:B:24:GLN:HA	1:B:25:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.84	0.43
1:B:413:ALA:HA	1:B:424:ILE:O	2.18	0.43
1:D:15:GLU:HA	1:D:16:PRO:HD3	1.79	0.43
1:D:490:MET:HE2	1:E:136:LEU:HD21	2.01	0.43
1:F:71:MET:HG2	1:F:82:TRP:HZ2	1.83	0.43
1:F:87:GLU:OE1	1:F:113:ARG:NH2	2.51	0.43
1:G:130:ILE:O	1:G:130:ILE:HD13	2.18	0.43
1:G:185:TYR:O	1:G:188:GLN:HB3	2.17	0.43
1:G:415:ARG:HD3	1:G:423:TRP:CZ2	2.53	0.43
1:H:17:ILE:HG21	1:H:244:SER:HB2	1.99	0.43
1:C:18:HIS:O	1:C:20:PRO:HD3	2.18	0.43
1:D:32:LEU:HD21	1:D:59:LEU:HD21	2.00	0.43
1:D:65:GLY:HA2	1:D:66:PRO:HD3	1.81	0.43
1:D:187:GLY:HA3	1:D:435:ILE:CD1	2.49	0.43
1:D:353:ASP:O	1:D:367:ARG:HD3	2.19	0.43
1:G:346:ILE:O	1:G:426:TRP:CZ3	2.72	0.43
1:A:45:ILE:HG22	1:A:49:LEU:HD12	2.00	0.43
1:A:179:ARG:H	1:A:182:LEU:HD12	1.83	0.43
1:D:15:GLU:OE2	1:D:245:PRO:HD2	2.19	0.43
1:E:33:ARG:HG2	1:E:37:MET:HB3	1.99	0.43
1:E:158:ASP:OD1	1:E:278:HIS:CE1	2.72	0.43
1:F:190:TYR:HA	1:F:191:PRO:HD3	1.83	0.43
2:G:900:BLA:HMB3	2:G:900:BLA:C3A	2.48	0.43
1:H:250:TYR:O	1:H:250:TYR:HD1	2.02	0.43
1:A:208:ILE:H	1:A:208:ILE:CD1	2.29	0.43
1:B:130:ILE:HG12	1:B:131:ILE:N	2.33	0.43
1:D:243:VAL:CG1	1:D:244:SER:N	2.82	0.43
1:E:24:GLN:HA	1:E:25:PRO:HD3	1.82	0.43
1:E:201:ARG:NH1	1:E:205:GLN:HG3	2.34	0.43
1:F:44:ASN:HB3	1:F:219:MET:SD	2.58	0.43
1:G:86:VAL:HG12	1:G:87:GLU:N	2.34	0.43
1:G:133:GLN:HE21	1:G:150:GLU:HB2	1.82	0.43
1:G:407:ASP:OD2	1:G:407:ASP:N	2.51	0.43
1:H:25:PRO:HD3	1:H:216:TYR:HD2	1.83	0.43
1:A:130:ILE:CG1	1:A:150:GLU:HG2	2.48	0.43
1:A:305:ARG:HB3	1:A:305:ARG:HE	1.73	0.43
1:B:42:SER:O	1:B:45:ILE:HG13	2.19	0.43
1:B:164:ARG:HB3	1:B:164:ARG:CZ	2.49	0.43
1:B:346:ILE:HD13	1:B:357:VAL:HG23	1.99	0.43
1:B:486:ARG:HH11	1:B:487:LEU:HD12	1.84	0.43
2:D:900:BLA:HBD2	2:D:900:BLA:HMD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:PRO:HG3	1:E:223:PRO:HD3	1.99	0.43
1:F:152:ARG:HD3	1:F:177:SER:O	2.19	0.43
1:F:203:TYR:HD2	1:F:273:LEU:CD2	2.32	0.43
1:G:424:ILE:HD12	1:G:485:LEU:HD13	1.99	0.43
1:H:328:ARG:HB3	1:H:338:ALA:HB1	2.01	0.43
1:A:85:SER:HB2	1:A:286:TYR:HE2	1.81	0.43
1:A:441:PRO:HB3	1:A:443:LYS:CD	2.48	0.43
1:B:222:PHE:HA	1:B:223:PRO:C	2.39	0.43
1:C:134:VAL:HG11	1:C:302:ILE:HG12	1.97	0.43
1:D:40:ALA:HB2	1:D:223:PRO:HD2	2.01	0.43
1:D:358:MET:HB3	1:D:358:MET:HE2	1.62	0.43
1:G:15:GLU:HA	1:G:16:PRO:HD3	1.75	0.43
1:G:152:ARG:HB2	1:G:160:VAL:CG1	2.49	0.43
1:G:210:LEU:HD23	1:G:259:SER:O	2.19	0.43
1:A:5:THR:HA	1:A:6:PRO:HD2	1.86	0.42
1:B:65:GLY:O	1:B:69:LEU:HD12	2.19	0.42
1:B:157:TYR:CE1	1:B:284:ILE:HD11	2.54	0.42
1:B:324:ALA:HB1	1:B:328:ARG:HH21	1.83	0.42
1:C:371:GLU:O	1:C:371:GLU:HG2	2.19	0.42
1:D:239:VAL:HG12	1:D:289:ARG:HH12	1.84	0.42
1:D:317:VAL:HG23	1:D:318:SER:N	2.34	0.42
1:G:214:VAL:HG23	1:G:257:ARG:O	2.19	0.42
1:G:349:LEU:CD1	1:G:485:LEU:HG	2.49	0.42
1:D:161:MET:O	1:D:274:PHE:HA	2.19	0.42
1:F:87:GLU:HB3	1:F:113:ARG:HH12	1.73	0.42
1:H:440:LYS:O	1:H:441:PRO:C	2.58	0.42
1:A:288:VAL:C	1:A:290:MET:N	2.71	0.42
1:B:278:HIS:HD2	1:B:280:SER:O	2.03	0.42
1:C:33:ARG:HB3	1:C:39:LEU:HD11	2.00	0.42
1:D:113:ARG:HH11	1:D:285:PRO:HB3	1.85	0.42
1:D:171:GLY:O	1:D:189:ARG:HA	2.19	0.42
1:D:479:LEU:O	1:D:483:GLU:HB2	2.19	0.42
1:F:17:ILE:O	1:F:241:ARG:HD2	2.20	0.42
1:F:209:ARG:O	1:F:260:MET:HA	2.20	0.42
1:G:440:LYS:HB3	1:G:440:LYS:HE3	1.85	0.42
1:H:15:GLU:HA	1:H:16:PRO:HD3	1.81	0.42
1:H:179:ARG:HD2	1:H:181:ASP:OD2	2.19	0.42
1:A:194:ASP:HB3	2:A:900:BLA:HHB	2.00	0.42
1:A:327:ARG:HH11	1:A:328:ARG:NE	2.18	0.42
1:A:330:ARG:CD	1:B:330:ARG:HB2	2.49	0.42
1:B:71:MET:SD	1:B:86:VAL:HG23	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:THR:HG22	1:C:107:TYR:CD1	2.54	0.42
1:D:9:LEU:HD22	1:D:9:LEU:N	2.35	0.42
1:D:210:LEU:HD23	1:D:211:ILE:N	2.34	0.42
1:D:361:GLY:O	1:H:440:LYS:HD3	2.18	0.42
1:E:54:SER:O	1:E:55:PRO:C	2.56	0.42
1:E:72:LEU:O	1:E:76:LEU:HD13	2.19	0.42
1:E:217:THR:HA	1:E:218:PRO:HD3	1.83	0.42
1:E:305:ARG:HB3	1:E:305:ARG:HE	1.66	0.42
1:F:49:LEU:CD1	1:F:63:GLN:HE21	2.33	0.42
1:F:367:ARG:HA	1:F:367:ARG:HD3	1.61	0.42
1:H:191:PRO:HG3	1:H:463:TRP:CA	2.49	0.42
1:C:132:ALA:O	1:C:136:LEU:HG	2.18	0.42
1:C:251:LEU:HD22	1:C:256:VAL:CG1	2.49	0.42
1:C:301:ALA:O	1:C:305:ARG:HD2	2.19	0.42
1:E:118:LEU:HD23	1:E:118:LEU:HA	1.91	0.42
1:E:172:GLU:HA	1:E:188:GLN:O	2.20	0.42
2:E:900:BLA:HMB3	2:E:900:BLA:HMA2	2.01	0.42
1:H:435:ILE:HG13	1:H:435:ILE:O	2.19	0.42
1:A:92:GLU:HG3	1:A:93:HIS:N	2.35	0.42
1:B:165:PHE:CD1	1:B:272:GLY:HA2	2.54	0.42
1:B:186:LEU:HD23	1:B:186:LEU:HA	1.83	0.42
1:C:15:GLU:HA	1:C:16:PRO:HD3	1.77	0.42
1:C:183:GLU:H	1:C:443:LYS:HE3	1.84	0.42
1:D:19:VAL:CG1	1:D:234:ASP:HA	2.38	0.42
1:E:43:GLU:HB3	1:E:222:PHE:CE2	2.55	0.42
1:F:9:LEU:HD21	1:F:450:SER:HB2	2.02	0.42
1:F:103:LYS:HD3	1:F:103:LYS:HA	1.70	0.42
1:F:464:GLU:O	1:F:468:ARG:HG2	2.20	0.42
1:F:488:ASP:O	1:F:492:LEU:HD13	2.20	0.42
1:G:322:ARG:NH1	1:G:484:LYS:HB3	2.35	0.42
1:G:335:LEU:HD22	1:G:335:LEU:HA	1.78	0.42
1:A:286:TYR:N	1:A:287:PRO:CD	2.83	0.42
1:A:311:ILE:HD13	1:A:312:ALA:N	2.35	0.42
1:D:433:HIS:NE2	1:D:460:PHE:HE1	2.18	0.42
1:E:288:VAL:HG12	1:E:292:PHE:CE2	2.55	0.42
1:F:431:GLU:O	1:F:432:VAL:C	2.57	0.42
1:G:67:GLU:CD	1:G:67:GLU:H	2.23	0.42
1:G:139:ASP:HB2	1:G:142:SER:CB	2.42	0.42
1:G:210:LEU:HD12	1:G:289:ARG:HD3	2.01	0.42
1:G:434:ARG:NH2	1:G:435:ILE:HD11	2.33	0.42
1:H:122:SER:O	1:H:126:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:GLU:O	1:H:154:MET:HG3	2.19	0.42
1:A:36:GLY:HA2	1:A:76:LEU:HD21	2.01	0.42
1:A:143:LEU:HD22	1:A:302:ILE:CG2	2.49	0.42
1:B:214:VAL:C	1:B:216:TYR:H	2.21	0.42
1:D:140:THR:HB	1:D:306:LEU:HD23	2.02	0.42
1:D:278:HIS:HD2	1:D:280:SER:O	2.02	0.42
1:F:165:PHE:CD1	1:F:272:GLY:HA2	2.55	0.42
1:F:249:GLU:CD	1:F:449:PRO:HD2	2.40	0.42
1:G:9:LEU:H	1:G:9:LEU:HD22	1.85	0.42
1:H:83:SER:HA	1:H:99:GLY:O	2.20	0.42
1:H:249:GLU:OE1	1:H:449:PRO:HD2	2.19	0.42
1:D:353:ASP:O	1:D:367:ARG:CD	2.68	0.42
1:E:19:VAL:HG12	1:E:234:ASP:HA	2.02	0.42
1:E:90:ILE:HD11	1:E:97:VAL:HG21	2.00	0.42
1:E:166:ARG:NH2	1:E:172:GLU:OE1	2.53	0.42
1:F:18:HIS:CG	1:F:198:GLN:NE2	2.88	0.42
1:G:305:ARG:CA	1:G:308:GLN:HG2	2.49	0.42
1:G:347:ALA:HB2	1:G:366:ILE:CD1	2.31	0.42
1:H:25:PRO:HD3	1:H:216:TYR:CD2	2.54	0.42
1:H:135:GLN:N	1:H:135:GLN:NE2	2.68	0.42
1:A:59:LEU:H	1:A:59:LEU:CD2	2.31	0.42
1:B:322:ARG:HH22	1:B:484:LYS:HD2	1.85	0.42
1:B:356:LEU:HD13	1:B:357:VAL:N	2.35	0.42
1:C:45:ILE:CD1	1:C:46:GLN:N	2.79	0.42
1:C:59:LEU:HD12	1:C:64:VAL:HG21	2.02	0.42
1:D:54:SER:HA	1:D:55:PRO:HD3	1.90	0.42
1:D:326:ALA:C	1:D:328:ARG:H	2.23	0.42
1:E:220:ARG:HB2	1:E:222:PHE:CZ	2.54	0.42
1:G:39:LEU:O	1:G:223:PRO:HD2	2.20	0.42
1:G:139:ASP:HB2	1:G:142:SER:N	2.33	0.42
1:G:226:ASN:HA	1:G:227:PRO:HD3	1.88	0.42
1:H:17:ILE:H	1:H:17:ILE:HG13	1.64	0.42
1:H:208:ILE:HG13	1:H:289:ARG:HD2	2.00	0.42
1:A:305:ARG:HH21	1:B:138:ASN:ND2	2.18	0.41
1:A:428:ARG:NH2	1:A:474:TRP:CE3	2.75	0.41
1:B:356:LEU:HB3	1:B:425:PHE:HB2	2.02	0.41
1:D:19:VAL:N	1:D:20:PRO:HD3	2.35	0.41
1:D:31:THR:C	1:D:32:LEU:HD12	2.40	0.41
1:D:201:ARG:O	1:D:201:ARG:HD3	2.19	0.41
1:D:264:ILE:HD11	1:D:274:PHE:CE1	2.55	0.41
1:E:346:ILE:O	1:E:426:TRP:HZ3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:ARG:O	1:E:453:ARG:CD	2.62	0.41
1:F:311:ILE:C	1:F:313:GLU:H	2.23	0.41
1:G:44:ASN:HB3	1:G:219:MET:HG2	2.01	0.41
1:G:182:LEU:HD13	1:G:279:MET:CE	2.50	0.41
1:H:126:ASN:HD22	1:H:126:ASN:HA	1.55	0.41
1:H:165:PHE:CE1	1:H:272:GLY:HA2	2.54	0.41
1:H:366:ILE:H	1:H:366:ILE:HG12	1.62	0.41
1:B:49:LEU:HD22	1:B:90:ILE:CD1	2.50	0.41
1:E:124:THR:HG23	1:F:294:ILE:HD12	2.02	0.41
1:E:414:ILE:HG21	1:E:482:ALA:O	2.20	0.41
1:F:410:GLY:O	1:F:427:PHE:HA	2.19	0.41
1:G:262:ILE:CD1	1:G:292:PHE:HB3	2.50	0.41
1:H:207:PRO:HB3	1:H:293:GLN:HG3	2.01	0.41
1:A:382:GLN:HA	1:A:382:GLN:HE21	1.84	0.41
1:B:59:LEU:N	1:B:59:LEU:HD22	2.36	0.41
1:B:112:ILE:HD13	1:B:112:ILE:N	2.34	0.41
1:B:157:TYR:CG	1:B:276:CYS:HB3	2.56	0.41
1:B:366:ILE:O	1:B:367:ARG:HB2	2.20	0.41
1:C:386:GLU:HG2	1:G:269:LYS:HA	2.02	0.41
1:C:419:GLN:HG3	1:G:237:TYR:OH	2.20	0.41
1:C:467:VAL:O	1:C:468:ARG:C	2.58	0.41
1:D:7:VAL:HG11	1:D:15:GLU:HB2	2.02	0.41
1:D:7:VAL:HG11	1:D:15:GLU:HG3	2.02	0.41
1:E:143:LEU:HD13	1:E:147:VAL:HG11	2.02	0.41
1:E:155:THR:HG22	1:E:292:PHE:CZ	2.55	0.41
1:E:354:GLY:HA3	1:E:370:PHE:HE1	1.86	0.41
1:F:84:ASN:ND2	1:F:85:SER:H	2.17	0.41
1:F:265:VAL:HG12	1:F:267:GLY:O	2.21	0.41
1:H:339:LEU:O	1:H:346:ILE:HG12	2.19	0.41
1:A:186:LEU:HD22	1:A:187:GLY:N	2.35	0.41
1:B:208:ILE:H	1:B:208:ILE:CD1	2.27	0.41
1:C:67:GLU:HA	1:C:70:ARG:HB2	2.03	0.41
1:C:86:VAL:HG12	1:C:88:THR:HG22	2.02	0.41
1:D:150:GLU:OE2	1:D:154:MET:HG3	2.20	0.41
1:E:335:LEU:O	1:E:337:GLY:N	2.54	0.41
1:F:49:LEU:HD22	1:F:90:ILE:CG2	2.51	0.41
1:F:74:GLU:HA	1:F:77:THR:OG1	2.21	0.41
1:F:194:ASP:OD2	1:F:453:ARG:NH2	2.54	0.41
1:F:311:ILE:C	1:F:313:GLU:N	2.74	0.41
1:F:454:LEU:O	1:F:455:THR:HG23	2.20	0.41
1:G:160:VAL:HA	1:G:275:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:MET:HB3	1:H:276:CYS:HB2	2.01	0.41
1:A:330:ARG:HD3	1:B:330:ARG:CB	2.51	0.41
1:B:95:PHE:CD2	1:B:112:ILE:HA	2.56	0.41
1:B:208:ILE:HD12	1:B:293:GLN:CG	2.47	0.41
1:C:229:THR:HG23	1:C:231:GLU:H	1.85	0.41
1:C:347:ALA:HB3	1:C:366:ILE:HD11	2.03	0.41
1:D:475:SER:O	1:D:478:ASP:HB2	2.20	0.41
1:G:28:ALA:CB	1:G:48:LEU:HD23	2.50	0.41
1:G:214:VAL:C	1:G:216:TYR:H	2.24	0.41
1:H:68:VAL:HG21	1:H:88:THR:HG21	2.02	0.41
1:H:112:ILE:HD13	1:H:112:ILE:N	2.25	0.41
1:H:165:PHE:CD1	1:H:272:GLY:HA2	2.56	0.41
1:H:433:HIS:CE1	1:H:460:PHE:HE1	2.39	0.41
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.71	0.41
1:A:433:HIS:HD2	1:A:436:ARG:HG2	1.86	0.41
1:B:45:ILE:O	1:B:49:LEU:HB2	2.20	0.41
1:B:59:LEU:HB3	1:B:69:LEU:HD21	2.02	0.41
1:B:62:GLU:OE1	1:B:62:GLU:HA	2.20	0.41
1:C:257:ARG:CG	1:C:257:ARG:NH1	2.57	0.41
1:D:460:PHE:CD2	1:D:460:PHE:C	2.94	0.41
1:F:30:VAL:HG12	1:F:32:LEU:CD1	2.51	0.41
1:F:98:ILE:HG21	1:F:286:TYR:CE1	2.55	0.41
1:F:468:ARG:HH11	1:F:469:GLY:H	1.68	0.41
1:G:8:THR:O	1:G:12:CYS:N	2.53	0.41
1:G:142:SER:O	1:G:146:ASN:HB2	2.20	0.41
1:G:200:ARG:O	1:G:204:ILE:HG13	2.20	0.41
1:G:341:HIS:HA	1:G:342:PRO:HD3	1.93	0.41
1:A:43:GLU:HG3	1:A:222:PHE:HE2	1.86	0.41
1:A:106:PHE:CD2	1:A:107:TYR:N	2.88	0.41
1:B:19:VAL:HG12	1:B:233:PHE:O	2.21	0.41
1:B:94:LEU:C	1:B:94:LEU:HD22	2.41	0.41
1:C:159:ARG:NH1	1:C:183:GLU:O	2.54	0.41
1:D:275:SER:OG	2:D:900:BLA:CGA	2.68	0.41
1:F:117:THR:O	1:F:117:THR:HG23	2.20	0.41
1:F:126:ASN:HD22	1:F:126:ASN:HA	1.54	0.41
1:G:45:ILE:HG13	1:G:45:ILE:H	1.70	0.41
1:H:199:ALA:O	1:H:203:TYR:CD1	2.73	0.41
1:A:159:ARG:HD3	1:A:161:MET:CG	2.51	0.41
1:A:189:ARG:NH2	1:A:463:TRP:NE1	2.69	0.41
1:A:315:LEU:HD22	1:A:315:LEU:HA	1.74	0.41
1:A:411:VAL:HG22	1:A:427:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:O	1:C:105:VAL:HG13	2.21	0.41
1:C:208:ILE:HA	1:C:261:SER:O	2.20	0.41
1:C:308:GLN:O	1:C:311:ILE:HD13	2.21	0.41
1:D:45:ILE:HG13	1:D:45:ILE:H	1.57	0.41
1:E:158:ASP:OD2	1:E:279:MET:HG2	2.21	0.41
1:F:44:ASN:CG	1:F:219:MET:HG2	2.41	0.41
1:G:124:THR:CG2	1:H:291:SER:HA	2.51	0.41
1:G:412:LEU:O	1:G:426:TRP:HD1	2.04	0.41
1:H:18:HIS:HB3	1:H:202:LEU:HD11	2.03	0.41
1:H:164:ARG:O	1:H:171:GLY:HA2	2.19	0.41
1:A:7:VAL:CG2	1:A:245:PRO:HG2	2.47	0.41
1:A:190:TYR:HA	1:A:191:PRO:HD3	1.86	0.41
1:A:261:SER:HB2	1:A:273:LEU:HD13	2.02	0.41
1:A:307:GLU:O	1:A:311:ILE:HG23	2.21	0.41
1:A:415:ARG:HD3	1:A:423:TRP:CE2	2.51	0.41
1:B:90:ILE:HD12	1:B:95:PHE:CD1	2.55	0.41
1:B:127:ALA:O	1:B:131:ILE:HG13	2.21	0.41
1:B:262:ILE:CD1	1:B:292:PHE:HB3	2.50	0.41
1:B:314:LEU:O	1:B:318:SER:HB2	2.20	0.41
1:B:382:GLN:O	1:H:197:ALA:CB	2.68	0.41
1:C:137:HIS:O	1:D:305:ARG:NH2	2.54	0.41
1:C:302:ILE:O	1:C:306:LEU:HB2	2.20	0.41
1:C:306:LEU:HD11	1:D:305:ARG:HH21	1.85	0.41
1:D:349:LEU:HD11	1:D:481:ILE:CG2	2.51	0.41
1:E:313:GLU:O	1:E:317:VAL:HG13	2.20	0.41
1:F:220:ARG:CG	1:F:220:ARG:NH1	2.75	0.41
1:G:247:HIS:CD2	2:G:900:BLA:CBD	3.03	0.41
1:A:163:TYR:HA	1:A:172:GLU:O	2.21	0.41
1:C:194:ASP:OD2	1:C:453:ARG:NH2	2.51	0.41
1:E:123:PHE:CD2	1:E:123:PHE:C	2.94	0.41
1:E:186:LEU:CD2	1:E:187:GLY:N	2.84	0.41
1:E:194:ASP:HB3	2:E:900:BLA:CHB	2.48	0.41
1:F:214:VAL:HG12	1:F:252:THR:CG2	2.50	0.41
1:G:84:ASN:ND2	1:G:85:SER:H	2.19	0.41
1:A:331:ASP:CG	1:B:495:ASN:HD21	2.25	0.40
1:A:362:ARG:HG3	1:G:441:PRO:HG2	2.03	0.40
1:A:366:ILE:H	1:A:366:ILE:HG12	1.72	0.40
1:B:95:PHE:HE2	1:B:112:ILE:HG22	1.86	0.40
1:B:243:VAL:HB	1:B:248:CYS:SG	2.61	0.40
1:B:266:VAL:O	1:B:266:VAL:CG2	2.68	0.40
1:C:119:SER:C	1:D:120:ILE:HD11	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:HA	1:C:166:ARG:HD3	1.88	0.40
1:C:168:ASP:OD2	1:C:170:SER:HB3	2.21	0.40
1:C:467:VAL:O	1:C:470:HIS:N	2.49	0.40
1:D:431:GLU:HG3	1:D:467:VAL:HB	2.02	0.40
1:E:169:ASP:HB3	1:E:200:ARG:CZ	2.51	0.40
1:F:63:GLN:O	1:F:90:ILE:HG23	2.21	0.40
1:F:356:LEU:HD11	1:F:358:MET:HG3	2.03	0.40
1:H:107:TYR:O	1:H:108:LEU:HD22	2.21	0.40
1:H:201:ARG:HA	1:H:201:ARG:HD2	1.90	0.40
1:H:339:LEU:HD23	1:H:339:LEU:HA	1.93	0.40
1:H:387:ARG:NH1	1:H:389:ILE:O	2.54	0.40
1:A:389:ILE:HD11	1:A:483:GLU:HG2	2.02	0.40
1:A:486:ARG:O	1:A:486:ARG:HG2	2.22	0.40
1:C:42:SER:HA	1:C:221:VAL:HA	2.03	0.40
1:C:250:TYR:CD2	1:C:454:LEU:O	2.74	0.40
1:C:390:TYR:HH	1:C:395:TRP:HZ3	1.67	0.40
1:D:132:ALA:O	1:D:136:LEU:HD23	2.21	0.40
1:D:157:TYR:CD2	1:D:278:HIS:HB2	2.57	0.40
1:D:217:THR:HG23	1:D:217:THR:O	2.20	0.40
1:E:51:PHE:CD1	1:E:63:GLN:HB3	2.56	0.40
1:E:120:ILE:HG13	1:F:120:ILE:CD1	2.52	0.40
1:E:210:LEU:HD23	1:E:210:LEU:C	2.42	0.40
1:F:162:ALA:CB	1:F:175:ALA:HB3	2.48	0.40
1:G:7:VAL:HG11	1:G:15:GLU:OE2	2.21	0.40
1:G:208:ILE:HD12	1:G:293:GLN:HE21	1.86	0.40
1:G:311:ILE:HD13	1:G:311:ILE:C	2.42	0.40
1:G:365:SER:OG	1:G:368:GLY:O	2.37	0.40
1:H:19:VAL:N	1:H:20:PRO:HD3	2.36	0.40
1:A:94:LEU:HD21	1:A:113:ARG:HH11	1.87	0.40
1:A:378:LEU:O	1:A:378:LEU:HD23	2.21	0.40
1:B:32:LEU:HD21	1:B:59:LEU:CD2	2.52	0.40
1:B:136:LEU:HB2	1:B:137:HIS:CE1	2.56	0.40
1:B:191:PRO:HG3	1:B:463:TRP:N	2.37	0.40
1:B:430:GLU:OE2	1:B:468:ARG:HA	2.21	0.40
1:C:427:PHE:N	1:C:427:PHE:CD1	2.89	0.40
1:D:155:THR:O	1:D:282:LYS:HE2	2.21	0.40
1:D:316:ARG:HE	1:D:316:ARG:HB3	1.69	0.40
1:D:325:LEU:HD12	1:D:325:LEU:C	2.42	0.40
1:D:344:ASP:OD1	1:D:344:ASP:N	2.54	0.40
1:E:29:LEU:HD12	1:E:108:LEU:O	2.21	0.40
1:E:168:ASP:OD2	1:E:170:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:VAL:HA	1:F:395:TRP:CH2	2.56	0.40
1:G:164:ARG:HH11	1:G:166:ARG:HH21	1.70	0.40
1:H:148:THR:HG23	1:H:160:VAL:O	2.21	0.40
1:H:208:ILE:HG22	1:H:262:ILE:HD13	2.03	0.40
1:H:209:ARG:NH1	2:H:900:BLA:CGD	2.85	0.40
1:H:416:PHE:HE1	1:H:424:ILE:CG1	2.33	0.40
1:A:117:THR:CG2	1:A:118:LEU:H	2.34	0.40
1:A:413:ALA:HA	1:A:424:ILE:O	2.21	0.40
1:B:5:THR:N	1:B:6:PRO:HD3	2.37	0.40
1:B:152:ARG:NH2	1:B:179:ARG:HB2	2.36	0.40
1:D:13:GLU:OE2	2:D:900:BLA:HBC1	2.21	0.40
1:D:42:SER:HA	1:D:221:VAL:HA	2.02	0.40
1:E:297:GLN:HB2	1:F:131:ILE:CD1	2.51	0.40
1:F:42:SER:HA	1:F:221:VAL:HA	2.04	0.40
1:F:209:ARG:HA	1:F:209:ARG:HD2	1.91	0.40
1:A:121:THR:HG21	1:B:85:SER:OG	2.22	0.40
1:A:307:GLU:C	1:A:309:GLY:N	2.74	0.40
1:B:98:ILE:HG13	1:B:109:GLU:HB2	2.03	0.40
1:B:262:ILE:HD12	1:B:292:PHE:HB3	2.04	0.40
1:C:366:ILE:HA	1:E:434:ARG:O	2.22	0.40
1:C:395:TRP:HB3	1:C:409:CYS:HA	2.04	0.40
1:D:118:LEU:HD13	1:D:118:LEU:HA	1.96	0.40
1:D:209:ARG:NH1	2:D:900:BLA:O1D	2.53	0.40
1:E:89:ARG:HB2	1:E:94:LEU:HD23	2.03	0.40
1:E:129:ARG:O	1:E:133:GLN:HB2	2.22	0.40
1:E:157:TYR:CD2	1:E:278:HIS:HB2	2.56	0.40
1:E:189:ARG:HB3	1:E:189:ARG:NH2	2.35	0.40
1:E:391:HIS:HA	1:E:411:VAL:O	2.21	0.40
1:F:19:VAL:N	1:F:20:PRO:CD	2.82	0.40
1:F:24:GLN:HA	1:F:25:PRO:HD3	1.95	0.40
1:G:305:ARG:HG3	1:H:305:ARG:HB2	2.03	0.40
1:H:17:ILE:HG22	1:H:244:SER:HB2	2.04	0.40
1:H:96:ASP:HB2	1:H:111:GLU:HB3	2.02	0.40
1:H:187:GLY:HA3	1:H:435:ILE:CG1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:O	1:C:47:ALA:O[7_445]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/505 (94%)	428 (90%)	42 (9%)	4 (1%)	19	51
1	B	462/505 (92%)	434 (94%)	25 (5%)	3 (1%)	25	58
1	C	478/505 (95%)	439 (92%)	37 (8%)	2 (0%)	34	66
1	D	472/505 (94%)	443 (94%)	29 (6%)	0	100	100
1	E	463/505 (92%)	425 (92%)	36 (8%)	2 (0%)	34	66
1	F	461/505 (91%)	433 (94%)	28 (6%)	0	100	100
1	G	479/505 (95%)	443 (92%)	33 (7%)	3 (1%)	25	58
1	H	476/505 (94%)	427 (90%)	47 (10%)	2 (0%)	34	66
All	All	3765/4040 (93%)	3472 (92%)	277 (7%)	16 (0%)	34	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	ASP
1	C	442	GLU
1	A	289	ARG
1	E	333	ASP
1	H	196	PRO
1	A	20	PRO
1	E	267	GLY
1	G	421	SER
1	H	342	PRO
1	B	452	PRO
1	B	19	VAL
1	B	449	PRO
1	G	66	PRO
1	G	449	PRO
1	A	16	PRO
1	A	207	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	407/431 (94%)	366 (90%)	41 (10%)	7 23
1	B	398/431 (92%)	351 (88%)	47 (12%)	5 16
1	C	410/431 (95%)	353 (86%)	57 (14%)	3 10
1	D	408/431 (95%)	367 (90%)	41 (10%)	7 23
1	E	400/431 (93%)	357 (89%)	43 (11%)	6 20
1	F	400/431 (93%)	351 (88%)	49 (12%)	4 14
1	G	411/431 (95%)	353 (86%)	58 (14%)	3 10
1	H	409/431 (95%)	367 (90%)	42 (10%)	7 22
All	All	3243/3448 (94%)	2865 (88%)	378 (12%)	5 16

All (378) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	13	GLU
1	A	17	ILE
1	A	45	ILE
1	A	59	LEU
1	A	72	LEU
1	A	88	THR
1	A	93	HIS
1	A	108	LEU
1	A	112	ILE
1	A	120	ILE
1	A	126	ASN
1	A	136	LEU
1	A	137	HIS
1	A	140	THR
1	A	149	ASP
1	A	160	VAL
1	A	181	ASP
1	A	186	LEU

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Mol	Chain	Res	Type
1	A	198	GLN
1	A	201	ARG
1	A	208	ILE
1	A	216	TYR
1	A	230	ASN
1	A	232	SER
1	A	260	MET
1	A	261	SER
1	A	305	ARG
1	A	311	ILE
1	A	315	LEU
1	A	327	ARG
1	A	364	LEU
1	A	366	ILE
1	A	388	ASP
1	A	393	ASP
1	A	395	TRP
1	A	412	LEU
1	A	426	TRP
1	A	440	LYS
1	A	450	SER
1	A	453	ARG
1	B	11	ASN
1	B	13	GLU
1	B	32	LEU
1	B	35	ASP
1	B	45	ILE
1	B	67	GLU
1	B	77	THR
1	B	94	LEU
1	B	112	ILE
1	B	114	THR
1	B	116	ASP
1	B	117	THR
1	B	119	SER
1	B	125	LEU
1	B	130	ILE
1	B	142	SER
1	B	160	VAL
1	B	177	SER
1	B	181	ASP
1	B	201	ARG

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Mol	Chain	Res	Type
1	B	208	ILE
1	B	216	TYR
1	B	230	ASN
1	B	239	VAL
1	B	250	TYR
1	B	273	LEU
1	B	304	GLU
1	B	305	ARG
1	B	311	ILE
1	B	317	VAL
1	B	318	SER
1	B	325	LEU
1	B	327	ARG
1	B	344	ASP
1	B	349	LEU
1	B	362	ARG
1	B	363	THR
1	B	364	LEU
1	B	366	ILE
1	B	393	ASP
1	B	412	LEU
1	B	426	TRP
1	B	446	THR
1	B	476	GLU
1	B	485	LEU
1	B	488	ASP
1	B	491	GLU
1	C	9	LEU
1	C	12	CYS
1	C	13	GLU
1	C	49	LEU
1	C	64	VAL
1	C	77	THR
1	C	84	ASN
1	C	88	THR
1	C	94	LEU
1	C	98	ILE
1	C	112	ILE
1	C	120	ILE
1	C	130	ILE
1	C	138	ASN
1	C	140	THR

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	147	VAL
1	C	160	VAL
1	C	164	ARG
1	C	188	GLN
1	C	210	LEU
1	C	216	TYR
1	C	217	THR
1	C	221	VAL
1	C	225	LEU
1	C	230	ASN
1	C	252	THR
1	C	257	ARG
1	C	259	SER
1	C	260	MET
1	C	262	ILE
1	C	298	VAL
1	C	305	ARG
1	C	306	LEU
1	C	311	ILE
1	C	315	LEU
1	C	321	ARG
1	C	323	LEU
1	C	330	ARG
1	C	349	LEU
1	C	356	LEU
1	C	363	THR
1	C	364	LEU
1	C	366	ILE
1	C	380	ARG
1	C	393	ASP
1	C	409	CYS
1	C	412	LEU
1	C	425	PHE
1	C	426	TRP
1	C	429	HIS
1	C	436	ARG
1	C	445	LEU
1	C	479	LEU
1	C	483	GLU
1	C	485	LEU
1	C	487	LEU

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Mol	Chain	Res	Type
1	D	7	VAL
1	D	17	ILE
1	D	35	ASP
1	D	67	GLU
1	D	77	THR
1	D	84	ASN
1	D	94	LEU
1	D	112	ILE
1	D	113	ARG
1	D	114	THR
1	D	116	ASP
1	D	117	THR
1	D	136	LEU
1	D	137	HIS
1	D	138	ASN
1	D	140	THR
1	D	160	VAL
1	D	163	TYR
1	D	201	ARG
1	D	208	ILE
1	D	210	LEU
1	D	230	ASN
1	D	239	VAL
1	D	250	TYR
1	D	260	MET
1	D	273	LEU
1	D	311	ILE
1	D	316	ARG
1	D	343	ASP
1	D	344	ASP
1	D	364	LEU
1	D	384	ASP
1	D	393	ASP
1	D	395	TRP
1	D	412	LEU
1	D	435	ILE
1	D	436	ARG
1	D	444	LEU
1	D	446	THR
1	D	483	GLU
1	D	485	LEU
1	E	12	CYS

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Mol	Chain	Res	Type
1	E	17	ILE
1	E	59	LEU
1	E	64	VAL
1	E	70	ARG
1	E	84	ASN
1	E	103	LYS
1	E	104	GLU
1	E	108	LEU
1	E	112	ILE
1	E	135	GLN
1	E	140	THR
1	E	143	LEU
1	E	146	ASN
1	E	154	MET
1	E	160	VAL
1	E	179	ARG
1	E	186	LEU
1	E	201	ARG
1	E	208	ILE
1	E	216	TYR
1	E	229	THR
1	E	294	ILE
1	E	302	ILE
1	E	305	ARG
1	E	311	ILE
1	E	315	LEU
1	E	317	VAL
1	E	325	LEU
1	E	330	ARG
1	E	349	LEU
1	E	356	LEU
1	E	380	ARG
1	E	381	LEU
1	E	393	ASP
1	E	394	ASN
1	E	426	TRP
1	E	434	ARG
1	E	447	ILE
1	E	450	SER
1	E	468	ARG
1	E	483	GLU
1	E	485	LEU

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Mol	Chain	Res	Type
1	F	11	ASN
1	F	12	CYS
1	F	13	GLU
1	F	35	ASP
1	F	59	LEU
1	F	61	GLN
1	F	64	VAL
1	F	67	GLU
1	F	76	LEU
1	F	84	ASN
1	F	94	LEU
1	F	98	ILE
1	F	112	ILE
1	F	117	THR
1	F	126	ASN
1	F	129	ARG
1	F	134	VAL
1	F	137	HIS
1	F	152	ARG
1	F	160	VAL
1	F	208	ILE
1	F	210	LEU
1	F	216	TYR
1	F	230	ASN
1	F	238	SER
1	F	239	VAL
1	F	257	ARG
1	F	260	MET
1	F	298	VAL
1	F	311	ILE
1	F	315	LEU
1	F	316	ARG
1	F	318	SER
1	F	335	LEU
1	F	343	ASP
1	F	349	LEU
1	F	363	THR
1	F	366	ILE
1	F	367	ARG
1	F	393	ASP
1	F	409	CYS
1	F	412	LEU

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Mol	Chain	Res	Type
1	F	426	TRP
1	F	447	ILE
1	F	453	ARG
1	F	466	VAL
1	F	468	ARG
1	F	472	THR
1	F	488	ASP
1	G	13	GLU
1	G	17	ILE
1	G	32	LEU
1	G	57	SER
1	G	61	GLN
1	G	67	GLU
1	G	84	ASN
1	G	93	HIS
1	G	94	LEU
1	G	98	ILE
1	G	108	LEU
1	G	112	ILE
1	G	118	LEU
1	G	121	THR
1	G	130	ILE
1	G	136	LEU
1	G	142	SER
1	G	143	LEU
1	G	146	ASN
1	G	149	ASP
1	G	160	VAL
1	G	179	ARG
1	G	182	LEU
1	G	201	ARG
1	G	208	ILE
1	G	210	LEU
1	G	216	TYR
1	G	217	THR
1	G	230	ASN
1	G	259	SER
1	G	295	PHE
1	G	304	GLU
1	G	305	ARG
1	G	306	LEU
1	G	311	ILE

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Mol	Chain	Res	Type
1	G	315	LEU
1	G	321	ARG
1	G	323	LEU
1	G	327	ARG
1	G	335	LEU
1	G	356	LEU
1	G	362	ARG
1	G	363	THR
1	G	364	LEU
1	G	365	SER
1	G	366	ILE
1	G	367	ARG
1	G	373	GLN
1	G	393	ASP
1	G	407	ASP
1	G	426	TRP
1	G	444	LEU
1	G	453	ARG
1	G	459	SER
1	G	483	GLU
1	G	485	LEU
1	G	487	LEU
1	G	494	LEU
1	H	64	VAL
1	H	77	THR
1	H	79	ASN
1	H	84	ASN
1	H	93	HIS
1	H	94	LEU
1	H	112	ILE
1	H	114	THR
1	H	126	ASN
1	H	130	ILE
1	H	134	VAL
1	H	135	GLN
1	H	146	ASN
1	H	160	VAL
1	H	163	TYR
1	H	181	ASP
1	H	208	ILE
1	H	210	LEU
1	H	230	ASN

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Mol	Chain	Res	Type
1	H	250	TYR
1	H	260	MET
1	H	273	LEU
1	H	305	ARG
1	H	314	LEU
1	H	315	LEU
1	H	341	HIS
1	H	349	LEU
1	H	357	VAL
1	H	366	ILE
1	H	378	LEU
1	H	387	ARG
1	H	409	CYS
1	H	412	LEU
1	H	437	TRP
1	H	445	LEU
1	H	446	THR
1	H	447	ILE
1	H	454	LEU
1	H	472	THR
1	H	477	THR
1	H	483	GLU
1	H	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	24	GLN
1	A	26	HIS
1	A	128	GLN
1	A	137	HIS
1	A	138	ASN
1	A	146	ASN
1	A	198	GLN
1	A	205	GLN
1	A	230	ASN
1	A	293	GLN
1	A	382	GLN
1	A	394	ASN
1	A	433	HIS
1	B	11	ASN

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Mol	Chain	Res	Type
1	B	24	GLN
1	B	26	HIS
1	B	138	ASN
1	B	198	GLN
1	B	205	GLN
1	B	230	ASN
1	B	277	HIS
1	B	278	HIS
1	B	293	GLN
1	B	308	GLN
1	B	373	GLN
1	B	495	ASN
1	C	24	GLN
1	C	63	GLN
1	C	84	ASN
1	C	128	GLN
1	C	133	GLN
1	C	137	HIS
1	C	138	ASN
1	C	146	ASN
1	C	205	GLN
1	C	230	ASN
1	C	278	HIS
1	C	394	ASN
1	C	417	HIS
1	C	495	ASN
1	D	11	ASN
1	D	24	GLN
1	D	61	GLN
1	D	79	ASN
1	D	84	ASN
1	D	126	ASN
1	D	128	GLN
1	D	135	GLN
1	D	138	ASN
1	D	146	ASN
1	D	205	GLN
1	D	230	ASN
1	D	293	GLN
1	D	373	GLN
1	E	84	ASN
1	E	93	HIS

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Mol	Chain	Res	Type
1	E	128	GLN
1	E	188	GLN
1	E	205	GLN
1	E	230	ASN
1	E	293	GLN
1	E	308	GLN
1	E	394	ASN
1	E	417	HIS
1	E	433	HIS
1	E	470	HIS
1	F	11	ASN
1	F	24	GLN
1	F	26	HIS
1	F	63	GLN
1	F	84	ASN
1	F	126	ASN
1	F	128	GLN
1	F	135	GLN
1	F	138	ASN
1	F	146	ASN
1	F	188	GLN
1	F	205	GLN
1	F	206	ASN
1	F	230	ASN
1	F	293	GLN
1	F	394	ASN
1	G	11	ASN
1	G	46	GLN
1	G	84	ASN
1	G	126	ASN
1	G	205	GLN
1	G	230	ASN
1	G	247	HIS
1	G	293	GLN
1	G	373	GLN
1	G	394	ASN
1	G	417	HIS
1	G	433	HIS
1	G	496	HIS
1	H	11	ASN
1	H	46	GLN
1	H	61	GLN

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Mol	Chain	Res	Type
1	H	63	GLN
1	H	79	ASN
1	H	84	ASN
1	H	93	HIS
1	H	126	ASN
1	H	133	GLN
1	H	137	HIS
1	H	138	ASN
1	H	146	ASN
1	H	230	ASN
1	H	278	HIS
1	H	391	HIS
1	H	394	ASN
1	H	433	HIS
1	H	496	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BLA	E	900	1	42,46,46	3.17	19 (45%)	53,67,67	2.01	13 (24%)
2	BLA	H	900	1	42,46,46	2.81	17 (40%)	53,67,67	2.10	13 (24%)
2	BLA	F	900	1	42,46,46	2.87	16 (38%)	53,67,67	2.07	13 (24%)
2	BLA	C	900	1	42,46,46	3.16	18 (42%)	53,67,67	2.26	14 (26%)
2	BLA	B	900	1	42,46,46	3.05	19 (45%)	53,67,67	2.03	14 (26%)
2	BLA	G	900	1	42,46,46	2.91	15 (35%)	53,67,67	2.06	14 (26%)
2	BLA	A	900	1	42,46,46	2.92	16 (38%)	53,67,67	2.07	13 (24%)
2	BLA	D	900	1	42,46,46	2.99	17 (40%)	53,67,67	2.12	14 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	E	900	1	-	11/26/74/74	0/4/4/4
2	BLA	H	900	1	-	9/26/74/74	0/4/4/4
2	BLA	F	900	1	-	9/26/74/74	0/4/4/4
2	BLA	C	900	1	-	10/26/74/74	0/4/4/4
2	BLA	B	900	1	-	8/26/74/74	0/4/4/4
2	BLA	G	900	1	-	8/26/74/74	0/4/4/4
2	BLA	A	900	1	-	8/26/74/74	0/4/4/4
2	BLA	D	900	1	-	9/26/74/74	0/4/4/4

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	900	BLA	CHB-C1B	9.75	1.54	1.34
2	G	900	BLA	CHB-C1B	9.69	1.54	1.34
2	D	900	BLA	CHB-C1B	9.61	1.54	1.34
2	E	900	BLA	CHB-C1B	9.54	1.54	1.34
2	B	900	BLA	CHB-C1B	9.52	1.54	1.34
2	F	900	BLA	CHB-C1B	9.39	1.54	1.34
2	A	900	BLA	CHB-C1B	9.35	1.53	1.34
2	C	900	BLA	CHB-C1B	9.24	1.53	1.34
2	C	900	BLA	C4D-C3D	-8.27	1.32	1.45
2	B	900	BLA	CHA-C4D	7.11	1.41	1.35
2	E	900	BLA	CHA-C4D	6.98	1.40	1.35
2	E	900	BLA	C4D-C3D	-6.79	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	900	BLA	CHD-C4C	6.42	1.53	1.38
2	A	900	BLA	CHD-C4C	6.41	1.53	1.38
2	D	900	BLA	CHD-C4C	6.22	1.52	1.38
2	B	900	BLA	CHD-C4C	6.20	1.52	1.38
2	E	900	BLA	CHD-C4C	6.16	1.52	1.38
2	G	900	BLA	CHD-C4C	6.12	1.52	1.38
2	H	900	BLA	CHD-C4C	6.12	1.52	1.38
2	A	900	BLA	CHA-C4D	6.10	1.40	1.35
2	D	900	BLA	CHA-C4D	6.04	1.40	1.35
2	G	900	BLA	CHD-C1D	5.86	1.54	1.40
2	A	900	BLA	CHD-C1D	5.82	1.54	1.40
2	C	900	BLA	CHA-C4D	5.77	1.39	1.35
2	B	900	BLA	CHD-C1D	5.74	1.53	1.40
2	E	900	BLA	CHD-C1D	5.74	1.53	1.40
2	F	900	BLA	CHD-C1D	5.69	1.53	1.40
2	C	900	BLA	CHD-C4C	5.65	1.51	1.38
2	D	900	BLA	CHD-C1D	5.64	1.53	1.40
2	B	900	BLA	C4D-C3D	-5.29	1.37	1.45
2	C	900	BLA	CHD-C1D	5.21	1.52	1.40
2	D	900	BLA	C4D-C3D	-5.17	1.37	1.45
2	H	900	BLA	CHD-C1D	5.13	1.52	1.40
2	F	900	BLA	CHA-C4D	5.10	1.39	1.35
2	G	900	BLA	CHA-C4D	4.99	1.39	1.35
2	C	900	BLA	C1D-C2D	-4.88	1.35	1.45
2	E	900	BLA	CBC-CAC	4.82	1.54	1.30
2	C	900	BLA	CBC-CAC	4.80	1.54	1.30
2	F	900	BLA	CBC-CAC	4.77	1.53	1.30
2	B	900	BLA	CBC-CAC	4.74	1.53	1.30
2	A	900	BLA	CBC-CAC	4.69	1.53	1.30
2	G	900	BLA	CBC-CAC	4.69	1.53	1.30
2	H	900	BLA	CBC-CAC	4.65	1.53	1.30
2	D	900	BLA	CBC-CAC	4.64	1.53	1.30
2	G	900	BLA	C4D-C3D	-4.26	1.38	1.45
2	E	900	BLA	C1D-C2D	-4.16	1.36	1.45
2	A	900	BLA	C4D-C3D	-4.02	1.39	1.45
2	B	900	BLA	C1D-C2D	-3.90	1.37	1.45
2	D	900	BLA	C1D-C2D	-3.87	1.37	1.45
2	H	900	BLA	CHA-C4D	3.85	1.38	1.35
2	D	900	BLA	C4A-CHB	3.75	1.55	1.41
2	H	900	BLA	C4D-C3D	-3.65	1.39	1.45
2	H	900	BLA	C1D-C2D	-3.60	1.38	1.45
2	C	900	BLA	C4A-CHB	3.57	1.55	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	900	BLA	C1D-C2D	-3.57	1.38	1.45
2	A	900	BLA	C1D-C2D	-3.56	1.38	1.45
2	E	900	BLA	C4A-CHB	3.54	1.54	1.41
2	H	900	BLA	C3C-C4C	-3.51	1.39	1.45
2	H	900	BLA	C4A-CHB	3.51	1.54	1.41
2	C	900	BLA	C1C-C2C	-3.50	1.38	1.47
2	F	900	BLA	CAB-C3B	-3.47	1.38	1.47
2	G	900	BLA	C4A-CHB	3.45	1.54	1.41
2	F	900	BLA	C3C-C4C	-3.44	1.39	1.45
2	G	900	BLA	C1C-C2C	-3.40	1.38	1.47
2	F	900	BLA	C1D-C2D	-3.39	1.38	1.45
2	F	900	BLA	C1C-C2C	-3.39	1.38	1.47
2	C	900	BLA	C4D-ND	-3.38	1.31	1.38
2	A	900	BLA	C3C-C4C	-3.36	1.40	1.45
2	F	900	BLA	C4A-CHB	3.34	1.54	1.41
2	B	900	BLA	C4A-CHB	3.34	1.54	1.41
2	A	900	BLA	C4A-CHB	3.31	1.54	1.41
2	H	900	BLA	C1C-C2C	-3.31	1.38	1.47
2	D	900	BLA	C3C-C4C	-3.29	1.40	1.45
2	E	900	BLA	C1C-C2C	-3.29	1.38	1.47
2	B	900	BLA	C3C-C4C	-3.28	1.40	1.45
2	B	900	BLA	C1C-C2C	-3.27	1.38	1.47
2	E	900	BLA	C3C-C4C	-3.25	1.40	1.45
2	D	900	BLA	C1C-C2C	-3.24	1.38	1.47
2	F	900	BLA	C4D-C3D	-3.19	1.40	1.45
2	H	900	BLA	C3B-C4B	-3.18	1.38	1.47
2	B	900	BLA	C3B-C4B	-3.16	1.38	1.47
2	A	900	BLA	CAB-C3B	-3.16	1.38	1.47
2	A	900	BLA	C1C-C2C	-3.13	1.39	1.47
2	G	900	BLA	C3B-C4B	-3.10	1.38	1.47
2	C	900	BLA	C3B-C4B	-3.08	1.38	1.47
2	C	900	BLA	C3C-C4C	-3.07	1.40	1.45
2	C	900	BLA	CAB-C3B	-3.07	1.39	1.47
2	F	900	BLA	C3B-C4B	-3.06	1.38	1.47
2	G	900	BLA	C3C-C4C	-3.04	1.40	1.45
2	G	900	BLA	CAB-C3B	-3.03	1.39	1.47
2	H	900	BLA	CAB-C3B	-3.02	1.39	1.47
2	D	900	BLA	C3B-C4B	-3.02	1.38	1.47
2	A	900	BLA	C3B-C4B	-3.00	1.38	1.47
2	E	900	BLA	C3B-C4B	-3.00	1.38	1.47
2	D	900	BLA	CAB-C3B	-3.00	1.39	1.47
2	C	900	BLA	C4C-NC	-2.94	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	BLA	CAB-C3B	-2.87	1.39	1.47
2	B	900	BLA	CAB-C3B	-2.86	1.39	1.47
2	B	900	BLA	C1B-C2B	-2.76	1.40	1.45
2	E	900	BLA	C1B-C2B	-2.75	1.40	1.45
2	E	900	BLA	CAC-C3C	2.75	1.54	1.47
2	G	900	BLA	CAC-C3C	2.74	1.54	1.47
2	D	900	BLA	C1B-C2B	-2.70	1.40	1.45
2	G	900	BLA	C1B-C2B	-2.68	1.40	1.45
2	C	900	BLA	C1B-C2B	-2.66	1.40	1.45
2	E	900	BLA	C4D-ND	-2.65	1.32	1.38
2	F	900	BLA	C1B-C2B	-2.65	1.40	1.45
2	C	900	BLA	CAC-C3C	2.63	1.54	1.47
2	A	900	BLA	C1B-C2B	-2.60	1.40	1.45
2	H	900	BLA	CAC-C3C	2.54	1.54	1.47
2	F	900	BLA	CAC-C3C	2.49	1.54	1.47
2	B	900	BLA	CAC-C3C	2.49	1.54	1.47
2	H	900	BLA	C1B-C2B	-2.47	1.40	1.45
2	D	900	BLA	C4D-ND	-2.45	1.33	1.38
2	A	900	BLA	CAC-C3C	2.44	1.54	1.47
2	E	900	BLA	C4C-NC	-2.37	1.33	1.37
2	B	900	BLA	C4D-ND	-2.33	1.33	1.38
2	A	900	BLA	C4D-ND	-2.28	1.33	1.38
2	D	900	BLA	CAC-C3C	2.25	1.53	1.47
2	H	900	BLA	C4D-ND	-2.25	1.33	1.38
2	D	900	BLA	C4C-NC	-2.25	1.34	1.37
2	H	900	BLA	C4C-NC	-2.24	1.34	1.37
2	E	900	BLA	C1B-NB	-2.24	1.34	1.37
2	E	900	BLA	C1C-NC	-2.22	1.33	1.38
2	B	900	BLA	C4B-NB	-2.19	1.33	1.38
2	F	900	BLA	C1C-NC	-2.16	1.33	1.38
2	F	900	BLA	C4C-NC	-2.15	1.34	1.37
2	E	900	BLA	C4B-NB	-2.12	1.33	1.38
2	D	900	BLA	C1C-NC	-2.11	1.33	1.38
2	B	900	BLA	C4C-NC	-2.10	1.34	1.37
2	G	900	BLA	C4C-NC	-2.09	1.34	1.37
2	C	900	BLA	C1C-NC	-2.08	1.33	1.38
2	H	900	BLA	C4B-NB	-2.08	1.33	1.38
2	A	900	BLA	C4C-NC	-2.08	1.34	1.37
2	B	900	BLA	C1C-NC	-2.07	1.33	1.38
2	C	900	BLA	C4B-NB	-2.02	1.33	1.38
2	B	900	BLA	C1B-NB	-2.01	1.34	1.37

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	900	BLA	C1A-CHA-C4D	-9.79	117.12	128.81
2	G	900	BLA	C1A-CHA-C4D	-9.02	118.04	128.81
2	D	900	BLA	C1A-CHA-C4D	-8.90	118.17	128.81
2	A	900	BLA	C1A-CHA-C4D	-8.79	118.31	128.81
2	E	900	BLA	C1A-CHA-C4D	-8.56	118.58	128.81
2	H	900	BLA	C1A-CHA-C4D	-8.40	118.78	128.81
2	F	900	BLA	C1A-CHA-C4D	-8.20	119.02	128.81
2	B	900	BLA	C1A-CHA-C4D	-7.82	119.47	128.81
2	H	900	BLA	C4C-CHD-C1D	-6.44	112.34	128.08
2	D	900	BLA	C4C-CHD-C1D	-6.07	113.24	128.08
2	F	900	BLA	C4C-CHD-C1D	-5.94	113.57	128.08
2	B	900	BLA	C4C-CHD-C1D	-5.74	114.05	128.08
2	E	900	BLA	C4C-CHD-C1D	-5.62	114.34	128.08
2	G	900	BLA	C4C-CHD-C1D	-5.23	115.30	128.08
2	C	900	BLA	CAD-C3D-C4D	4.85	133.58	125.01
2	A	900	BLA	C4C-CHD-C1D	-4.76	116.44	128.08
2	C	900	BLA	C4C-CHD-C1D	-4.25	117.70	128.08
2	H	900	BLA	CMB-C2B-C1B	4.04	129.22	124.17
2	C	900	BLA	CAD-C3D-C2D	-3.91	120.59	127.88
2	A	900	BLA	CMB-C2B-C1B	3.74	128.84	124.17
2	C	900	BLA	CHD-C1D-ND	3.59	132.46	124.93
2	E	900	BLA	CAD-C3D-C4D	3.50	131.20	125.01
2	C	900	BLA	CMB-C2B-C1B	3.46	128.49	124.17
2	B	900	BLA	CAD-C3D-C4D	3.34	130.92	125.01
2	F	900	BLA	CMB-C2B-C1B	3.28	128.27	124.17
2	D	900	BLA	CBC-CAC-C3C	-3.25	111.47	127.62
2	F	900	BLA	CBA-CAA-C2A	3.21	118.10	112.62
2	D	900	BLA	CMB-C2B-C1B	3.18	128.13	124.17
2	G	900	BLA	CMB-C2B-C1B	3.10	128.03	124.17
2	F	900	BLA	CAD-C3D-C4D	3.02	130.35	125.01
2	D	900	BLA	CAD-C3D-C4D	3.00	130.32	125.01
2	D	900	BLA	CBA-CAA-C2A	2.97	117.68	112.62
2	B	900	BLA	CBC-CAC-C3C	-2.89	113.25	127.62
2	B	900	BLA	CMB-C2B-C1B	2.86	127.74	124.17
2	C	900	BLA	CHB-C1B-NB	-2.85	120.84	130.40
2	A	900	BLA	CBC-CAC-C3C	-2.81	113.64	127.62
2	E	900	BLA	CMB-C2B-C1B	2.78	127.64	124.17
2	A	900	BLA	CAD-C3D-C4D	2.76	129.90	125.01
2	A	900	BLA	CHD-C1D-ND	2.76	130.71	124.93
2	F	900	BLA	CBC-CAC-C3C	-2.75	113.94	127.62
2	G	900	BLA	CHD-C1D-ND	2.75	130.68	124.93
2	A	900	BLA	CHB-C1B-NB	-2.72	121.28	130.40
2	C	900	BLA	CBC-CAC-C3C	-2.70	114.17	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	BLA	CHB-C1B-NB	-2.68	121.39	130.40
2	E	900	BLA	CAD-C3D-C2D	-2.65	122.94	127.88
2	G	900	BLA	CHA-C4D-C3D	-2.64	119.23	125.32
2	H	900	BLA	CHB-C1B-NB	-2.64	121.55	130.40
2	H	900	BLA	CBC-CAC-C3C	-2.61	114.65	127.62
2	F	900	BLA	CHD-C1D-ND	2.57	130.32	124.93
2	C	900	BLA	C2D-C1D-ND	-2.55	105.08	110.53
2	C	900	BLA	C3B-C4B-NB	2.53	109.05	106.19
2	H	900	BLA	CAD-C3D-C4D	2.53	129.48	125.01
2	B	900	BLA	C3B-C4B-NB	2.52	109.03	106.19
2	F	900	BLA	CBD-CAD-C3D	-2.51	105.65	112.63
2	B	900	BLA	CBA-CAA-C2A	2.50	116.88	112.62
2	D	900	BLA	C3B-C4B-NB	2.49	109.00	106.19
2	E	900	BLA	CBC-CAC-C3C	-2.49	115.24	127.62
2	G	900	BLA	CBC-CAC-C3C	-2.48	115.27	127.62
2	C	900	BLA	O1D-CGD-CBD	-2.48	115.13	123.08
2	B	900	BLA	CHD-C1D-ND	2.48	130.11	124.93
2	E	900	BLA	CHB-C1B-NB	-2.47	122.10	130.40
2	H	900	BLA	CHB-C1B-C2B	2.43	131.76	126.97
2	B	900	BLA	CAD-C3D-C2D	-2.42	123.36	127.88
2	E	900	BLA	C3B-C4B-NB	2.42	108.92	106.19
2	G	900	BLA	CHB-C1B-NB	-2.42	122.29	130.40
2	A	900	BLA	CMC-C2C-C1C	2.41	127.06	121.39
2	G	900	BLA	CHA-C4D-ND	2.40	132.15	128.83
2	A	900	BLA	C1D-C2D-C3D	2.36	109.22	106.51
2	H	900	BLA	C4D-ND-C1D	2.36	110.96	106.51
2	A	900	BLA	C4D-ND-C1D	2.34	110.92	106.51
2	C	900	BLA	CHB-C1B-C2B	2.34	131.59	126.97
2	D	900	BLA	CMC-C2C-C1C	2.29	126.78	121.39
2	F	900	BLA	O1D-CGD-CBD	-2.27	115.78	123.08
2	G	900	BLA	C3B-C4B-NB	2.26	108.74	106.19
2	E	900	BLA	C3C-C4C-NC	2.26	110.33	106.80
2	B	900	BLA	CHB-C1B-C2B	2.25	131.40	126.97
2	H	900	BLA	CHA-C4D-ND	2.23	131.92	128.83
2	F	900	BLA	CHB-C1B-NB	-2.23	122.92	130.40
2	B	900	BLA	C1D-C2D-C3D	2.22	109.06	106.51
2	D	900	BLA	CAD-C3D-C2D	-2.20	123.77	127.88
2	H	900	BLA	CHD-C1D-ND	2.19	129.52	124.93
2	C	900	BLA	C1D-C2D-C3D	2.18	109.01	106.51
2	H	900	BLA	CHA-C4D-C3D	-2.17	120.30	125.32
2	E	900	BLA	CBA-CAA-C2A	2.16	116.31	112.62
2	A	900	BLA	C3B-C4B-NB	2.16	108.63	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	900	BLA	C1D-C2D-C3D	2.12	108.94	106.51
2	D	900	BLA	C4D-ND-C1D	2.11	110.49	106.51
2	H	900	BLA	C3B-C4B-NB	2.11	108.57	106.19
2	E	900	BLA	CHD-C1D-ND	2.10	129.33	124.93
2	F	900	BLA	CAD-C3D-C2D	-2.09	123.98	127.88
2	G	900	BLA	CAD-C3D-C4D	2.09	128.70	125.01
2	H	900	BLA	O1D-CGD-CBD	-2.09	116.37	123.08
2	G	900	BLA	C1D-C2D-C3D	2.08	108.90	106.51
2	B	900	BLA	O1D-CGD-CBD	-2.07	116.43	123.08
2	A	900	BLA	O1D-CGD-CBD	-2.07	116.44	123.08
2	D	900	BLA	CHB-C1B-NB	-2.07	123.46	130.40
2	C	900	BLA	C3C-C4C-NC	2.07	110.03	106.80
2	D	900	BLA	O1D-CGD-CBD	-2.05	116.49	123.08
2	F	900	BLA	C4D-ND-C1D	2.04	110.36	106.51
2	E	900	BLA	O1D-CGD-CBD	-2.04	116.52	123.08
2	G	900	BLA	C3C-C4C-NC	2.04	109.99	106.80
2	B	900	BLA	C2D-C1D-ND	-2.04	106.18	110.53
2	E	900	BLA	C2D-C1D-ND	-2.03	106.18	110.53
2	D	900	BLA	O1A-CGA-CBA	-2.03	116.55	123.08
2	G	900	BLA	CBA-CAA-C2A	2.03	116.08	112.62
2	G	900	BLA	C4C-NC-C1C	-2.02	108.10	110.67
2	D	900	BLA	C1D-C2D-C3D	2.01	108.81	106.51
2	A	900	BLA	CHA-C4D-C3D	-2.01	120.68	125.32

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	A	900	BLA	NB-C1B-CHB-C4A
2	A	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	NB-C1B-CHB-C4A
2	B	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	NA-C4A-CHB-C1B
2	C	900	BLA	C3A-C4A-CHB-C1B
2	C	900	BLA	NB-C1B-CHB-C4A
2	C	900	BLA	C2B-C1B-CHB-C4A
2	D	900	BLA	NA-C4A-CHB-C1B
2	D	900	BLA	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
2	D	900	BLA	NB-C1B-CHB-C4A
2	D	900	BLA	C2B-C1B-CHB-C4A
2	E	900	BLA	NA-C4A-CHB-C1B
2	E	900	BLA	C3A-C4A-CHB-C1B
2	E	900	BLA	NB-C1B-CHB-C4A
2	E	900	BLA	C2B-C1B-CHB-C4A
2	F	900	BLA	NA-C4A-CHB-C1B
2	F	900	BLA	C3A-C4A-CHB-C1B
2	F	900	BLA	NB-C1B-CHB-C4A
2	F	900	BLA	C2B-C1B-CHB-C4A
2	G	900	BLA	C1A-C2A-CAA-CBA
2	G	900	BLA	C3A-C2A-CAA-CBA
2	G	900	BLA	NA-C4A-CHB-C1B
2	G	900	BLA	C3A-C4A-CHB-C1B
2	G	900	BLA	NB-C1B-CHB-C4A
2	G	900	BLA	C2B-C1B-CHB-C4A
2	H	900	BLA	NA-C4A-CHB-C1B
2	H	900	BLA	C3A-C4A-CHB-C1B
2	H	900	BLA	NB-C1B-CHB-C4A
2	H	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	NC-C4C-CHD-C1D
2	D	900	BLA	C2C-C3C-CAC-CBC
2	D	900	BLA	CAD-CBD-CGD-O2D
2	E	900	BLA	CAD-CBD-CGD-O2D
2	E	900	BLA	C4D-C3D-CAD-CBD
2	A	900	BLA	CAA-CBA-CGA-O1A
2	A	900	BLA	CAD-CBD-CGD-O1D
2	E	900	BLA	CAD-CBD-CGD-O1D
2	E	900	BLA	C2D-C3D-CAD-CBD
2	A	900	BLA	CAD-CBD-CGD-O2D
2	H	900	BLA	CAD-CBD-CGD-O2D
2	H	900	BLA	CAD-CBD-CGD-O1D
2	C	900	BLA	C3C-C4C-CHD-C1D
2	A	900	BLA	CAA-CBA-CGA-O2A
2	E	900	BLA	ND-C1D-CHD-C4C
2	C	900	BLA	CAD-CBD-CGD-O2D
2	D	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O2D
2	C	900	BLA	CAD-CBD-CGD-O1D
2	E	900	BLA	CAA-CBA-CGA-O1A
2	H	900	BLA	CAA-CBA-CGA-O1A
2	B	900	BLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	C	900	BLA	CAA-CBA-CGA-O1A
2	F	900	BLA	CAA-CBA-CGA-O1A
2	G	900	BLA	CAD-CBD-CGD-O2D
2	H	900	BLA	C2D-C3D-CAD-CBD
2	F	900	BLA	CAD-CBD-CGD-O1D
2	F	900	BLA	CAD-CBD-CGD-O2D
2	D	900	BLA	C4C-C3C-CAC-CBC
2	C	900	BLA	CAA-CBA-CGA-O2A
2	B	900	BLA	CAA-CBA-CGA-O1A
2	E	900	BLA	CAA-CBA-CGA-O2A
2	G	900	BLA	CAD-CBD-CGD-O1D
2	H	900	BLA	CAA-CBA-CGA-O2A
2	F	900	BLA	CAA-CBA-CGA-O2A
2	F	900	BLA	NC-C4C-CHD-C1D
2	B	900	BLA	CAA-CBA-CGA-O2A
2	D	900	BLA	CAA-CBA-CGA-O1A

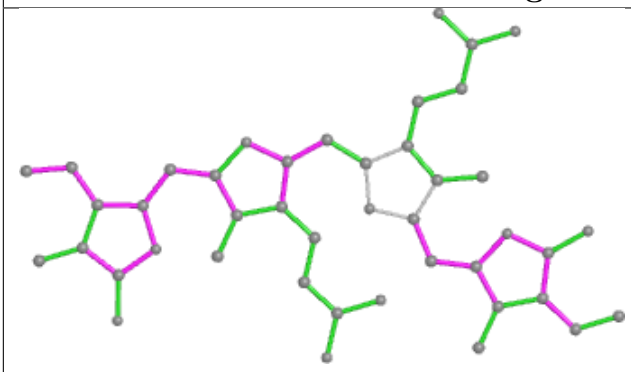
There are no ring outliers.

8 monomers are involved in 69 short contacts:

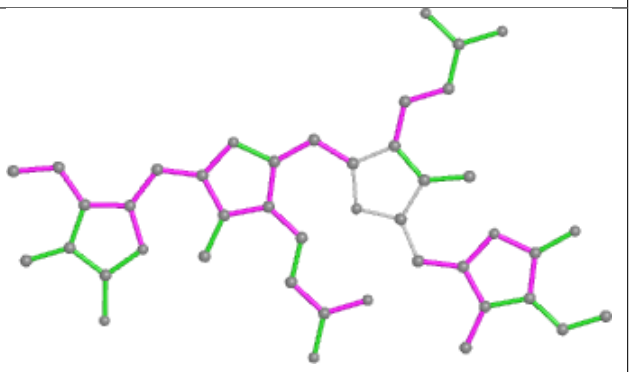
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	900	BLA	8	0
2	H	900	BLA	10	0
2	F	900	BLA	7	0
2	C	900	BLA	11	0
2	B	900	BLA	6	0
2	G	900	BLA	10	0
2	A	900	BLA	6	0
2	D	900	BLA	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

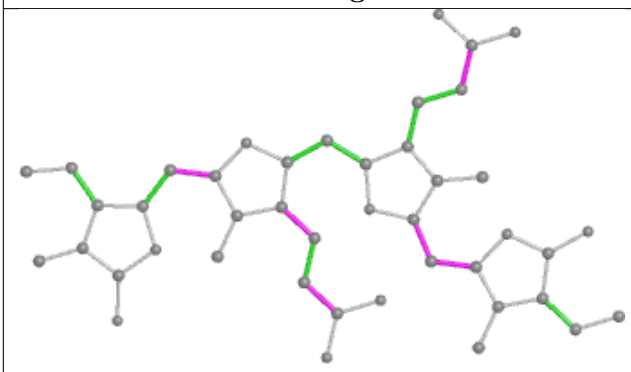
Ligand BLA E 900



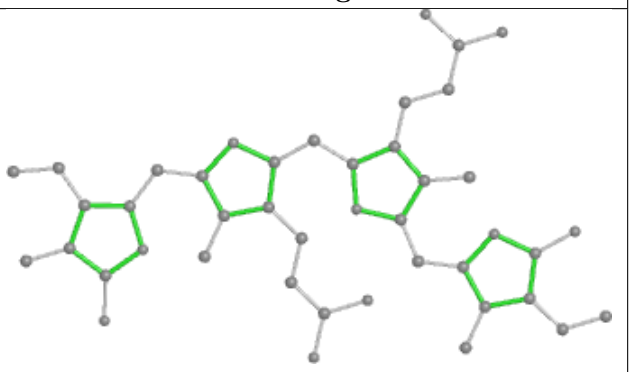
Bond lengths



Bond angles

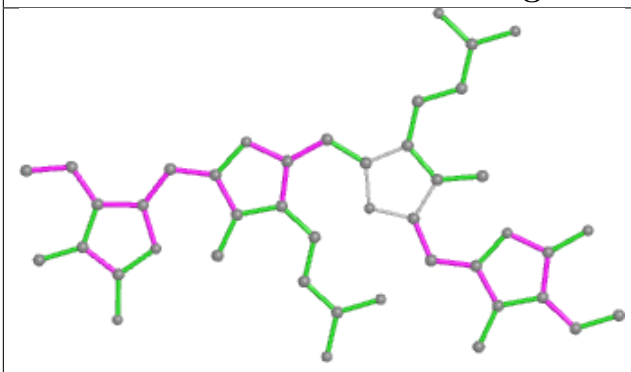


Torsions

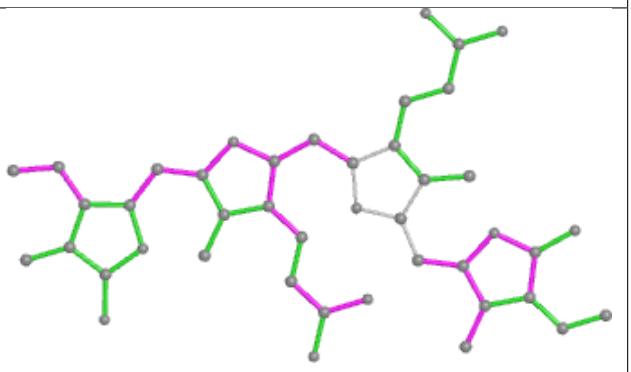


Rings

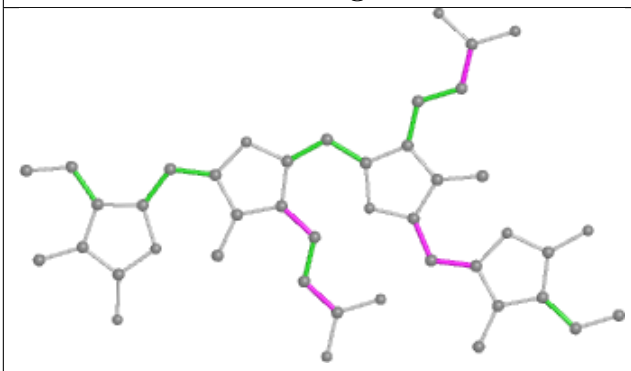
Ligand BLA H 900



Bond lengths



Bond angles



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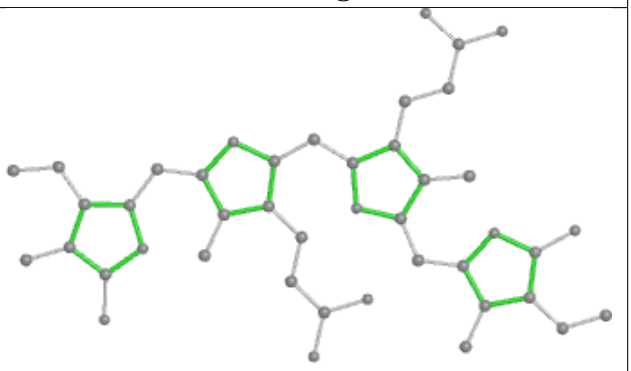
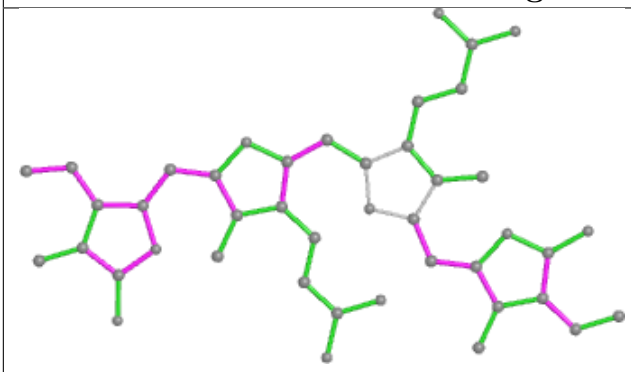
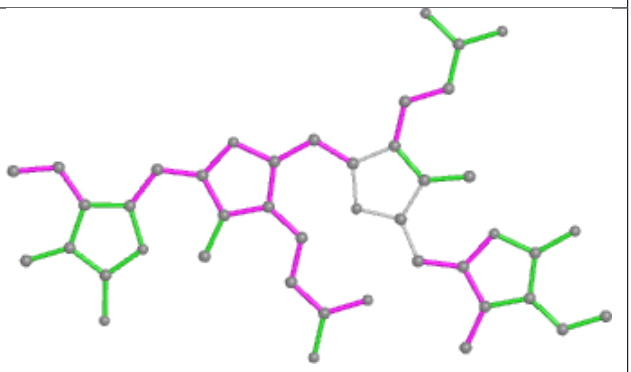


Rings

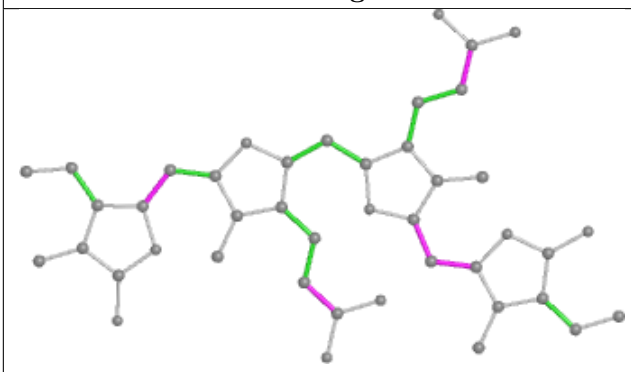
Ligand BLA F 900



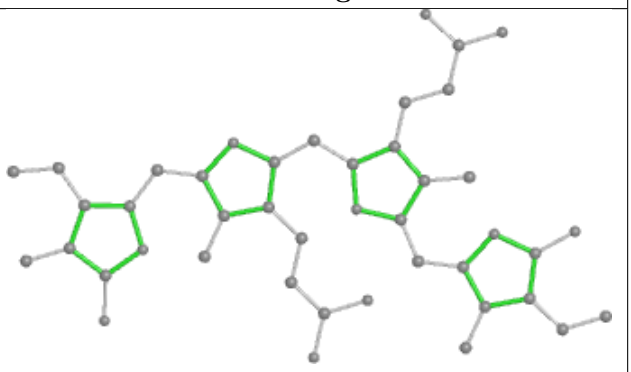
Bond lengths



Bond angles

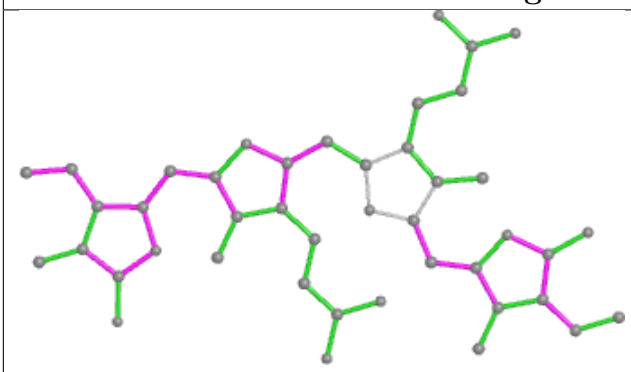


Torsions

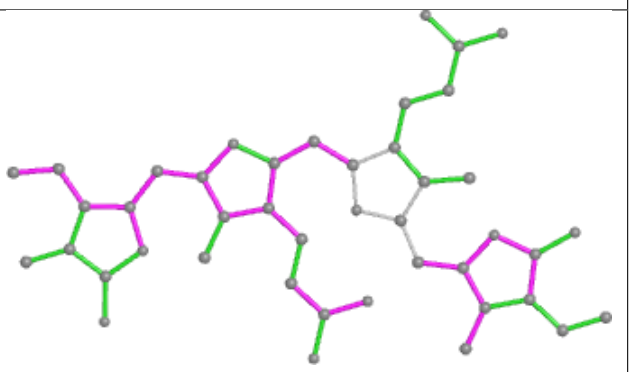


Rings

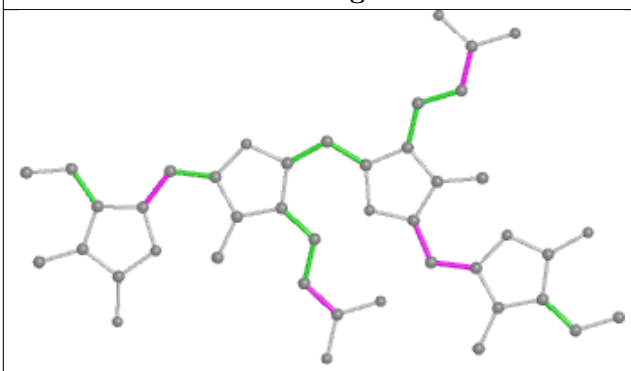
Ligand BLA C 900



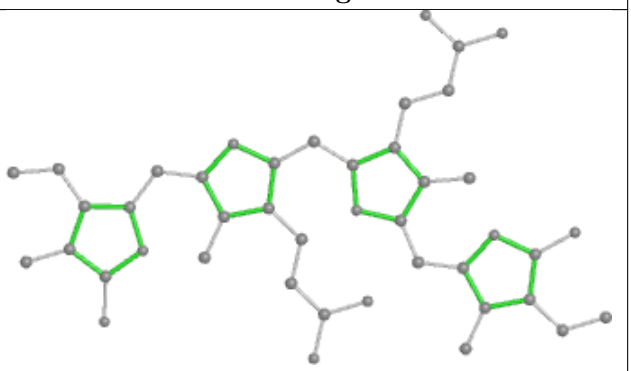
Bond lengths



Bond angles

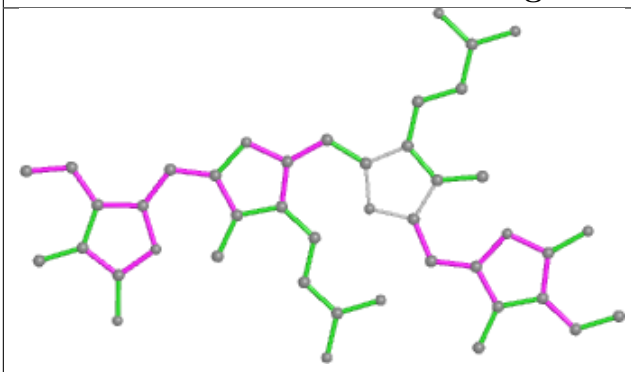


Torsions

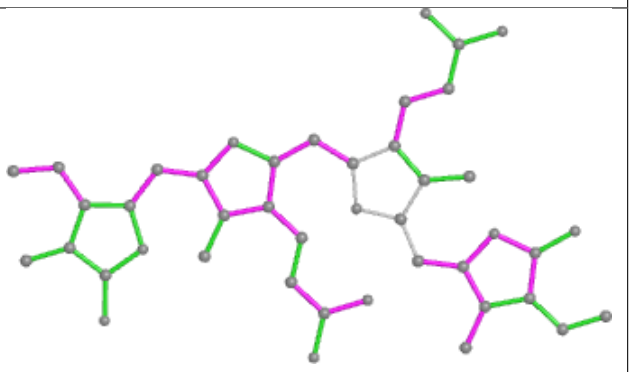


Rings

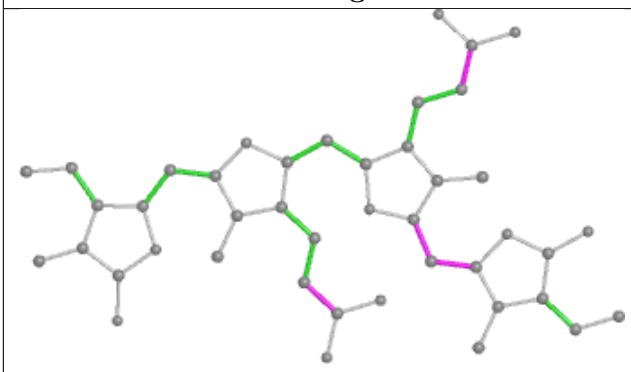
Ligand BLA B 900



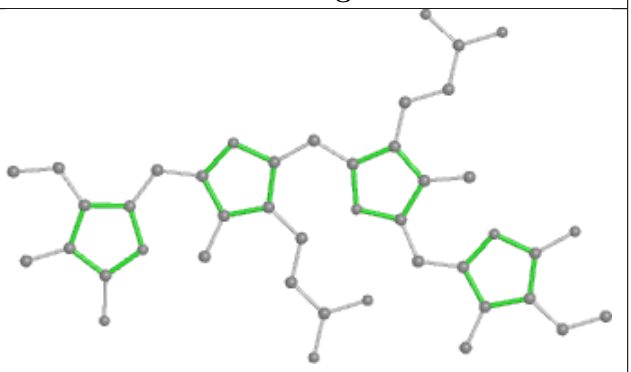
Bond lengths



Bond angles

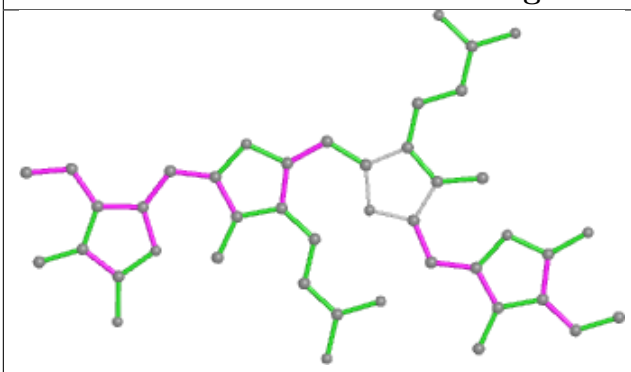


Torsions

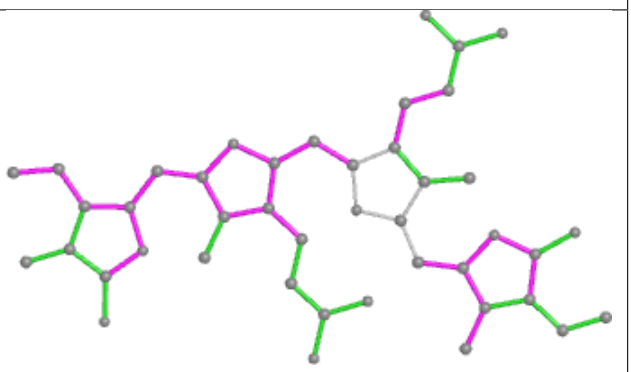


Rings

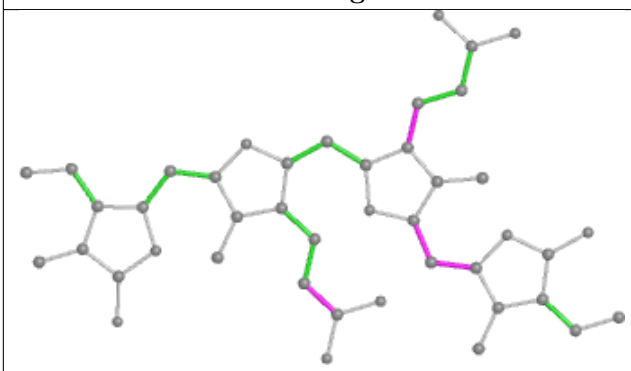
Ligand BLA G 900



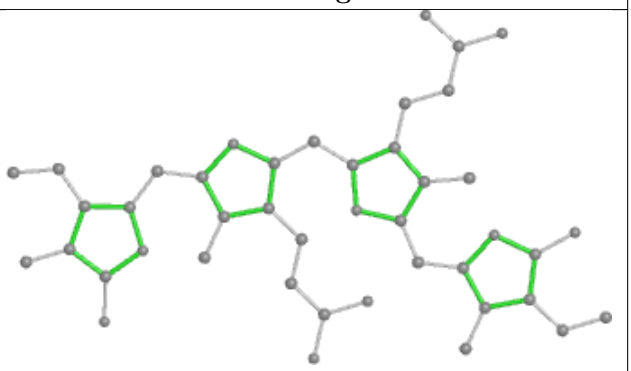
Bond lengths



Bond angles

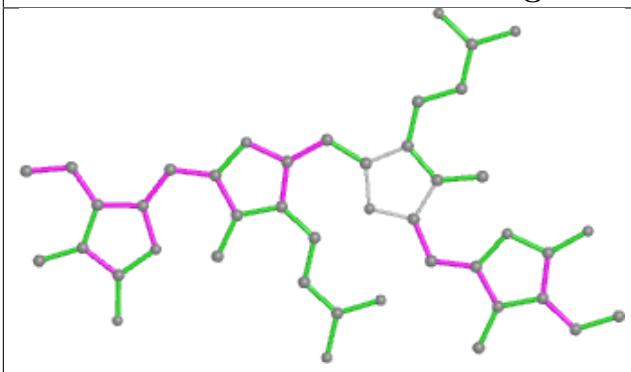


Torsions

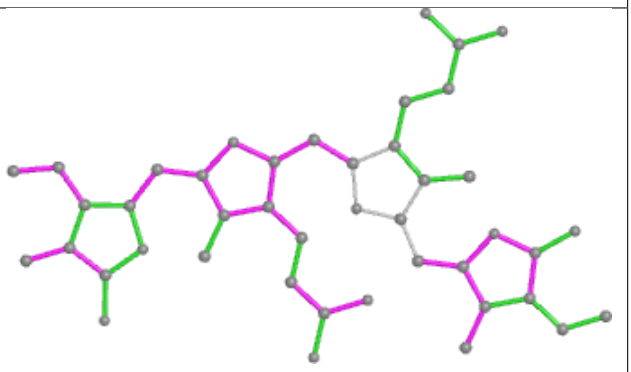


Rings

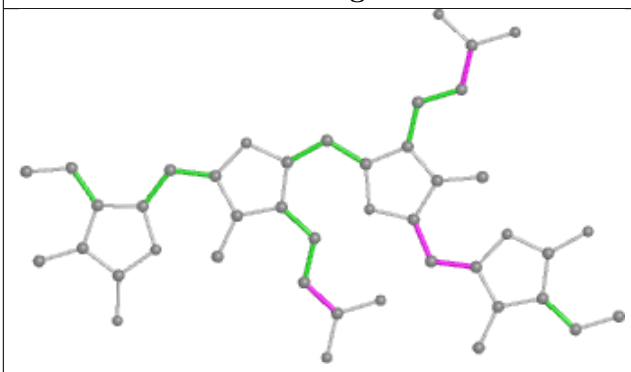
Ligand BLA A 900



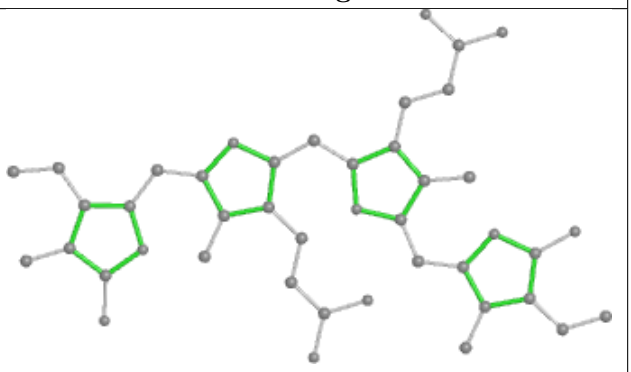
Bond lengths



Bond angles

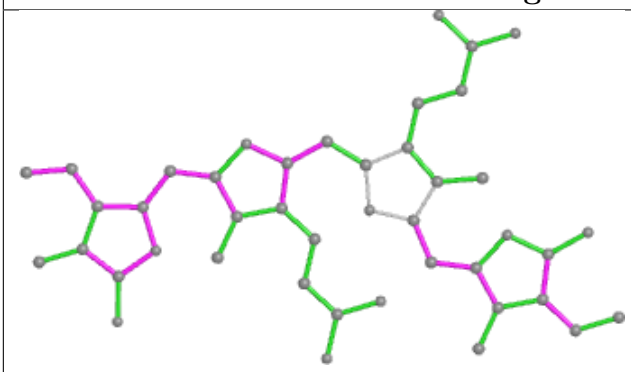


Torsions

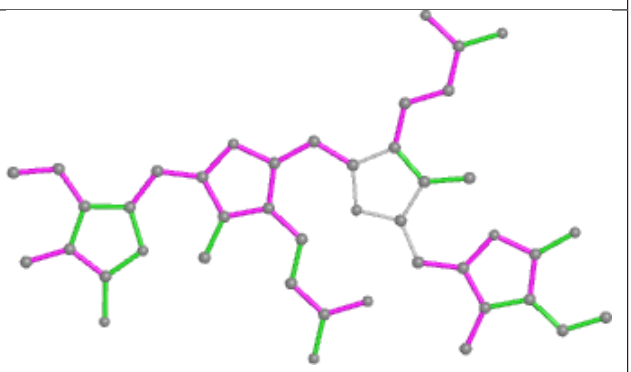


Rings

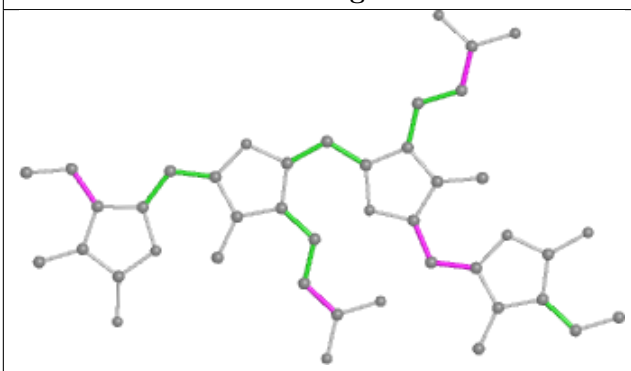
Ligand BLA D 900



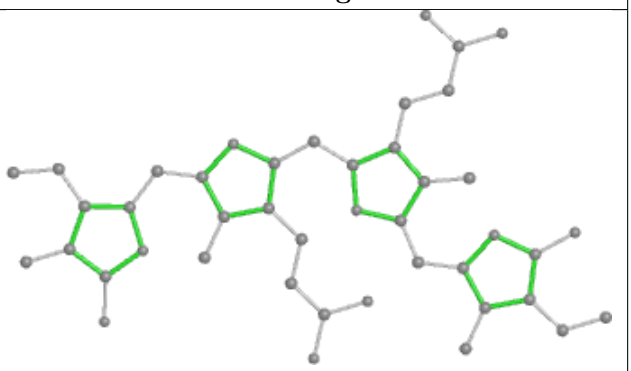
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	478/505 (94%)	-0.09	6 (1%) 77 77	67, 98, 155, 233	0
1	B	468/505 (92%)	0.33	31 (6%) 18 14	74, 129, 188, 243	0
1	C	482/505 (95%)	-0.10	5 (1%) 82 82	66, 99, 148, 206	0
1	D	478/505 (94%)	0.26	27 (5%) 24 20	83, 139, 194, 239	0
1	E	471/505 (93%)	0.27	31 (6%) 18 14	87, 139, 186, 225	0
1	F	469/505 (92%)	0.24	29 (6%) 20 16	80, 124, 203, 282	0
1	G	482/505 (95%)	-0.10	8 (1%) 70 69	66, 103, 152, 217	0
1	H	480/505 (95%)	0.50	50 (10%) 6 5	84, 139, 214, 274	0
All	All	3808/4040 (94%)	0.16	187 (4%) 29 26	66, 122, 191, 282	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	28	ALA	7.5
1	H	59	LEU	6.6
1	H	5	THR	5.8
1	F	222	PHE	5.2
1	H	29	LEU	5.2
1	H	95	PHE	5.1
1	B	30	VAL	4.9
1	H	49	LEU	4.8
1	A	330	ARG	4.6
1	H	30	VAL	4.6
1	D	53	ALA	4.5
1	D	60	THR	4.5
1	H	39	LEU	4.5
1	E	39	LEU	4.4
1	C	441	PRO	4.3
1	F	232	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	453	ARG	4.3
1	H	110	PHE	4.3
1	F	29	LEU	4.1
1	G	118	LEU	4.1
1	H	99	GLY	4.0
1	H	88	THR	3.9
1	B	447	ILE	3.8
1	G	116	ASP	3.8
1	B	58	TYR	3.8
1	A	93	HIS	3.8
1	F	225	LEU	3.7
1	F	30	VAL	3.7
1	H	390	TYR	3.7
1	B	69	LEU	3.7
1	A	89	ARG	3.7
1	F	63	GLN	3.7
1	E	230	ASN	3.7
1	B	452	PRO	3.7
1	H	90	ILE	3.6
1	F	53	ALA	3.6
1	H	51	PHE	3.5
1	B	53	ALA	3.5
1	H	53	ALA	3.5
1	H	96	ASP	3.5
1	F	110	PHE	3.5
1	F	32	LEU	3.5
1	D	427	PHE	3.5
1	D	59	LEU	3.5
1	H	32	LEU	3.4
1	D	90	ILE	3.4
1	H	418	ARG	3.4
1	H	496	HIS	3.4
1	F	108	LEU	3.3
1	E	31	THR	3.3
1	A	445	LEU	3.3
1	D	69	LEU	3.3
1	E	53	ALA	3.3
1	E	466	VAL	3.3
1	B	29	LEU	3.2
1	F	106	PHE	3.2
1	F	346	ILE	3.2
1	B	55	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	257	ARG	3.2
1	B	32	LEU	3.2
1	D	70	ARG	3.2
1	H	97	VAL	3.1
1	F	233	PHE	3.1
1	F	64	VAL	3.1
1	H	419	GLN	3.1
1	G	70	ARG	3.1
1	B	36	GLY	3.0
1	D	62	GLU	3.0
1	E	454	LEU	3.0
1	H	60	THR	3.0
1	H	89	ARG	3.0
1	H	64	VAL	2.9
1	D	30	VAL	2.9
1	H	31	THR	2.9
1	B	59	LEU	2.9
1	B	225	LEU	2.9
1	F	224	ALA	2.9
1	B	52	VAL	2.9
1	F	468	ARG	2.9
1	H	106	PHE	2.9
1	H	412	LEU	2.9
1	H	93	HIS	2.8
1	D	327	ARG	2.8
1	F	207	PRO	2.8
1	E	246	ILE	2.8
1	D	246	ILE	2.8
1	D	411	VAL	2.8
1	H	197	ALA	2.8
1	E	29	LEU	2.7
1	E	225	LEU	2.7
1	B	335	LEU	2.7
1	H	112	ILE	2.7
1	H	225	LEU	2.7
1	E	32	LEU	2.7
1	B	72	LEU	2.7
1	D	207	PRO	2.7
1	D	295	PHE	2.6
1	E	214	VAL	2.6
1	E	425	PHE	2.6
1	B	468	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	108	LEU	2.6
1	B	296	SER	2.6
1	E	64	VAL	2.6
1	D	222	PHE	2.6
1	D	469	GLY	2.6
1	H	22	ALA	2.6
1	H	330	ARG	2.6
1	E	112	ILE	2.6
1	D	95	PHE	2.6
1	E	129	ARG	2.6
1	B	93	HIS	2.6
1	E	381	LEU	2.6
1	H	206	ASN	2.6
1	D	442	GLU	2.5
1	H	52	VAL	2.5
1	H	296	SER	2.5
1	F	395	TRP	2.5
1	D	443	LYS	2.5
1	E	383	ARG	2.5
1	B	205	GLN	2.5
1	B	235	LEU	2.5
1	F	107	TYR	2.5
1	H	222	PHE	2.4
1	B	207	PRO	2.4
1	E	93	HIS	2.4
1	F	221	VAL	2.4
1	B	56	GLY	2.4
1	E	28	ALA	2.4
1	G	330	ARG	2.4
1	F	39	LEU	2.4
1	E	95	PHE	2.3
1	B	366	ILE	2.3
1	H	492	LEU	2.3
1	H	87	GLU	2.3
1	H	105	VAL	2.3
1	B	76	LEU	2.3
1	E	48	LEU	2.3
1	G	444	LEU	2.3
1	F	113	ARG	2.3
1	D	407	ASP	2.3
1	C	128	GLN	2.3
1	H	92	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	59	LEU	2.3
1	E	12	CYS	2.3
1	F	345	GLY	2.3
1	G	64	VAL	2.3
1	H	107	TYR	2.3
1	D	64	VAL	2.3
1	B	338	ALA	2.2
1	F	445	LEU	2.2
1	E	377	VAL	2.2
1	E	468	ARG	2.2
1	D	42	SER	2.2
1	G	59	LEU	2.2
1	H	427	PHE	2.2
1	H	98	ILE	2.2
1	B	450	SER	2.2
1	H	445	LEU	2.2
1	E	330	ARG	2.2
1	H	220	ARG	2.2
1	F	117	THR	2.2
1	B	106	PHE	2.2
1	H	210	LEU	2.1
1	B	206	ASN	2.1
1	G	128	GLN	2.1
1	D	395	TRP	2.1
1	F	40	ALA	2.1
1	C	440	LYS	2.1
1	D	206	ASN	2.1
1	C	53	ALA	2.1
1	D	338	ALA	2.1
1	E	161	MET	2.1
1	B	449	PRO	2.1
1	D	106	PHE	2.1
1	F	235	LEU	2.1
1	F	349	LEU	2.0
1	E	106	PHE	2.0
1	E	427	PHE	2.0
1	A	128	GLN	2.0
1	H	233	PHE	2.0
1	E	110	PHE	2.0
1	A	49	LEU	2.0
1	E	493	CYS	2.0
1	F	206	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	224	ALA	2.0
1	H	86	VAL	2.0
1	H	295	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

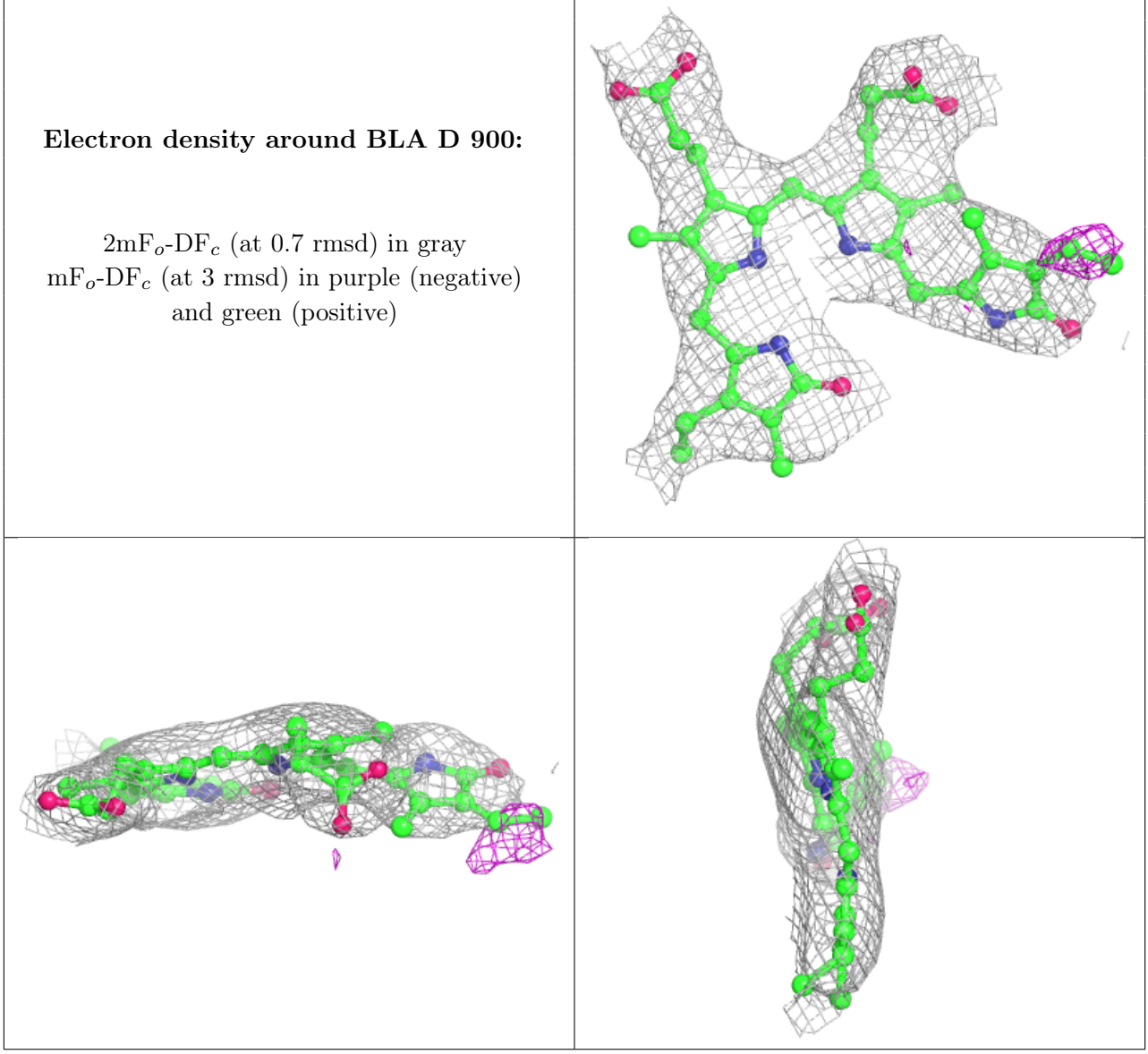
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BLA	D	900	43/43	0.88	0.25	99,123,140,148	0
2	BLA	B	900	43/43	0.90	0.22	105,121,135,145	0
2	BLA	E	900	43/43	0.90	0.46	100,144,164,174	0
2	BLA	H	900	43/43	0.91	0.22	79,121,140,148	0
2	BLA	G	900	43/43	0.94	0.24	67,93,104,128	0
2	BLA	C	900	43/43	0.94	0.21	64,88,102,108	0
2	BLA	F	900	43/43	0.95	0.24	74,102,118,132	0
2	BLA	A	900	43/43	0.96	0.22	60,83,113,119	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

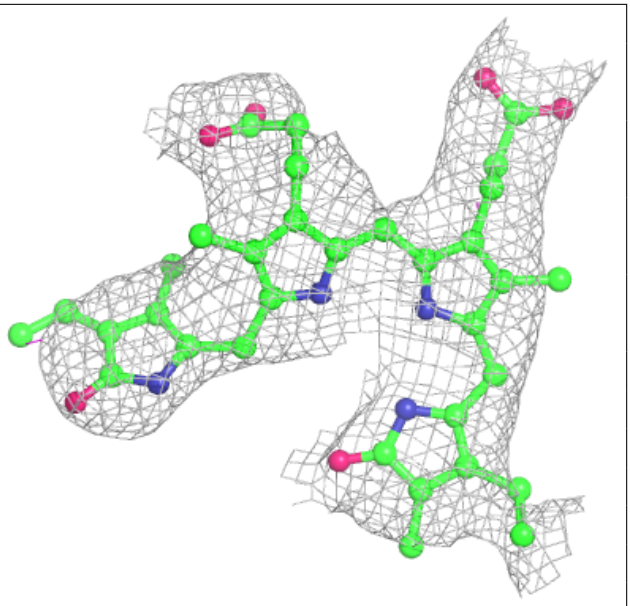
Electron density around BLA D 900:

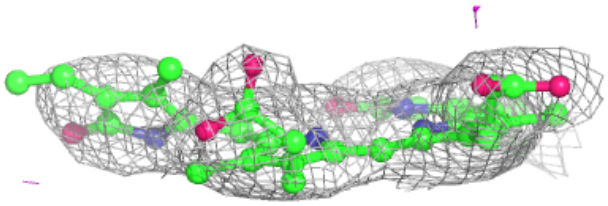
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

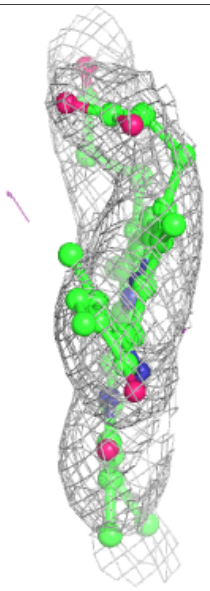


Electron density around BLA B 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

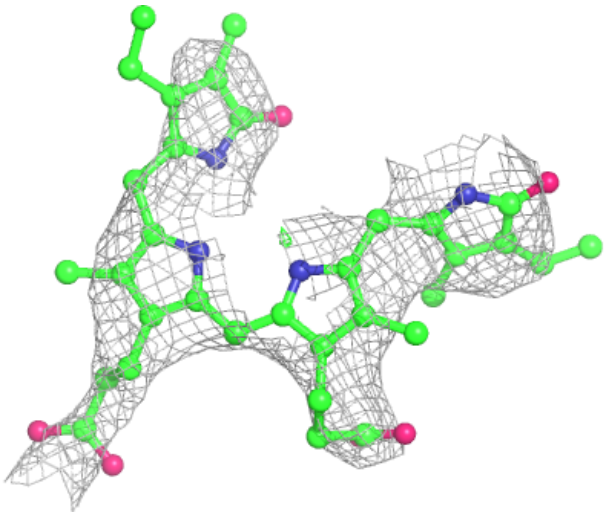


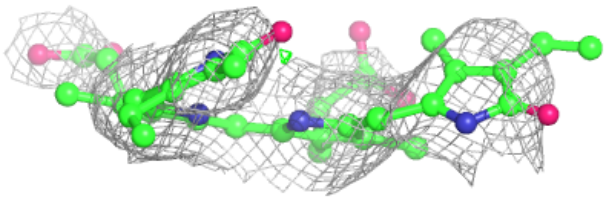


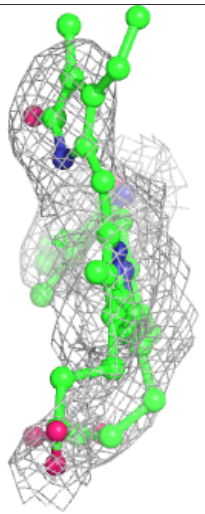


Electron density around BLA E 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

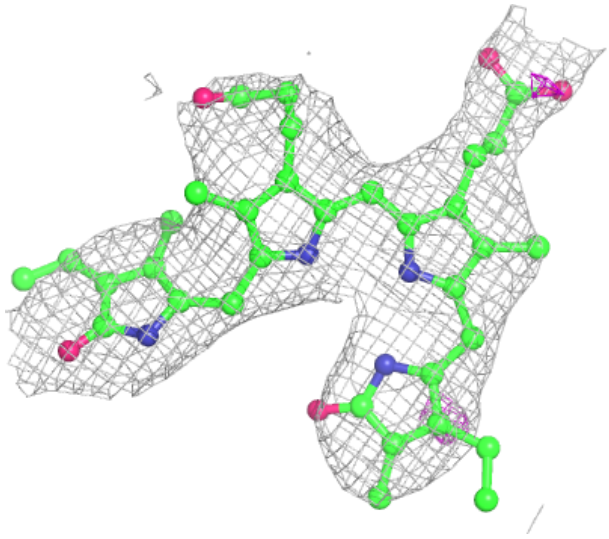


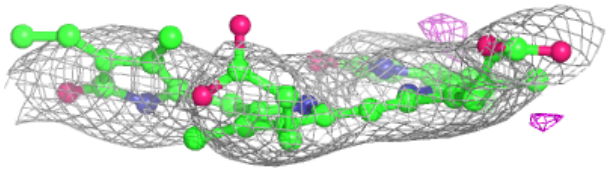


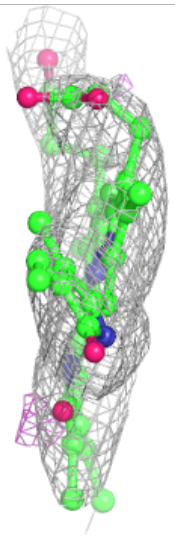


Electron density around BLA H 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

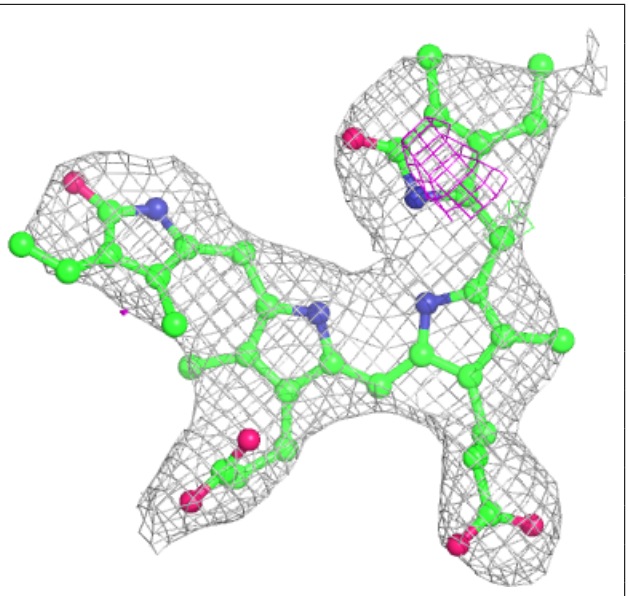


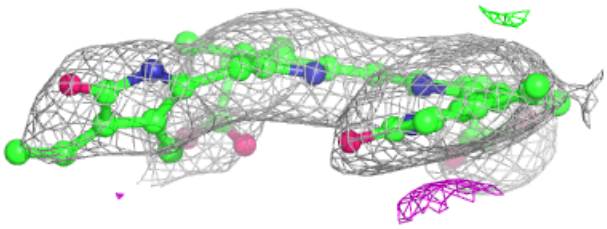


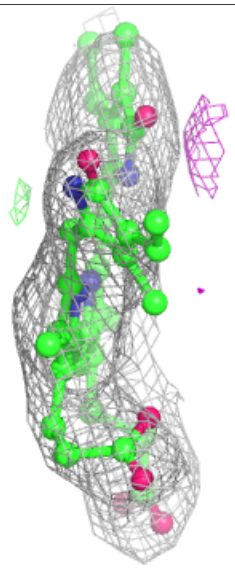


Electron density around BLA G 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

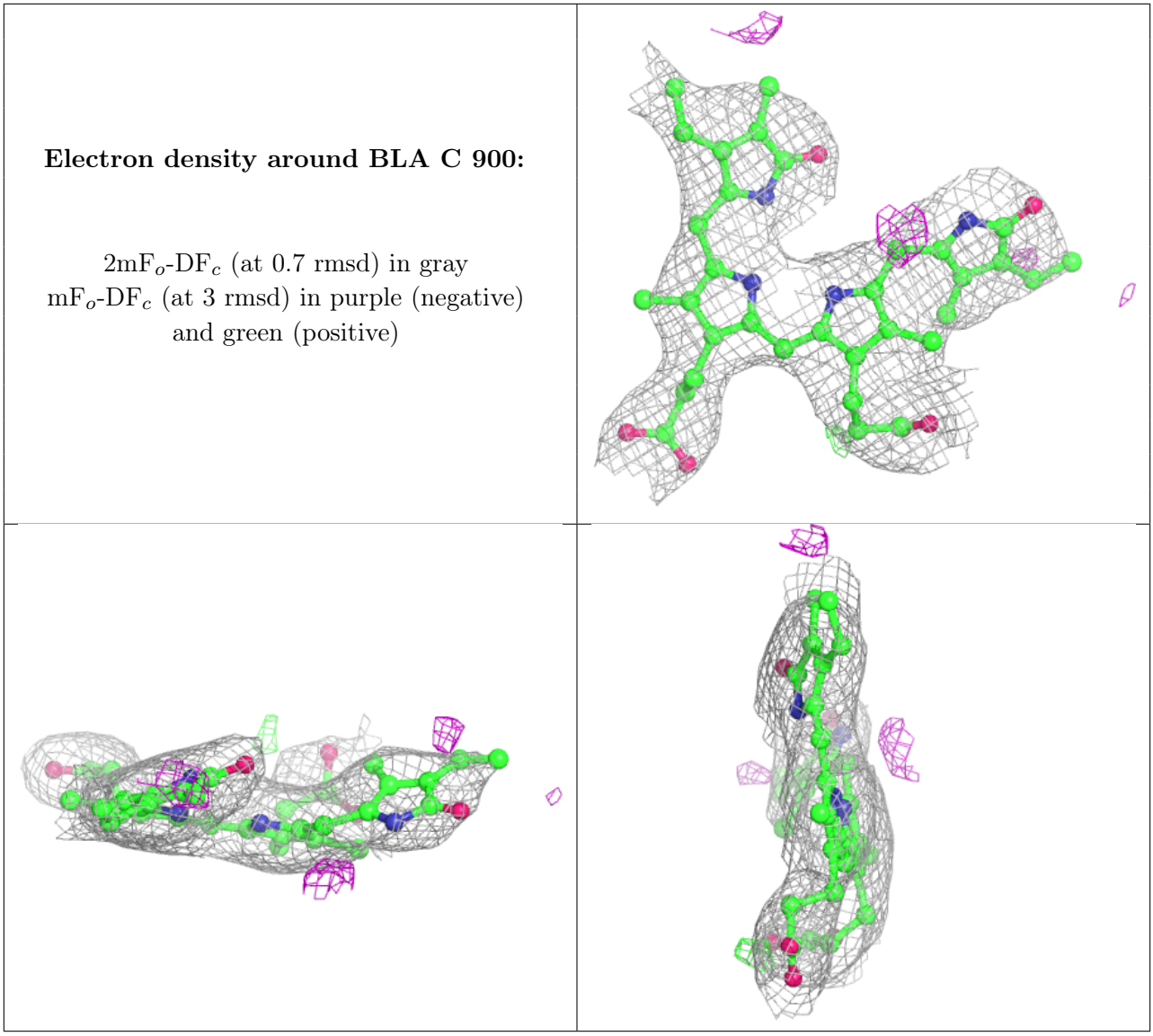






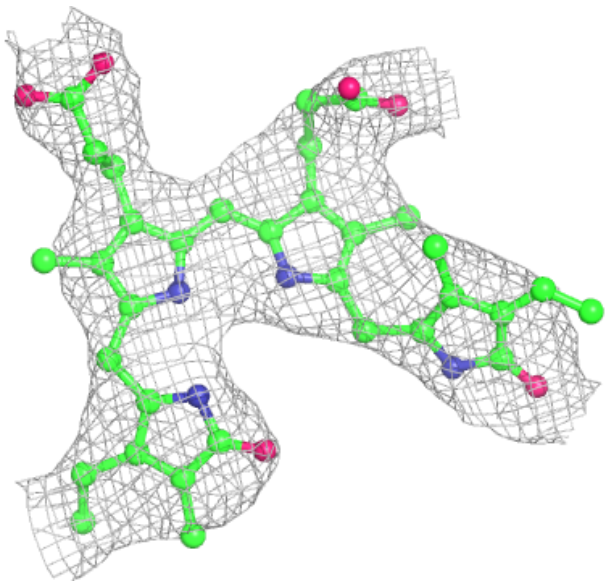
Electron density around BLA C 900:

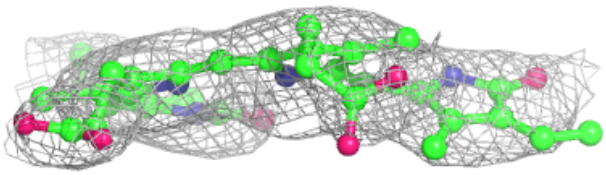
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

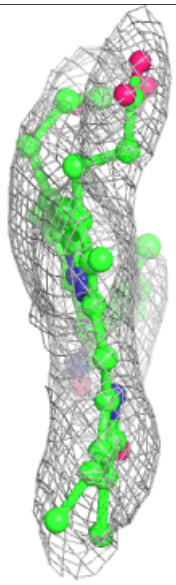


Electron density around BLA F 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

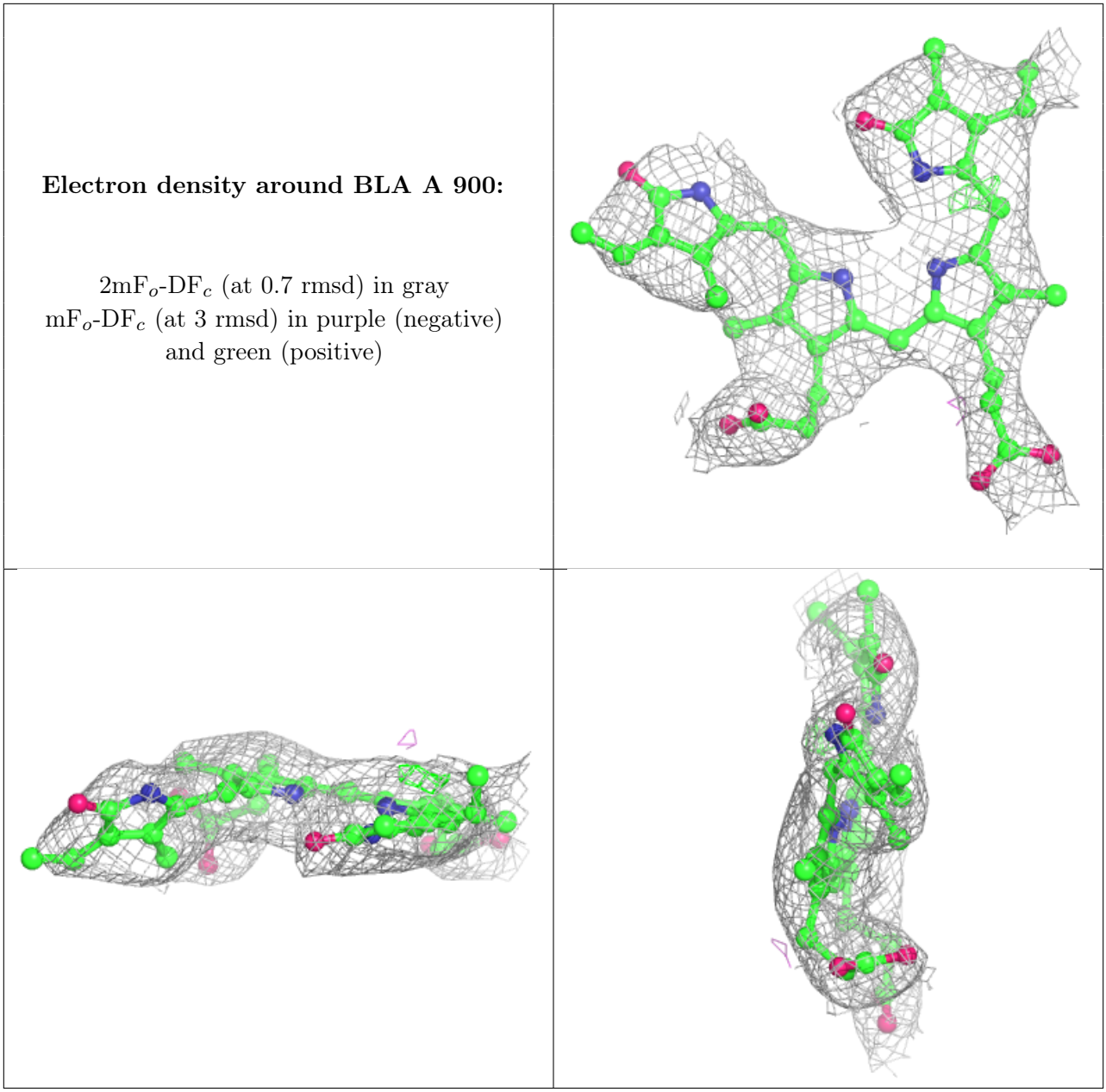






Electron density around BLA A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.