Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:57 PM EDT

PDB ID	:	5YC9
Title	:	Crystal structure of a Pseudomonas aeruginosa transcriptional regulator
Authors	:	Harikiran, R.; Rohan, S.
Deposited on	:	2017-09-07
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:

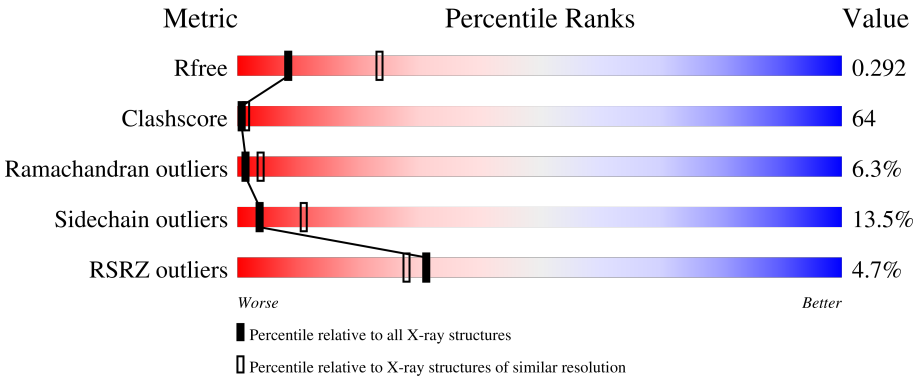
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	291	4% 37% 36% 11% • 14%
1	B	291	3% 35% 44% 8% • 13%
1	C	291	4% 29% 44% 10% • 14%
1	D	291	5% 30% 40% 16% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8286 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 C-di-GMP-binding multidrug transporter transcriptional regulator BrlR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			2048	1305	373	366	4			
1	B	254	Total	C	N	O	S	0	0	0
			2095	1340	379	371	5			
1	C	249	Total	C	N	O	S	0	0	0
			2048	1305	373	366	4			
1	D	254	Total	C	N	O	S	0	0	0
			2095	1340	379	371	5			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A0A069Q416
A	-18	GLY	-	expression tag	UNP A0A069Q416
A	-17	SER	-	expression tag	UNP A0A069Q416
A	-16	SER	-	expression tag	UNP A0A069Q416
A	-15	HIS	-	expression tag	UNP A0A069Q416
A	-14	HIS	-	expression tag	UNP A0A069Q416
A	-13	HIS	-	expression tag	UNP A0A069Q416
A	-12	HIS	-	expression tag	UNP A0A069Q416
A	-11	HIS	-	expression tag	UNP A0A069Q416
A	-10	HIS	-	expression tag	UNP A0A069Q416
A	-9	SER	-	expression tag	UNP A0A069Q416
A	-8	SER	-	expression tag	UNP A0A069Q416
A	-7	GLY	-	expression tag	UNP A0A069Q416
A	-6	LEU	-	expression tag	UNP A0A069Q416
A	-5	VAL	-	expression tag	UNP A0A069Q416
A	-4	PRO	-	expression tag	UNP A0A069Q416
A	-3	ARG	-	expression tag	UNP A0A069Q416
A	-2	GLY	-	expression tag	UNP A0A069Q416
A	-1	SER	-	expression tag	UNP A0A069Q416
A	0	HIS	-	expression tag	UNP A0A069Q416

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Chain	Residue	Modelled	Actual	Comment	Reference
A	271	GLY	-	expression tag	UNP A0A069Q416
B	-19	MET	-	expression tag	UNP A0A069Q416
B	-18	GLY	-	expression tag	UNP A0A069Q416
B	-17	SER	-	expression tag	UNP A0A069Q416
B	-16	SER	-	expression tag	UNP A0A069Q416
B	-15	HIS	-	expression tag	UNP A0A069Q416
B	-14	HIS	-	expression tag	UNP A0A069Q416
B	-13	HIS	-	expression tag	UNP A0A069Q416
B	-12	HIS	-	expression tag	UNP A0A069Q416
B	-11	HIS	-	expression tag	UNP A0A069Q416
B	-10	HIS	-	expression tag	UNP A0A069Q416
B	-9	SER	-	expression tag	UNP A0A069Q416
B	-8	SER	-	expression tag	UNP A0A069Q416
B	-7	GLY	-	expression tag	UNP A0A069Q416
B	-6	LEU	-	expression tag	UNP A0A069Q416
B	-5	VAL	-	expression tag	UNP A0A069Q416
B	-4	PRO	-	expression tag	UNP A0A069Q416
B	-3	ARG	-	expression tag	UNP A0A069Q416
B	-2	GLY	-	expression tag	UNP A0A069Q416
B	-1	SER	-	expression tag	UNP A0A069Q416
B	0	HIS	-	expression tag	UNP A0A069Q416
B	271	GLY	-	expression tag	UNP A0A069Q416
C	-19	MET	-	expression tag	UNP A0A069Q416
C	-18	GLY	-	expression tag	UNP A0A069Q416
C	-17	SER	-	expression tag	UNP A0A069Q416
C	-16	SER	-	expression tag	UNP A0A069Q416
C	-15	HIS	-	expression tag	UNP A0A069Q416
C	-14	HIS	-	expression tag	UNP A0A069Q416
C	-13	HIS	-	expression tag	UNP A0A069Q416
C	-12	HIS	-	expression tag	UNP A0A069Q416
C	-11	HIS	-	expression tag	UNP A0A069Q416
C	-10	HIS	-	expression tag	UNP A0A069Q416
C	-9	SER	-	expression tag	UNP A0A069Q416
C	-8	SER	-	expression tag	UNP A0A069Q416
C	-7	GLY	-	expression tag	UNP A0A069Q416
C	-6	LEU	-	expression tag	UNP A0A069Q416
C	-5	VAL	-	expression tag	UNP A0A069Q416
C	-4	PRO	-	expression tag	UNP A0A069Q416
C	-3	ARG	-	expression tag	UNP A0A069Q416
C	-2	GLY	-	expression tag	UNP A0A069Q416
C	-1	SER	-	expression tag	UNP A0A069Q416
C	0	HIS	-	expression tag	UNP A0A069Q416

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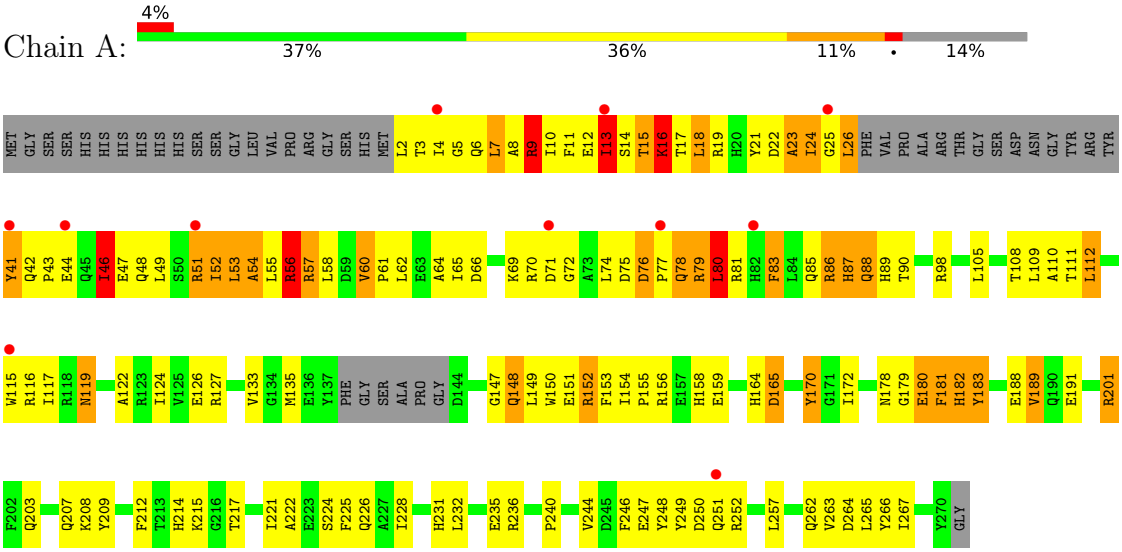
Chain	Residue	Modelled	Actual	Comment	Reference
C	271	GLY	-	expression tag	UNP A0A069Q416
D	-19	MET	-	expression tag	UNP A0A069Q416
D	-18	GLY	-	expression tag	UNP A0A069Q416
D	-17	SER	-	expression tag	UNP A0A069Q416
D	-16	SER	-	expression tag	UNP A0A069Q416
D	-15	HIS	-	expression tag	UNP A0A069Q416
D	-14	HIS	-	expression tag	UNP A0A069Q416
D	-13	HIS	-	expression tag	UNP A0A069Q416
D	-12	HIS	-	expression tag	UNP A0A069Q416
D	-11	HIS	-	expression tag	UNP A0A069Q416
D	-10	HIS	-	expression tag	UNP A0A069Q416
D	-9	SER	-	expression tag	UNP A0A069Q416
D	-8	SER	-	expression tag	UNP A0A069Q416
D	-7	GLY	-	expression tag	UNP A0A069Q416
D	-6	LEU	-	expression tag	UNP A0A069Q416
D	-5	VAL	-	expression tag	UNP A0A069Q416
D	-4	PRO	-	expression tag	UNP A0A069Q416
D	-3	ARG	-	expression tag	UNP A0A069Q416
D	-2	GLY	-	expression tag	UNP A0A069Q416
D	-1	SER	-	expression tag	UNP A0A069Q416
D	0	HIS	-	expression tag	UNP A0A069Q416
D	271	GLY	-	expression tag	UNP A0A069Q416

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.

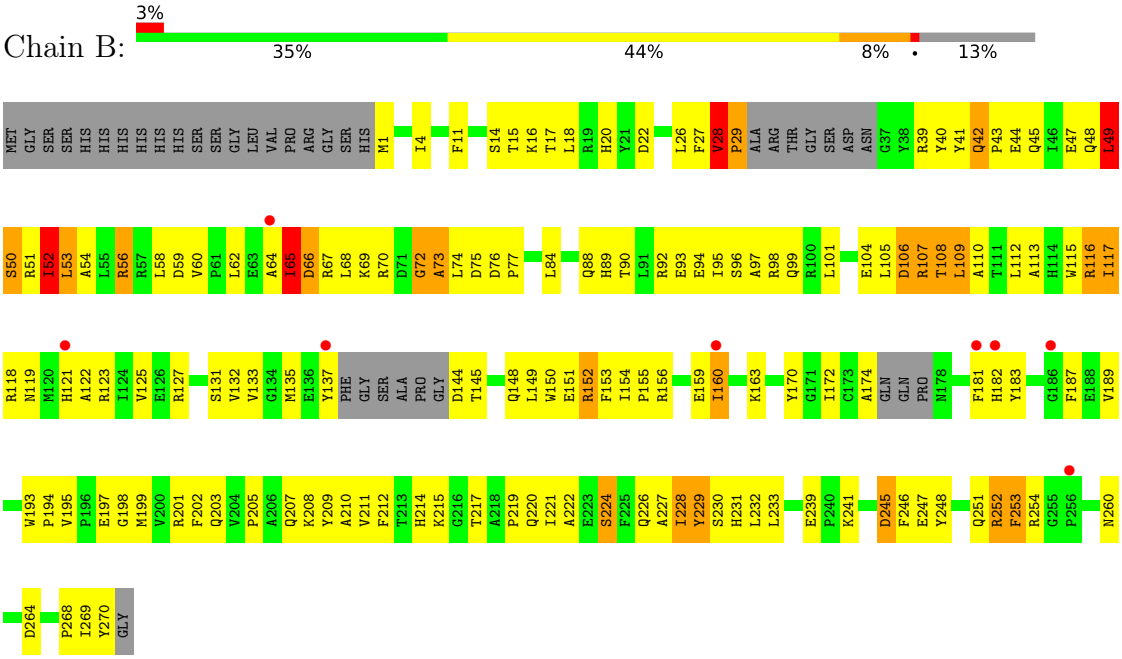
• Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR

Chain A:



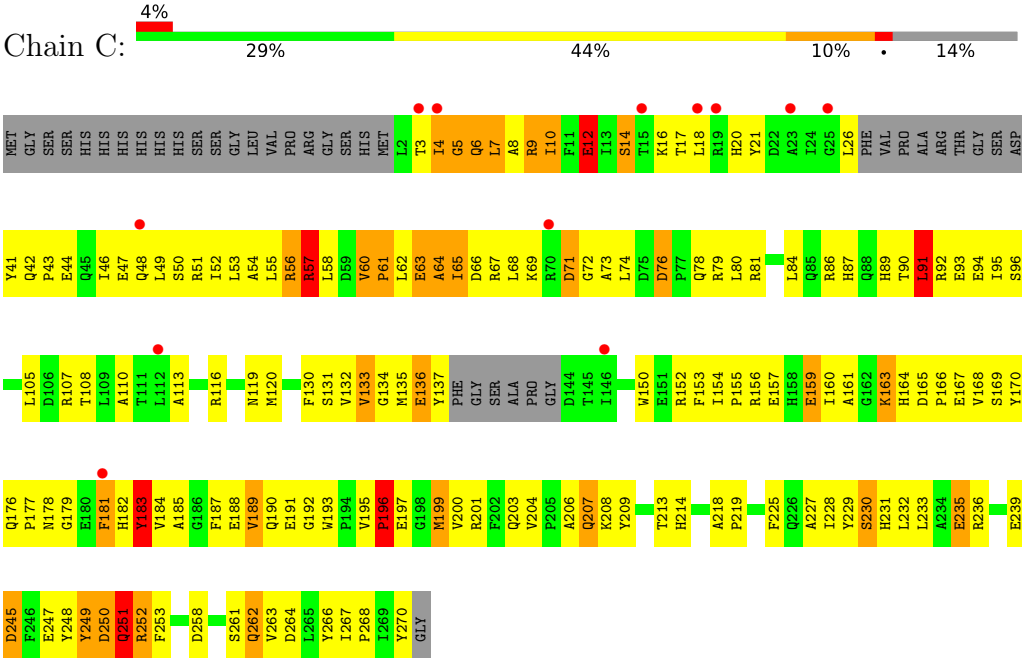
• Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR

Chain B:



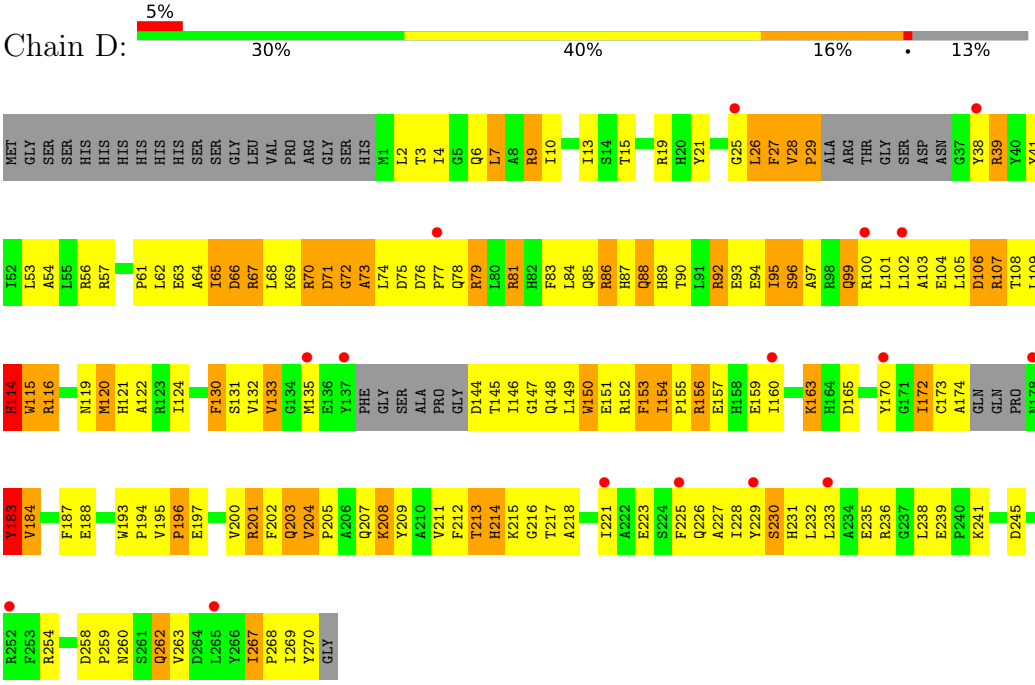
• Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR

Chain C:



• Molecule 1: C-di-GMP-binding multidrug transporter transcriptional regulator BrlR

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	111.64Å 111.64Å 261.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.32 – 2.90 38.85 – 2.90	Depositor EDS
% Data completeness (in resolution range)	74.8 (34.32-2.90) 86.0 (38.85-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.90Å)	Xtriage
Refinement program	PHENIX (dev_2875)	Depositor
R, R_{free}	0.268 , 0.307 0.258 , 0.292	Depositor DCC
R_{free} test set	1987 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 21.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.427 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 (i)

5.1 Standard geometry (i)

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	1.04	8/2099 (0.4%)	0.90	6/2842 (0.2%)
1	B	1.05	0/2148	0.97	10/2906 (0.3%)
1	C	1.44	16/2099 (0.8%)	1.07	12/2842 (0.4%)
1	D	1.15	3/2148 (0.1%)	1.03	8/2906 (0.3%)
All	All	1.18	27/8494 (0.3%)	1.00	36/11496 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	TYR	CE1-CZ	-10.09	1.25	1.38
1	C	170	TYR	CE1-CZ	-8.82	1.27	1.38
1	C	266	TYR	CE1-CZ	-8.69	1.27	1.38
1	A	183	TYR	CE1-CZ	-8.13	1.27	1.38
1	A	170	TYR	CE2-CZ	-8.02	1.28	1.38
1	C	249	TYR	CE1-CZ	-7.73	1.28	1.38
1	A	170	TYR	CG-CD2	-7.69	1.29	1.39
1	A	266	TYR	CE1-CZ	-7.50	1.28	1.38
1	C	249	TYR	CG-CD1	-7.18	1.29	1.39
1	C	248	TYR	CE1-CZ	-6.36	1.30	1.38
1	D	183	TYR	CE1-CZ	-6.28	1.30	1.38
1	C	183	TYR	CE1-CZ	-6.08	1.30	1.38
1	C	266	TYR	CE2-CZ	-6.07	1.30	1.38
1	A	266	TYR	CG-CD1	-5.90	1.31	1.39
1	A	266	TYR	CE2-CZ	-5.86	1.30	1.38
1	C	209	TYR	CE1-CZ	-5.78	1.31	1.38
1	C	266	TYR	CG-CD1	-5.63	1.31	1.39
1	C	249	TYR	CE2-CZ	-5.50	1.31	1.38
1	A	170	TYR	CG-CD1	-5.48	1.32	1.39
1	C	229	TYR	CE1-CZ	-5.39	1.31	1.38
1	C	248	TYR	CE2-CZ	-5.26	1.31	1.38
1	C	248	TYR	CG-CD1	-5.26	1.32	1.39
1	D	21	TYR	CG-CD1	-5.19	1.32	1.39
1	D	21	TYR	CE1-CZ	-5.19	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	TYR	CG-CD2	-5.15	1.32	1.39
1	C	207	GLN	C-O	-5.15	1.13	1.23
1	C	241	LYS	C-O	-5.14	1.13	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	60	VAL	C-N-CD	-14.02	89.75	120.60
1	D	72	GLY	N-CA-C	-10.34	87.25	113.10
1	D	76	ASP	C-N-CD	-9.83	98.97	120.60
1	B	72	GLY	N-CA-C	-9.28	89.90	113.10
1	B	76	ASP	N-CA-C	-8.44	88.22	111.00
1	C	5	GLY	N-CA-C	-7.72	93.81	113.10
1	C	91	LEU	N-CA-C	-7.19	91.58	111.00
1	D	165	ASP	N-CA-C	-6.97	92.18	111.00
1	A	12	GLU	N-CA-C	-6.61	93.16	111.00
1	C	57	ARG	N-CA-C	-6.33	93.90	111.00
1	C	250	ASP	N-CA-C	-6.25	94.11	111.00
1	A	189	VAL	CB-CA-C	-6.18	99.65	111.40
1	C	251	GLN	C-N-CA	-6.08	106.50	121.70
1	C	251	GLN	CB-CA-C	-5.88	98.65	110.40
1	D	28	VAL	C-N-CD	5.85	140.69	128.40
1	B	28	VAL	C-N-CD	5.79	140.55	128.40
1	B	49	LEU	CA-CB-CG	5.68	128.38	115.30
1	B	76	ASP	C-N-CD	5.68	140.33	128.40
1	D	2	LEU	N-CA-C	5.66	126.29	111.00
1	B	65	ILE	N-CA-C	-5.58	95.93	111.00
1	A	60	VAL	C-N-CD	5.53	140.01	128.40
1	A	124	ILE	CG1-CB-CG2	-5.49	99.32	111.40
1	B	193	TRP	C-N-CD	5.47	139.88	128.40
1	C	176	GLN	C-N-CD	5.46	139.87	128.40
1	C	258	ASP	C-N-CD	5.43	139.80	128.40
1	D	29	PRO	CA-N-CD	-5.38	103.97	111.50
1	D	76	ASP	N-CA-C	-5.38	96.47	111.00
1	C	239	GLU	C-N-CD	5.38	139.69	128.40
1	B	194	PRO	CA-N-CD	-5.28	104.11	111.50
1	C	208	LYS	N-CA-C	-5.27	96.78	111.00
1	A	165	ASP	C-N-CD	5.19	139.29	128.40
1	D	204	VAL	C-N-CD	5.17	139.26	128.40
1	A	265	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	C	196	PRO	CA-N-CD	-5.11	104.35	111.50
1	B	77	PRO	CA-N-CD	-5.09	104.37	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	ILE	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2048	0	2011	276	5
1	B	2095	0	2057	256	5
1	C	2048	0	2009	238	2
1	D	2095	0	2058	357	2
All	All	8286	0	8135	1055	7

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 64.

All (1055) 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:4:ILE:HD11	1:C:41:TYR:CZ	1.33	1.62
1:D:27:PHE:HE2	1:D:49:LEU:CD2	1.14	1.55
1:D:29:PRO:HG2	1:D:41:TYR:CE1	1.03	1.55
1:A:60:VAL:CG1	1:A:65:ILE:HD11	1.42	1.50
1:D:27:PHE:CD2	1:D:49:LEU:HD11	1.44	1.49
1:B:214:HIS:CE1	1:B:221:ILE:HG22	1.44	1.48
1:D:27:PHE:CE2	1:D:49:LEU:CD1	1.96	1.48
1:D:27:PHE:CE2	1:D:49:LEU:HD11	1.48	1.48
1:D:64:ALA:O	1:D:67:ARG:CD	1.64	1.45
1:D:27:PHE:CE2	1:D:49:LEU:CD2	2.00	1.44
1:D:29:PRO:CG	1:D:41:TYR:CE1	1.99	1.43
1:C:4:ILE:CD1	1:C:41:TYR:CE1	2.01	1.42
1:D:88:GLN:HE21	1:D:92:ARG:NH1	1.13	1.41
1:D:51:ARG:HH22	1:D:75:ASP:CG	1.23	1.41
1:A:51:ARG:NH1	1:A:80:LEU:CD1	1.82	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:THR:CG2	1:D:6:GLN:HG2	1.51	1.39
1:D:27:PHE:CE2	1:D:49:LEU:HD21	1.55	1.39
1:D:51:ARG:NH2	1:D:75:ASP:CG	1.72	1.38
1:C:4:ILE:HD12	1:C:41:TYR:CE1	1.59	1.36
1:B:254:ARG:NH2	1:B:260:ASN:O	1.59	1.33
1:A:17:THR:O	1:A:21:TYR:CD1	1.81	1.33
1:D:88:GLN:NE2	1:D:92:ARG:NH1	1.78	1.32
1:D:108:THR:O	1:D:112:LEU:HD23	1.24	1.32
1:D:51:ARG:CZ	1:D:75:ASP:OD2	1.76	1.31
1:C:4:ILE:HD11	1:C:41:TYR:OH	1.15	1.30
1:A:51:ARG:NH1	1:A:80:LEU:HD12	1.39	1.30
1:C:133:VAL:CG2	1:C:200:VAL:O	1.80	1.28
1:D:3:THR:CG2	1:D:6:GLN:CG	2.13	1.27
1:D:104:GLU:OE1	1:D:105:LEU:CD1	1.82	1.25
1:D:64:ALA:O	1:D:67:ARG:NE	1.68	1.22
1:C:4:ILE:CD1	1:C:41:TYR:OH	1.88	1.21
1:C:4:ILE:CD1	1:C:41:TYR:CZ	2.16	1.21
1:A:52:ILE:O	1:A:54:ALA:N	1.73	1.21
1:B:104:GLU:OE2	1:B:107:ARG:CZ	1.90	1.20
1:A:214:HIS:CD2	1:A:221:ILE:HG12	1.76	1.19
1:B:214:HIS:ND1	1:B:221:ILE:HG22	1.53	1.19
1:D:104:GLU:OE1	1:D:105:LEU:HD13	1.40	1.19
1:A:47:GLU:O	1:A:51:ARG:CG	1.92	1.18
1:B:135:MET:HE1	1:B:152:ARG:O	1.43	1.17
1:D:25:GLY:O	1:D:69:LYS:NZ	1.77	1.17
1:D:133:VAL:CG2	1:D:201:ARG:HA	1.73	1.17
1:D:64:ALA:O	1:D:67:ARG:HD2	1.35	1.17
1:A:51:ARG:HH12	1:A:80:LEU:CD1	1.49	1.16
1:A:61:PRO:O	1:A:65:ILE:HD13	1.41	1.16
1:B:48:GLN:NE2	1:B:75:ASP:OD1	1.78	1.16
1:D:72:GLY:HA3	1:D:73:ALA:HB2	1.18	1.16
1:D:133:VAL:HG23	1:D:201:ARG:CA	1.69	1.16
1:D:3:THR:HG23	1:D:6:GLN:HG2	1.17	1.15
1:A:60:VAL:CG1	1:A:65:ILE:CD1	2.24	1.15
1:C:53:LEU:O	1:C:57:ARG:NH2	1.79	1.15
1:D:153:PHE:O	1:D:155:PRO:N	1.78	1.14
1:A:47:GLU:O	1:A:51:ARG:HG2	1.46	1.14
1:C:90:THR:O	1:C:91:LEU:O	1.64	1.14
1:B:228:ILE:HA	1:B:232:LEU:HB2	1.25	1.13
1:C:134:GLY:O	1:C:199:MET:CB	1.96	1.13
1:A:60:VAL:HG12	1:A:65:ILE:CD1	1.77	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:HD11	1:C:41:TYR:CE1	1.73	1.12
1:D:29:PRO:HG2	1:D:41:TYR:CD1	1.83	1.12
1:D:108:THR:O	1:D:112:LEU:CD2	1.96	1.12
1:A:60:VAL:HG11	1:A:65:ILE:HD11	1.21	1.12
1:C:163:LYS:HA	1:C:189:VAL:HG13	1.13	1.11
1:D:160:ILE:O	1:D:163:LYS:NZ	1.82	1.11
1:D:172:ILE:CD1	1:D:202:PHE:CE1	2.33	1.11
1:B:135:MET:CE	1:B:152:ARG:O	1.99	1.10
1:C:133:VAL:HG22	1:C:200:VAL:O	1.52	1.10
1:B:214:HIS:CE1	1:B:221:ILE:CG2	2.33	1.10
1:D:29:PRO:HG2	1:D:41:TYR:CZ	1.85	1.10
1:D:3:THR:HG22	1:D:6:GLN:HE21	1.05	1.10
1:D:172:ILE:HD11	1:D:202:PHE:CE1	1.86	1.09
1:C:163:LYS:CA	1:C:189:VAL:HG13	1.81	1.09
1:A:17:THR:O	1:A:21:TYR:CE1	2.03	1.09
1:A:54:ALA:HB1	1:A:57:ARG:HD3	1.32	1.09
1:C:133:VAL:HG23	1:C:200:VAL:O	1.43	1.09
1:A:85:GLN:OE1	1:A:88:GLN:CG	2.01	1.08
1:D:27:PHE:CE2	1:D:49:LEU:CG	2.36	1.08
1:D:104:GLU:CD	1:D:105:LEU:HD12	1.74	1.08
1:B:116:ARG:O	1:B:119:ASN:N	1.87	1.07
1:D:153:PHE:O	1:D:155:PRO:CD	2.01	1.07
1:C:9:ARG:HG3	1:C:10:ILE:N	1.62	1.07
1:D:172:ILE:HD11	1:D:202:PHE:HE1	1.09	1.07
1:B:108:THR:O	1:B:112:LEU:HD21	1.56	1.06
1:C:133:VAL:HG23	1:C:201:ARG:HA	1.36	1.06
1:D:3:THR:HG22	1:D:6:GLN:NE2	1.68	1.06
1:B:116:ARG:NH1	1:B:117:ILE:N	2.04	1.05
1:A:51:ARG:HH11	1:A:80:LEU:HD12	0.95	1.05
1:A:60:VAL:HG12	1:A:65:ILE:HD11	1.33	1.05
1:C:133:VAL:HG23	1:C:200:VAL:C	1.77	1.05
1:B:116:ARG:O	1:B:118:ARG:N	1.88	1.05
1:C:251:GLN:OE1	1:C:251:GLN:N	1.88	1.05
1:A:51:ARG:HH12	1:A:80:LEU:HD13	1.22	1.04
1:A:115:TRP:CE2	1:D:77:PRO:HG3	1.93	1.04
1:D:172:ILE:HD13	1:D:202:PHE:CD1	1.92	1.03
1:D:4:ILE:HD12	1:D:4:ILE:H	1.23	1.03
1:D:92:ARG:O	1:D:96:SER:OG	1.75	1.03
1:C:133:VAL:HG23	1:C:201:ARG:CA	1.88	1.03
1:B:11:PHE:CE2	1:B:49:LEU:HD13	1.93	1.02
1:D:27:PHE:HE2	1:D:49:LEU:CG	1.71	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ALA:HB2	1:D:212:PHE:CE1	1.94	1.02
1:D:214:HIS:CE1	1:D:216:GLY:HA3	1.94	1.02
1:A:55:LEU:O	1:A:58:LEU:N	1.93	1.01
1:D:65:ILE:O	1:D:68:LEU:N	1.92	1.01
1:A:85:GLN:OE1	1:A:88:GLN:CD	1.99	1.00
1:B:116:ARG:HH12	1:B:117:ILE:HA	1.22	1.00
1:D:131:SER:OG	1:D:203:GLN:OE1	1.77	1.00
1:D:214:HIS:HE1	1:D:216:GLY:HA3	1.23	0.99
1:B:72:GLY:HA3	1:B:73:ALA:HB2	1.45	0.98
1:D:27:PHE:HE2	1:D:49:LEU:HD22	1.24	0.98
1:A:115:TRP:CD2	1:D:77:PRO:HG3	1.97	0.98
1:C:9:ARG:HG3	1:C:10:ILE:H	1.18	0.98
1:B:116:ARG:HH12	1:B:117:ILE:CA	1.77	0.98
1:A:115:TRP:CH2	1:D:77:PRO:HD3	1.99	0.97
1:A:13:ILE:HD13	1:A:13:ILE:H	1.28	0.97
1:C:53:LEU:HD13	1:C:57:ARG:HH21	1.25	0.97
1:A:41:TYR:OH	1:B:239:GLU:OE2	1.81	0.97
1:C:133:VAL:CG2	1:C:200:VAL:C	2.33	0.97
1:D:72:GLY:CA	1:D:73:ALA:HB2	1.93	0.97
1:D:122:ALA:HB2	1:D:212:PHE:HE1	1.24	0.97
1:A:46:ILE:HG23	1:A:47:GLU:N	1.80	0.96
1:B:29:PRO:HB3	1:B:41:TYR:CE1	2.00	0.96
1:B:148:GLN:O	1:B:152:ARG:NH2	1.98	0.96
1:D:27:PHE:CD2	1:D:49:LEU:CD1	2.32	0.96
1:C:134:GLY:O	1:C:199:MET:HB3	1.63	0.96
1:A:58:LEU:HD12	1:A:60:VAL:HG22	1.45	0.95
1:B:48:GLN:HE22	1:B:75:ASP:CG	1.70	0.95
1:A:86:ARG:O	1:A:89:HIS:HB3	1.66	0.95
1:C:90:THR:C	1:C:91:LEU:O	1.89	0.95
1:D:3:THR:HG23	1:D:6:GLN:CG	1.88	0.95
1:B:115:TRP:O	1:B:118:ARG:HG2	1.67	0.94
1:A:214:HIS:HD2	1:A:221:ILE:HG12	1.22	0.94
1:A:42:GLN:HG3	1:A:43:PRO:HD2	1.46	0.94
1:A:46:ILE:HG23	1:A:47:GLU:H	1.32	0.94
1:C:4:ILE:HD12	1:C:41:TYR:HE1	0.79	0.94
1:C:197:GLU:N	1:C:197:GLU:OE1	2.00	0.94
1:C:95:ILE:HG22	1:C:99:GLN:NE2	1.83	0.94
1:C:163:LYS:HA	1:C:189:VAL:CG1	1.98	0.94
1:C:4:ILE:CD1	1:C:41:TYR:HE1	1.57	0.93
1:D:72:GLY:HA3	1:D:73:ALA:CB	1.98	0.93
1:D:104:GLU:OE1	1:D:105:LEU:HD12	1.64	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:O	1:A:51:ARG:HG3	1.67	0.93
1:A:48:GLN:O	1:A:52:ILE:HG13	1.68	0.93
1:A:58:LEU:HD12	1:A:60:VAL:CG2	1.97	0.93
1:C:91:LEU:O	1:C:93:GLU:N	2.00	0.93
1:D:3:THR:HG21	1:D:6:GLN:HG2	1.50	0.92
1:D:29:PRO:CG	1:D:41:TYR:CD1	2.48	0.92
1:C:196:PRO:HG2	1:C:199:MET:CE	1.99	0.92
1:D:65:ILE:O	1:D:67:ARG:N	2.03	0.92
1:D:149:LEU:HA	1:D:152:ARG:CD	2.00	0.92
1:C:196:PRO:HB2	1:C:199:MET:HE2	1.50	0.92
1:D:88:GLN:NE2	1:D:92:ARG:HH12	1.66	0.92
1:D:3:THR:CG2	1:D:6:GLN:HE21	1.81	0.92
1:A:87:HIS:O	1:A:90:THR:N	2.03	0.92
1:C:87:HIS:HE1	1:C:91:LEU:HD11	1.34	0.91
1:A:215:LYS:CE	1:A:262:GLN:OE1	2.19	0.91
1:B:112:LEU:HD23	1:B:112:LEU:H	1.36	0.91
1:D:106:ASP:HA	1:D:109:LEU:CD2	2.00	0.91
1:B:49:LEU:HD22	1:B:53:LEU:CD2	2.00	0.91
1:C:214:HIS:O	1:C:262:GLN:HA	1.71	0.91
1:D:104:GLU:OE2	1:D:105:LEU:HD12	1.68	0.91
1:C:87:HIS:CE1	1:C:91:LEU:HD11	2.05	0.91
1:D:3:THR:HG22	1:D:6:GLN:CG	1.99	0.90
1:B:149:LEU:HA	1:B:152:ARG:HD3	1.52	0.90
1:D:27:PHE:CE2	1:D:49:LEU:HD13	2.05	0.90
1:C:61:PRO:C	1:C:62:LEU:HD12	1.91	0.90
1:A:13:ILE:HB	1:A:14:SER:HA	1.53	0.90
1:B:65:ILE:HD12	1:B:66:ASP:H	1.33	0.90
1:A:54:ALA:CB	1:A:57:ARG:HD3	2.01	0.89
1:A:88:GLN:OE1	1:D:106:ASP:OD1	1.89	0.89
1:A:15:THR:O	1:A:17:THR:N	2.05	0.89
1:B:65:ILE:O	1:B:67:ARG:N	2.04	0.89
1:C:73:ALA:HB2	1:C:79:ARG:HE	1.36	0.89
1:D:86:ARG:O	1:D:89:HIS:N	2.04	0.89
1:C:4:ILE:CG1	1:C:41:TYR:OH	2.20	0.89
1:D:133:VAL:HG23	1:D:201:ARG:HA	0.91	0.89
1:B:42:GLN:HG3	1:B:44:GLU:OE2	1.73	0.88
1:B:133:VAL:HG23	1:B:160:ILE:HD11	1.54	0.88
1:A:42:GLN:HE21	1:A:43:PRO:HD2	1.36	0.88
1:B:58:LEU:O	1:B:60:VAL:HG23	1.74	0.88
1:C:4:ILE:HD11	1:C:41:TYR:HH	1.30	0.88
1:D:88:GLN:HE21	1:D:92:ARG:HH11	0.93	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:VAL:CG2	1:D:201:ARG:CA	2.40	0.88
1:A:109:LEU:HA	1:A:112:LEU:CD2	2.04	0.88
1:A:252:ARG:HE	1:A:262:GLN:HE21	1.20	0.87
1:C:196:PRO:CB	1:C:199:MET:HE2	2.03	0.87
1:D:214:HIS:CE1	1:D:216:GLY:CA	2.56	0.87
1:D:27:PHE:CD2	1:D:49:LEU:HD21	2.09	0.87
1:D:29:PRO:HG2	1:D:41:TYR:HE1	1.10	0.87
1:B:123:ARG:HH21	1:B:125:VAL:HG21	1.37	0.87
1:D:104:GLU:CD	1:D:105:LEU:CD1	2.37	0.87
1:B:48:GLN:NE2	1:B:75:ASP:CG	2.28	0.87
1:C:5:GLY:O	1:C:7:LEU:N	2.08	0.86
1:D:67:ARG:O	1:D:71:ASP:HB3	1.75	0.86
1:A:13:ILE:CB	1:A:14:SER:HA	2.05	0.86
1:D:3:THR:CG2	1:D:6:GLN:NE2	2.36	0.86
1:D:172:ILE:HG22	1:D:184:VAL:O	1.75	0.86
1:D:149:LEU:HA	1:D:152:ARG:HD3	1.57	0.86
1:C:55:LEU:O	1:C:58:LEU:N	2.06	0.86
1:C:133:VAL:HG23	1:C:201:ARG:N	1.91	0.86
1:A:78:GLN:OE1	1:D:259:PRO:O	1.94	0.86
1:A:191:GLU:HA	1:A:201:ARG:NH2	1.90	0.86
1:D:153:PHE:C	1:D:155:PRO:HD2	1.96	0.86
1:A:42:GLN:NE2	1:A:43:PRO:HD2	1.89	0.86
1:D:172:ILE:HD13	1:D:202:PHE:CE1	2.05	0.86
1:B:107:ARG:HH21	1:C:57:ARG:NH1	1.74	0.85
1:C:196:PRO:HB2	1:C:199:MET:CE	2.05	0.85
1:D:69:LYS:CE	1:D:70:ARG:HH11	1.89	0.85
1:A:17:THR:O	1:A:21:TYR:HD1	1.33	0.85
1:A:80:LEU:HD23	1:A:80:LEU:H	1.41	0.85
1:B:133:VAL:CG2	1:B:160:ILE:HD11	2.07	0.85
1:D:153:PHE:O	1:D:155:PRO:HD2	1.76	0.85
1:B:49:LEU:HD22	1:B:53:LEU:HD23	1.56	0.84
1:B:116:ARG:HH11	1:B:117:ILE:N	1.71	0.84
1:C:87:HIS:CE1	1:C:91:LEU:CD1	2.60	0.84
1:C:214:HIS:O	1:C:262:GLN:CA	2.25	0.84
1:B:116:ARG:NH1	1:B:117:ILE:CA	2.39	0.84
1:B:228:ILE:HA	1:B:232:LEU:CB	2.07	0.84
1:D:214:HIS:CE1	1:D:216:GLY:N	2.46	0.84
1:C:53:LEU:CD1	1:C:57:ARG:HH21	1.90	0.83
1:A:15:THR:C	1:A:17:THR:H	1.80	0.83
1:C:192:GLY:H	1:C:201:ARG:HH12	1.26	0.83
1:A:215:LYS:HE3	1:A:262:GLN:OE1	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ASP:O	1:D:69:LYS:HB3	1.79	0.83
1:D:145:THR:HG22	1:D:148:GLN:OE1	1.78	0.83
1:B:65:ILE:CD1	1:B:66:ASP:H	1.90	0.83
1:B:104:GLU:OE2	1:B:107:ARG:NE	2.10	0.83
1:B:108:THR:O	1:B:112:LEU:CD2	2.27	0.83
1:B:116:ARG:NH1	1:B:117:ILE:HA	1.93	0.83
1:D:172:ILE:CD1	1:D:202:PHE:HE1	1.78	0.83
1:B:58:LEU:O	1:B:60:VAL:N	2.12	0.83
1:A:42:GLN:HG3	1:A:43:PRO:CD	2.08	0.82
1:D:90:THR:O	1:D:94:GLU:HG3	1.79	0.82
1:D:105:LEU:O	1:D:108:THR:HG22	1.79	0.82
1:D:214:HIS:HE1	1:D:216:GLY:CA	1.93	0.82
1:C:134:GLY:O	1:C:199:MET:HB2	1.78	0.82
1:D:69:LYS:HE3	1:D:70:ARG:HH11	1.45	0.81
1:A:109:LEU:HA	1:A:112:LEU:HD23	1.63	0.81
1:A:105:LEU:HD22	1:D:84:LEU:HD22	1.61	0.81
1:B:160:ILE:HG23	1:B:163:LYS:HD2	1.62	0.81
1:B:11:PHE:HE2	1:B:49:LEU:HD13	1.42	0.81
1:B:228:ILE:HG13	1:B:229:TYR:H	1.44	0.81
1:C:95:ILE:HG22	1:C:99:GLN:HE22	1.43	0.81
1:D:182:HIS:ND1	1:D:182:HIS:O	2.13	0.80
1:A:52:ILE:C	1:A:54:ALA:H	1.83	0.80
1:B:214:HIS:HD2	1:B:215:LYS:N	1.79	0.80
1:C:214:HIS:O	1:C:262:GLN:CB	2.29	0.80
1:D:88:GLN:HE21	1:D:92:ARG:HH12	1.14	0.80
1:D:106:ASP:HA	1:D:109:LEU:HD23	1.63	0.80
1:D:135:MET:CE	1:D:153:PHE:HD1	1.93	0.80
1:A:23:ALA:C	1:A:24:ILE:HG12	2.02	0.80
1:B:160:ILE:CG2	1:B:163:LYS:HD2	2.12	0.80
1:B:228:ILE:CA	1:B:232:LEU:HB2	2.10	0.79
1:D:95:ILE:O	1:D:99:GLN:HB2	1.82	0.79
1:B:29:PRO:CB	1:B:41:TYR:CE1	2.65	0.79
1:D:29:PRO:CB	1:D:41:TYR:CD1	2.65	0.79
1:A:215:LYS:HE2	1:A:262:GLN:OE1	1.82	0.79
1:B:214:HIS:HE1	1:B:221:ILE:HG22	1.42	0.79
1:A:60:VAL:CB	1:A:65:ILE:HD11	2.12	0.79
1:D:29:PRO:HB2	1:D:41:TYR:CD1	2.18	0.79
1:B:69:LYS:CG	1:B:74:LEU:HD23	2.13	0.79
1:B:116:ARG:O	1:B:117:ILE:C	2.16	0.79
1:A:85:GLN:OE1	1:A:88:GLN:HG2	1.83	0.79
1:A:115:TRP:CE2	1:D:77:PRO:CG	2.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD13	1:B:105:LEU:O	1.83	0.79
1:A:54:ALA:N	1:A:55:LEU:HB3	1.98	0.78
1:A:58:LEU:CD1	1:A:60:VAL:HG22	2.13	0.78
1:C:60:VAL:HG23	1:C:61:PRO:O	1.82	0.78
1:B:106:ASP:OD2	1:D:103:ALA:O	2.01	0.78
1:A:115:TRP:CZ2	1:D:77:PRO:HD3	2.19	0.78
1:A:85:GLN:OE1	1:A:88:GLN:CB	2.33	0.77
1:B:214:HIS:ND1	1:B:221:ILE:CG2	2.43	0.77
1:D:152:ARG:O	1:D:155:PRO:HG2	1.85	0.77
1:C:105:LEU:HD12	1:C:105:LEU:O	1.85	0.77
1:C:214:HIS:O	1:C:262:GLN:HB3	1.85	0.77
1:D:153:PHE:O	1:D:156:ARG:N	2.18	0.77
1:D:69:LYS:O	1:D:72:GLY:O	2.00	0.77
1:A:46:ILE:CG2	1:A:47:GLU:H	1.98	0.76
1:B:148:GLN:O	1:B:152:ARG:HD2	1.85	0.76
1:A:115:TRP:CZ2	1:D:77:PRO:CD	2.67	0.76
1:B:131:SER:HB3	1:B:201:ARG:HD2	1.67	0.76
1:C:89:HIS:O	1:C:91:LEU:O	2.04	0.76
1:D:228:ILE:HD13	1:D:267:ILE:HG12	1.68	0.76
1:A:42:GLN:CG	1:A:43:PRO:HD2	2.15	0.76
1:A:60:VAL:HG11	1:A:65:ILE:CD1	2.04	0.76
1:D:207:GLN:HG3	1:D:209:TYR:CE1	2.20	0.76
1:C:231:HIS:O	1:C:235:GLU:HG3	1.85	0.76
1:A:51:ARG:NH1	1:A:80:LEU:HD11	2.00	0.75
1:C:71:ASP:H	1:C:72:GLY:HA2	1.50	0.75
1:B:28:VAL:HG23	1:B:29:PRO:HD2	1.68	0.75
1:A:2:LEU:HD12	1:A:7:LEU:HB2	1.66	0.75
1:B:227:ALA:C	1:B:232:LEU:HD12	2.07	0.75
1:B:228:ILE:N	1:B:232:LEU:HD12	2.00	0.75
1:C:196:PRO:HG2	1:C:199:MET:HE3	1.68	0.75
1:D:214:HIS:ND1	1:D:215:LYS:N	2.35	0.75
1:B:72:GLY:CA	1:B:73:ALA:HB2	2.15	0.75
1:A:13:ILE:CG1	1:A:14:SER:HA	2.17	0.75
1:D:64:ALA:O	1:D:67:ARG:CG	2.34	0.75
1:A:57:ARG:O	1:D:101:LEU:HD21	1.87	0.74
1:A:55:LEU:O	1:A:57:ARG:N	2.19	0.74
1:A:80:LEU:HA	1:A:83:PHE:HB3	1.67	0.74
1:B:18:LEU:CD2	1:B:41:TYR:OH	2.35	0.74
1:B:135:MET:HE3	1:B:152:ARG:O	1.86	0.74
1:A:13:ILE:H	1:A:13:ILE:CD1	1.97	0.73
1:B:14:SER:OG	1:B:17:THR:OG1	1.98	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ALA:O	1:D:114:HIS:CD2	2.41	0.73
1:D:172:ILE:CG2	1:D:184:VAL:HB	2.17	0.73
1:C:178:ASN:H	1:C:179:GLY:HA2	1.52	0.73
1:A:7:LEU:CD2	1:A:9:ARG:NE	2.52	0.73
1:A:108:THR:O	1:A:112:LEU:CD2	2.36	0.73
1:B:52:ILE:O	1:B:54:ALA:N	2.22	0.72
1:A:76:ASP:C	1:A:78:GLN:H	1.90	0.72
1:C:9:ARG:NH1	1:D:225:PHE:CE2	2.56	0.72
1:A:191:GLU:HA	1:A:201:ARG:HH21	1.53	0.72
1:A:7:LEU:HD23	1:A:9:ARG:HE	1.52	0.72
1:B:229:TYR:OH	1:B:245:ASP:OD1	2.08	0.72
1:D:104:GLU:OE2	1:D:105:LEU:CD1	2.38	0.72
1:A:214:HIS:CD2	1:A:221:ILE:CG1	2.67	0.72
1:B:18:LEU:HD21	1:B:41:TYR:OH	1.89	0.72
1:C:64:ALA:O	1:C:66:ASP:N	2.22	0.72
1:A:2:LEU:HD12	1:A:7:LEU:CB	2.20	0.72
1:A:207:GLN:HE22	1:A:244:VAL:H	1.36	0.72
1:C:196:PRO:CG	1:C:199:MET:CE	2.68	0.72
1:A:248:TYR:HB3	1:A:264:ASP:HB2	1.70	0.72
1:D:7:LEU:O	1:D:10:ILE:HG13	1.89	0.72
1:B:107:ARG:HH21	1:C:57:ARG:HH11	1.35	0.72
1:B:65:ILE:CG1	1:B:66:ASP:H	2.03	0.71
1:B:69:LYS:HG3	1:B:74:LEU:HD23	1.71	0.71
1:A:9:ARG:NH1	1:A:9:ARG:HG2	2.06	0.71
1:D:215:LYS:HA	1:D:262:GLN:HA	1.72	0.71
1:B:115:TRP:O	1:B:118:ARG:CG	2.37	0.71
1:D:145:THR:OG1	1:D:146:ILE:N	2.24	0.71
1:A:80:LEU:HD23	1:A:80:LEU:N	2.04	0.71
1:B:65:ILE:HD12	1:B:66:ASP:N	2.04	0.71
1:D:200:VAL:HG22	1:D:201:ARG:N	2.05	0.71
1:B:42:GLN:CG	1:B:44:GLU:OE2	2.39	0.71
1:D:3:THR:CG2	1:D:6:GLN:CD	2.59	0.71
1:D:27:PHE:CE2	1:D:49:LEU:HD22	2.08	0.71
1:D:65:ILE:HG22	1:D:66:ASP:N	2.06	0.71
1:B:11:PHE:HE2	1:B:49:LEU:CD1	2.02	0.70
1:B:116:ARG:HA	1:B:119:ASN:HB2	1.71	0.70
1:C:227:ALA:CA	1:C:230:SER:OG	2.39	0.70
1:B:11:PHE:CD2	1:B:49:LEU:HD13	2.26	0.70
1:D:106:ASP:HA	1:D:109:LEU:HD21	1.72	0.70
1:B:29:PRO:CA	1:B:41:TYR:CE1	2.75	0.70
1:D:105:LEU:O	1:D:107:ARG:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:CD2	1:A:9:ARG:HE	2.04	0.70
1:D:78:GLN:HA	1:D:81:ARG:HG2	1.72	0.70
1:D:29:PRO:CB	1:D:41:TYR:CE1	2.75	0.70
1:A:52:ILE:HA	1:A:55:LEU:HG	1.74	0.69
1:B:98:ARG:HA	1:B:101:LEU:HB2	1.74	0.69
1:C:132:VAL:HG23	1:C:187:PHE:O	1.92	0.69
1:C:227:ALA:HA	1:C:230:SER:OG	1.92	0.69
1:A:15:THR:C	1:A:17:THR:N	2.44	0.69
1:C:7:LEU:CD1	1:C:41:TYR:CE1	2.75	0.69
1:C:245:ASP:N	1:C:245:ASP:OD1	2.25	0.69
1:D:4:ILE:H	1:D:4:ILE:CD1	1.96	0.69
1:C:206:ALA:C	1:C:207:GLN:HG3	2.13	0.69
1:D:86:ARG:O	1:D:88:GLN:N	2.25	0.69
1:B:214:HIS:CD2	1:B:215:LYS:N	2.59	0.69
1:D:3:THR:HG22	1:D:6:GLN:CD	2.12	0.69
1:B:65:ILE:O	1:B:68:LEU:N	2.18	0.69
1:C:130:PHE:CZ	1:C:204:VAL:HG21	2.28	0.69
1:B:67:ARG:HH11	1:B:67:ARG:HG2	1.58	0.68
1:C:133:VAL:CG2	1:C:201:ARG:HA	2.19	0.68
1:A:7:LEU:HD23	1:A:9:ARG:NE	2.09	0.68
1:C:65:ILE:HA	1:C:68:LEU:HB3	1.75	0.68
1:D:69:LYS:HE3	1:D:70:ARG:HD2	1.74	0.68
1:D:172:ILE:HD13	1:D:202:PHE:HD1	1.57	0.68
1:D:81:ARG:O	1:D:85:GLN:HB3	1.93	0.68
1:C:53:LEU:HD13	1:C:57:ARG:NH2	2.05	0.68
1:A:178:ASN:H	1:A:179:GLY:HA2	1.58	0.68
1:B:14:SER:OG	1:B:17:THR:CB	2.42	0.68
1:B:132:VAL:HG11	1:B:172:ILE:HD11	1.75	0.68
1:C:110:ALA:O	1:C:113:ALA:HB3	1.94	0.68
1:A:252:ARG:NE	1:A:262:GLN:HE21	1.92	0.67
1:C:196:PRO:CG	1:C:199:MET:HE2	2.24	0.67
1:A:87:HIS:O	1:A:88:GLN:C	2.31	0.67
1:C:5:GLY:O	1:C:8:ALA:N	2.26	0.67
1:C:236:ARG:O	1:C:236:ARG:HG3	1.94	0.67
1:C:53:LEU:CD1	1:C:57:ARG:NH2	2.57	0.67
1:C:182:HIS:CD2	1:C:183:TYR:H	2.12	0.67
1:D:69:LYS:HG2	1:D:70:ARG:N	2.09	0.67
1:A:180:GLU:HG3	1:A:181:PHE:H	1.59	0.67
1:D:65:ILE:O	1:D:67:ARG:HD2	1.94	0.67
1:A:7:LEU:HD22	1:A:7:LEU:O	1.95	0.67
1:D:122:ALA:CB	1:D:212:PHE:CE1	2.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASP:HA	1:B:148:GLN:HG2	1.75	0.67
1:B:160:ILE:HG23	1:B:163:LYS:CD	2.24	0.67
1:D:149:LEU:HD12	1:D:152:ARG:HH21	1.60	0.67
1:A:43:PRO:O	1:A:46:ILE:HG22	1.94	0.67
1:A:85:GLN:HA	1:A:88:GLN:HB3	1.77	0.67
1:C:79:ARG:HG3	1:C:80:LEU:HD12	1.76	0.67
1:C:247:GLU:OE1	1:D:9:ARG:NH2	2.27	0.67
1:D:112:LEU:N	1:D:112:LEU:HD22	2.09	0.67
1:B:28:VAL:HG23	1:B:29:PRO:CD	2.24	0.67
1:D:3:THR:CG2	1:D:6:GLN:HG3	2.23	0.67
1:A:2:LEU:HD12	1:A:7:LEU:CA	2.25	0.67
1:A:87:HIS:O	1:A:89:HIS:N	2.28	0.67
1:B:220:GLN:HE22	1:C:81:ARG:NH1	1.92	0.66
1:A:13:ILE:HD13	1:A:13:ILE:N	2.05	0.66
1:A:26:LEU:C	1:A:26:LEU:HD12	2.16	0.66
1:C:42:GLN:HG3	1:C:43:PRO:HD2	1.77	0.66
1:D:29:PRO:HB2	1:D:41:TYR:HD1	1.59	0.66
1:B:29:PRO:HA	1:B:41:TYR:CE1	2.30	0.66
1:D:88:GLN:NE2	1:D:92:ARG:HH11	1.59	0.66
1:B:108:THR:C	1:B:112:LEU:HD21	2.14	0.66
1:D:153:PHE:O	1:D:154:ILE:C	2.33	0.66
1:A:76:ASP:C	1:A:78:GLN:N	2.50	0.66
1:C:181:PHE:CE2	1:D:15:THR:HG23	2.31	0.65
1:A:60:VAL:HG12	1:A:65:ILE:HD13	1.72	0.65
1:A:115:TRP:CZ2	1:D:77:PRO:HG3	2.31	0.65
1:C:3:THR:O	1:C:7:LEU:HB2	1.96	0.65
1:C:96:SER:O	1:C:100:ARG:HG3	1.97	0.65
1:B:226:GLN:O	1:B:230:SER:HB3	1.96	0.65
1:D:214:HIS:N	1:D:263:VAL:O	2.29	0.65
1:B:153:PHE:O	1:B:156:ARG:N	2.21	0.65
1:C:161:ALA:O	1:C:189:VAL:HG11	1.96	0.65
1:A:75:ASP:HB2	1:D:115:TRP:CZ3	2.32	0.65
1:B:248:TYR:HB3	1:B:264:ASP:HB2	1.79	0.65
1:D:83:PHE:HD1	1:D:84:LEU:N	1.93	0.64
1:D:106:ASP:CA	1:D:109:LEU:HD23	2.27	0.64
1:D:152:ARG:O	1:D:155:PRO:CG	2.44	0.64
1:D:223:GLU:HA	1:D:226:GLN:HB3	1.78	0.64
1:B:195:VAL:HG22	1:B:199:MET:HB2	1.78	0.64
1:B:49:LEU:CD2	1:B:53:LEU:CD2	2.73	0.64
1:B:214:HIS:HE1	1:B:221:ILE:CG2	2.01	0.64
1:C:134:GLY:O	1:C:199:MET:CA	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TRP:O	1:B:154:ILE:HG13	1.98	0.64
1:A:13:ILE:HB	1:A:14:SER:CA	2.26	0.64
1:A:46:ILE:HD12	1:B:230:SER:HA	1.80	0.64
1:A:9:ARG:CD	1:A:9:ARG:H	2.11	0.64
1:B:11:PHE:CE2	1:B:49:LEU:CD1	2.75	0.64
1:D:160:ILE:O	1:D:163:LYS:CE	2.46	0.64
1:A:207:GLN:HB2	1:A:209:TYR:CZ	2.33	0.64
1:D:245:ASP:HB3	1:D:268:PRO:HD3	1.79	0.63
1:A:3:THR:O	1:A:7:LEU:HB2	1.99	0.63
1:B:14:SER:HG	1:B:17:THR:HG1	1.27	0.63
1:B:172:ILE:HD13	1:B:202:PHE:CD2	2.34	0.63
1:D:88:GLN:O	1:D:92:ARG:CD	2.46	0.63
1:B:109:LEU:HA	1:B:112:LEU:HD21	1.79	0.63
1:D:71:ASP:OD1	1:D:72:GLY:N	2.31	0.63
1:B:220:GLN:NE2	1:C:81:ARG:NH1	2.46	0.63
1:A:17:THR:O	1:A:21:TYR:HE1	1.79	0.63
1:D:132:VAL:HB	1:D:188:GLU:HA	1.79	0.63
1:A:115:TRP:CZ2	1:D:77:PRO:CG	2.82	0.63
1:D:4:ILE:HD12	1:D:4:ILE:N	2.05	0.62
1:D:181:PHE:O	1:D:182:HIS:HB2	1.98	0.62
1:A:78:GLN:OE1	1:D:260:ASN:HA	1.98	0.62
1:B:69:LYS:HG2	1:B:74:LEU:HD23	1.81	0.62
1:A:109:LEU:CA	1:A:112:LEU:HD23	2.28	0.62
1:C:87:HIS:ND1	1:C:91:LEU:HD12	2.15	0.62
1:D:73:ALA:HB1	1:D:79:ARG:HD2	1.81	0.62
1:D:172:ILE:HG21	1:D:184:VAL:HB	1.81	0.62
1:A:105:LEU:HD22	1:D:84:LEU:CD2	2.29	0.62
1:D:153:PHE:C	1:D:155:PRO:CD	2.61	0.62
1:A:191:GLU:CD	1:A:203:GLN:HE22	2.02	0.62
1:A:250:ASP:OD2	1:A:252:ARG:NH1	2.32	0.62
1:C:213:THR:OG1	1:C:264:ASP:OD1	2.13	0.62
1:B:116:ARG:C	1:B:118:ARG:N	2.52	0.62
1:D:149:LEU:HA	1:D:152:ARG:HD2	1.78	0.62
1:D:149:LEU:HD12	1:D:152:ARG:NH2	2.15	0.62
1:A:119:ASN:O	1:A:119:ASN:ND2	2.22	0.61
1:A:85:GLN:HG3	1:A:85:GLN:O	1.99	0.61
1:A:214:HIS:NE2	1:A:221:ILE:HA	2.14	0.61
1:C:133:VAL:CG2	1:C:201:ARG:CA	2.74	0.61
1:C:195:VAL:HG23	1:C:195:VAL:O	1.99	0.61
1:A:52:ILE:C	1:A:54:ALA:N	2.44	0.61
1:B:230:SER:OG	1:B:231:HIS:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HD12	1:C:69:LYS:HE3	1.83	0.61
1:C:71:ASP:OD1	1:C:72:GLY:O	2.18	0.61
1:D:69:LYS:CE	1:D:70:ARG:HD2	2.30	0.61
1:B:116:ARG:NH1	1:B:116:ARG:HG3	2.13	0.61
1:D:130:PHE:CE1	1:D:204:VAL:HG13	2.36	0.61
1:A:228:ILE:HG21	1:A:267:ILE:HD13	1.83	0.61
1:B:123:ARG:HH21	1:B:125:VAL:CG2	2.11	0.61
1:C:65:ILE:O	1:C:65:ILE:HG22	2.01	0.61
1:C:134:GLY:C	1:C:199:MET:HB3	2.20	0.61
1:A:23:ALA:O	1:A:25:GLY:N	2.29	0.60
1:A:53:LEU:HD23	1:A:53:LEU:O	2.01	0.60
1:D:124:ILE:CG2	1:D:208:LYS:NZ	2.64	0.60
1:D:214:HIS:O	1:D:263:VAL:N	2.32	0.60
1:B:69:LYS:HG3	1:B:74:LEU:CD2	2.29	0.60
1:C:9:ARG:CG	1:C:10:ILE:N	2.45	0.60
1:D:135:MET:HE1	1:D:153:PHE:HD1	1.66	0.60
1:A:115:TRP:CE3	1:D:77:PRO:HG3	2.36	0.60
1:A:180:GLU:HG3	1:A:181:PHE:N	2.15	0.60
1:B:116:ARG:HH11	1:B:116:ARG:C	2.05	0.60
1:D:130:PHE:CE1	1:D:204:VAL:CG1	2.84	0.60
1:D:28:VAL:O	1:D:28:VAL:HG13	2.02	0.60
1:A:70:ARG:HD3	1:A:74:LEU:HD12	1.82	0.60
1:A:71:ASP:N	1:A:72:GLY:HA2	2.15	0.60
1:A:149:LEU:HD12	1:A:149:LEU:H	1.66	0.59
1:C:62:LEU:HD12	1:C:62:LEU:N	2.15	0.59
1:D:83:PHE:CD1	1:D:84:LEU:N	2.70	0.59
1:D:170:TYR:HE2	1:D:188:GLU:HB2	1.66	0.59
1:A:46:ILE:O	1:A:49:LEU:N	2.36	0.59
1:C:55:LEU:HB3	1:C:60:VAL:HG11	1.84	0.59
1:D:214:HIS:ND1	1:D:216:GLY:N	2.50	0.59
1:A:65:ILE:N	1:A:65:ILE:HD12	2.17	0.59
1:A:105:LEU:CD2	1:D:84:LEU:CD2	2.81	0.59
1:C:47:GLU:HA	1:C:50:SER:HB3	1.84	0.59
1:C:87:HIS:CE1	1:C:91:LEU:HD12	2.36	0.59
1:B:149:LEU:HA	1:B:152:ARG:HH21	1.65	0.59
1:D:213:THR:HG23	1:D:213:THR:O	2.01	0.59
1:B:92:ARG:O	1:B:96:SER:N	2.31	0.59
1:D:200:VAL:HG22	1:D:201:ARG:H	1.67	0.59
1:D:135:MET:HE3	1:D:153:PHE:HD1	1.65	0.59
1:A:252:ARG:HE	1:A:262:GLN:NE2	1.97	0.59
1:B:88:GLN:NE2	1:B:92:ARG:HD3	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ARG:HE	1:D:104:GLU:HG3	1.66	0.59
1:B:56:ARG:HD2	1:B:62:LEU:HD21	1.83	0.59
1:C:65:ILE:HG12	1:C:68:LEU:HD23	1.85	0.59
1:D:228:ILE:HA	1:D:232:LEU:HB2	1.83	0.59
1:C:136:GLU:HG2	1:C:137:TYR:N	2.16	0.58
1:C:196:PRO:CB	1:C:199:MET:CE	2.70	0.58
1:B:29:PRO:CA	1:B:41:TYR:HE1	2.17	0.58
1:B:16:LYS:HE2	1:B:20:HIS:HB2	1.86	0.58
1:D:84:LEU:O	1:D:88:GLN:HB3	2.03	0.58
1:A:42:GLN:HG3	1:A:43:PRO:N	2.17	0.58
1:A:108:THR:O	1:A:112:LEU:HD21	2.04	0.58
1:D:26:LEU:HG	1:D:27:PHE:N	2.18	0.58
1:A:6:GLN:C	1:A:8:ALA:H	2.07	0.58
1:A:11:PHE:HD1	1:B:181:PHE:HE2	1.51	0.58
1:C:182:HIS:O	1:C:183:TYR:HB2	2.03	0.58
1:B:151:GLU:C	1:B:153:PHE:H	2.08	0.58
1:A:18:LEU:O	1:A:21:TYR:HB2	2.04	0.57
1:A:53:LEU:O	1:A:54:ALA:HB2	2.03	0.57
1:B:70:ARG:O	1:B:70:ARG:HG3	2.03	0.57
1:A:62:LEU:O	1:A:65:ILE:N	2.36	0.57
1:B:44:GLU:OE2	1:B:44:GLU:N	2.30	0.57
1:B:228:ILE:HA	1:B:232:LEU:HD12	1.86	0.57
1:D:207:GLN:OE1	1:D:209:TYR:HE1	1.87	0.57
1:A:80:LEU:H	1:A:80:LEU:CD2	2.08	0.57
1:B:18:LEU:HD22	1:B:41:TYR:OH	2.03	0.57
1:C:79:ARG:CG	1:C:80:LEU:HD12	2.35	0.57
1:C:253:PHE:HA	1:C:261:SER:HB2	1.86	0.57
1:A:77:PRO:HD3	1:D:115:TRP:HZ3	1.69	0.57
1:A:111:THR:HG22	1:A:111:THR:O	2.03	0.57
1:A:149:LEU:HD12	1:A:149:LEU:N	2.19	0.57
1:B:52:ILE:C	1:B:54:ALA:H	2.08	0.57
1:B:150:TRP:HE1	1:B:183:TYR:HE2	1.52	0.57
1:C:79:ARG:C	1:C:81:ARG:H	2.07	0.57
1:A:105:LEU:HD13	1:D:88:GLN:HB2	1.85	0.57
1:A:122:ALA:HB2	1:A:212:PHE:CE1	2.39	0.57
1:D:90:THR:HA	1:D:93:GLU:HB2	1.87	0.57
1:D:231:HIS:ND1	1:D:235:GLU:OE1	2.33	0.57
1:D:130:PHE:N	1:D:130:PHE:HD1	2.02	0.57
1:D:27:PHE:CZ	1:D:49:LEU:CD1	2.80	0.57
1:B:110:ALA:HB2	1:D:107:ARG:O	2.04	0.57
1:C:89:HIS:O	1:C:90:THR:C	2.41	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:PHE:N	1:D:130:PHE:CD1	2.71	0.57
1:B:49:LEU:O	1:B:51:ARG:N	2.37	0.56
1:B:241:LYS:HA	1:B:270:TYR:CE1	2.40	0.56
1:D:69:LYS:HE3	1:D:70:ARG:NH1	2.16	0.56
1:D:109:LEU:N	1:D:109:LEU:HD22	2.19	0.56
1:B:29:PRO:HA	1:B:41:TYR:CD1	2.39	0.56
1:D:106:ASP:C	1:D:109:LEU:HD23	2.25	0.56
1:D:172:ILE:HG22	1:D:184:VAL:HB	1.85	0.56
1:D:27:PHE:CD2	1:D:49:LEU:CG	2.78	0.56
1:C:178:ASN:N	1:C:179:GLY:HA2	2.18	0.56
1:D:72:GLY:CA	1:D:73:ALA:CB	2.63	0.56
1:B:97:ALA:O	1:B:101:LEU:HD23	2.05	0.56
1:B:228:ILE:CA	1:B:232:LEU:HD12	2.35	0.56
1:C:69:LYS:HB2	1:C:74:LEU:HA	1.86	0.56
1:D:51:ARG:NH2	1:D:75:ASP:OD2	0.47	0.56
1:A:126:GLU:HG2	1:A:208:LYS:HB2	1.87	0.56
1:B:64:ALA:O	1:B:65:ILE:O	2.24	0.56
1:B:65:ILE:CG1	1:B:66:ASP:N	2.69	0.56
1:B:172:ILE:O	1:B:183:TYR:HA	2.05	0.56
1:B:65:ILE:C	1:B:67:ARG:H	2.09	0.55
1:C:228:ILE:HG21	1:C:267:ILE:HD13	1.87	0.55
1:A:115:TRP:CH2	1:D:77:PRO:CD	2.81	0.55
1:A:214:HIS:HB3	1:A:263:VAL:HG22	1.87	0.55
1:A:58:LEU:CD1	1:A:60:VAL:CG2	2.79	0.55
1:B:104:GLU:OE2	1:B:107:ARG:NH2	2.34	0.55
1:B:127:ARG:NH2	1:B:170:TYR:OH	2.40	0.55
1:A:85:GLN:OE1	1:A:88:GLN:HB3	2.05	0.55
1:C:182:HIS:CD2	1:C:183:TYR:N	2.75	0.55
1:C:250:ASP:OD1	1:C:250:ASP:N	2.40	0.55
1:D:195:VAL:HG13	1:D:195:VAL:O	2.06	0.55
1:A:9:ARG:HG2	1:A:9:ARG:HH11	1.69	0.55
1:B:252:ARG:NH2	1:B:264:ASP:OD1	2.39	0.55
1:C:71:ASP:OD1	1:C:72:GLY:C	2.45	0.55
1:B:26:LEU:O	1:B:69:LYS:NZ	2.22	0.55
1:C:228:ILE:HA	1:C:232:LEU:HB2	1.88	0.55
1:D:159:GLU:HB3	1:D:196:PRO:HG2	1.89	0.55
1:B:148:GLN:O	1:B:152:ARG:CD	2.55	0.54
1:D:73:ALA:HB2	1:D:79:ARG:NH1	2.22	0.54
1:D:112:LEU:O	1:D:113:ALA:O	2.26	0.54
1:A:88:GLN:HA	1:D:102:LEU:HD21	1.90	0.54
1:C:190:GLN:O	1:C:193:TRP:HD1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:HG	1:D:108:THR:HG21	1.88	0.54
1:A:105:LEU:CD1	1:D:88:GLN:HB2	2.37	0.54
1:D:65:ILE:HG22	1:D:66:ASP:H	1.71	0.54
1:B:156:ARG:HA	1:B:159:GLU:OE1	2.08	0.54
1:C:250:ASP:OD2	1:C:252:ARG:CZ	2.55	0.54
1:D:149:LEU:HD12	1:D:152:ARG:HD2	1.88	0.54
1:D:214:HIS:O	1:D:262:GLN:HA	2.08	0.54
1:B:160:ILE:HG21	1:B:163:LYS:HD2	1.88	0.54
1:C:6:GLN:C	1:C:8:ALA:H	2.11	0.54
1:C:154:ILE:N	1:C:155:PRO:HD2	2.23	0.54
1:B:52:ILE:C	1:B:54:ALA:N	2.60	0.54
1:A:23:ALA:O	1:A:24:ILE:HG12	2.08	0.54
1:D:69:LYS:NZ	1:D:70:ARG:HH11	2.05	0.54
1:D:124:ILE:CG2	1:D:208:LYS:HZ3	2.20	0.54
1:A:42:GLN:CD	1:A:43:PRO:HD2	2.28	0.54
1:A:133:VAL:HG23	1:A:189:VAL:HG21	1.89	0.53
1:A:135:MET:SD	1:A:152:ARG:HD2	2.48	0.53
1:C:73:ALA:CB	1:C:79:ARG:HE	2.14	0.53
1:D:172:ILE:CG2	1:D:184:VAL:CB	2.84	0.53
1:D:172:ILE:CG2	1:D:184:VAL:HG23	2.39	0.53
1:A:65:ILE:HG22	1:A:65:ILE:O	2.07	0.53
1:B:137:TYR:HD2	1:B:183:TYR:HB3	1.73	0.53
1:C:10:ILE:HD13	1:D:226:GLN:HA	1.90	0.53
1:C:86:ARG:O	1:C:90:THR:HG23	2.08	0.53
1:D:69:LYS:HG2	1:D:70:ARG:H	1.73	0.53
1:A:55:LEU:HD13	1:A:56:ARG:N	2.22	0.53
1:B:107:ARG:NH2	1:C:57:ARG:NH1	2.51	0.53
1:D:130:PHE:CD1	1:D:204:VAL:HG13	2.44	0.53
1:B:228:ILE:C	1:B:230:SER:H	2.12	0.53
1:C:173:CYS:HB3	1:D:9:ARG:NH1	2.23	0.53
1:D:105:LEU:C	1:D:107:ARG:H	2.12	0.53
1:A:250:ASP:OD2	1:A:252:ARG:HG3	2.09	0.53
1:B:145:THR:H	1:B:148:GLN:HB2	1.74	0.53
1:B:151:GLU:O	1:B:155:PRO:HD2	2.08	0.53
1:A:56:ARG:CG	1:A:56:ARG:HH11	2.19	0.53
1:A:66:ASP:O	1:A:69:LYS:N	2.38	0.53
1:B:22:ASP:OD2	1:B:39:ARG:NH2	2.42	0.53
1:A:65:ILE:CD1	1:A:65:ILE:N	2.71	0.53
1:A:105:LEU:CD2	1:D:84:LEU:HD22	2.37	0.53
1:C:6:GLN:CD	1:C:6:GLN:H	2.13	0.53
1:C:131:SER:CB	1:C:203:GLN:HE22	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:C	1:A:24:ILE:CG1	2.76	0.53
1:A:55:LEU:HD13	1:A:55:LEU:C	2.29	0.53
1:D:149:LEU:CD1	1:D:152:ARG:NH2	2.72	0.53
1:D:207:GLN:CG	1:D:209:TYR:CE1	2.91	0.53
1:B:18:LEU:HD23	1:B:18:LEU:O	2.10	0.52
1:B:132:VAL:CG1	1:B:172:ILE:HD11	2.38	0.52
1:B:104:GLU:O	1:B:108:THR:HG23	2.09	0.52
1:B:174:ALA:HB3	1:B:182:HIS:HB3	1.90	0.52
1:C:73:ALA:CB	1:C:76:ASP:HB2	2.39	0.52
1:D:146:ILE:HG23	1:D:150:TRP:CB	2.39	0.52
1:D:172:ILE:O	1:D:183:TYR:HA	2.08	0.52
1:C:173:CYS:HB3	1:D:9:ARG:HH12	1.74	0.52
1:D:146:ILE:HG23	1:D:150:TRP:HB2	1.91	0.52
1:A:112:LEU:CD2	1:A:112:LEU:N	2.72	0.52
1:C:132:VAL:CG2	1:C:187:PHE:O	2.57	0.52
1:C:152:ARG:O	1:C:156:ARG:HG3	2.09	0.52
1:A:149:LEU:H	1:A:149:LEU:CD1	2.22	0.52
1:C:136:GLU:OE2	1:C:200:VAL:HG11	2.10	0.52
1:C:191:GLU:HG3	1:C:201:ARG:NH1	2.25	0.52
1:D:112:LEU:CD2	1:D:112:LEU:N	2.72	0.52
1:A:55:LEU:CD1	1:A:56:ARG:N	2.73	0.52
1:A:164:HIS:HD2	1:A:165:ASP:CG	2.12	0.52
1:B:28:VAL:HG23	1:B:29:PRO:N	2.25	0.52
1:B:241:LYS:HA	1:B:270:TYR:HE1	1.74	0.52
1:C:7:LEU:HD12	1:C:41:TYR:CE1	2.44	0.52
1:A:26:LEU:C	1:A:69:LYS:HE2	2.30	0.52
1:A:52:ILE:CA	1:A:55:LEU:HG	2.37	0.52
1:A:148:GLN:HE21	1:A:148:GLN:C	2.13	0.52
1:B:94:GLU:OE1	1:C:98:ARG:NH1	2.43	0.52
1:C:4:ILE:CD1	1:C:4:ILE:N	2.73	0.52
1:C:7:LEU:CD2	1:C:18:LEU:HD21	2.40	0.52
1:A:9:ARG:HH11	1:A:9:ARG:CG	2.22	0.52
1:A:10:ILE:HD12	1:B:222:ALA:O	2.10	0.52
1:B:116:ARG:NH1	1:B:117:ILE:H	2.05	0.52
1:D:116:ARG:O	1:D:119:ASN:N	2.43	0.52
1:D:173:CYS:O	1:D:174:ALA:HB2	2.09	0.52
1:A:47:GLU:HG2	1:D:115:TRP:CE2	2.45	0.52
1:B:116:ARG:HH11	1:B:116:ARG:HG3	1.75	0.52
1:B:149:LEU:HA	1:B:152:ARG:CD	2.32	0.52
1:C:7:LEU:HD12	1:C:41:TYR:CD1	2.44	0.52
1:A:156:ARG:HA	1:A:159:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LYS:NZ	1:D:70:ARG:NH1	2.58	0.51
1:B:26:LEU:HD12	1:B:69:LYS:HD2	1.92	0.51
1:D:27:PHE:CZ	1:D:49:LEU:HD13	2.46	0.51
1:D:109:LEU:CD2	1:D:109:LEU:N	2.73	0.51
1:D:152:ARG:O	1:D:155:PRO:HD2	2.10	0.51
1:A:23:ALA:O	1:A:24:ILE:CG1	2.58	0.51
1:A:109:LEU:HA	1:A:112:LEU:HD21	1.90	0.51
1:B:149:LEU:CA	1:B:152:ARG:HH21	2.23	0.51
1:C:150:TRP:O	1:C:154:ILE:HG12	2.10	0.51
1:D:15:THR:OG1	1:D:19:ARG:NH2	2.43	0.51
1:D:78:GLN:O	1:D:81:ARG:HG3	2.11	0.51
1:D:133:VAL:HG21	1:D:201:ARG:CA	2.34	0.51
1:A:172:ILE:O	1:A:183:TYR:HA	2.09	0.51
1:C:46:ILE:HG12	1:D:230:SER:HA	1.92	0.51
1:C:91:LEU:HA	1:C:94:GLU:HG3	1.91	0.51
1:D:29:PRO:CG	1:D:41:TYR:HE1	1.85	0.51
1:D:218:ALA:O	1:D:221:ILE:HG12	2.10	0.51
1:B:49:LEU:C	1:B:51:ARG:N	2.64	0.51
1:B:67:ARG:HG2	1:B:67:ARG:NH1	2.23	0.51
1:D:153:PHE:O	1:D:155:PRO:CG	2.59	0.51
1:A:112:LEU:N	1:A:112:LEU:HD22	2.26	0.51
1:C:227:ALA:C	1:C:230:SER:OG	2.48	0.51
1:D:135:MET:CE	1:D:153:PHE:CD1	2.84	0.51
1:B:42:GLN:O	1:B:45:GLN:HG2	2.11	0.51
1:B:105:LEU:O	1:B:109:LEU:HD12	2.10	0.51
1:C:76:ASP:HB3	1:C:78:GLN:OE1	2.11	0.51
1:D:88:GLN:O	1:D:92:ARG:HD2	2.09	0.51
1:B:253:PHE:C	1:B:254:ARG:HG3	2.30	0.51
1:C:4:ILE:CD1	1:C:41:TYR:HH	2.02	0.51
1:A:231:HIS:O	1:A:235:GLU:HG3	2.11	0.50
1:D:149:LEU:HD12	1:D:152:ARG:CD	2.41	0.50
1:D:200:VAL:CG2	1:D:201:ARG:N	2.74	0.50
1:A:13:ILE:HG12	1:A:14:SER:HA	1.94	0.50
1:A:251:GLN:OE1	1:A:251:GLN:N	2.33	0.50
1:B:228:ILE:HG13	1:B:229:TYR:N	2.20	0.50
1:A:148:GLN:O	1:A:151:GLU:N	2.45	0.50
1:B:253:PHE:C	1:B:253:PHE:CD1	2.85	0.50
1:C:16:LYS:O	1:C:20:HIS:HB2	2.11	0.50
1:C:65:ILE:CG1	1:C:68:LEU:HD23	2.40	0.50
1:C:192:GLY:N	1:C:201:ARG:HH12	2.03	0.50
1:A:56:ARG:CG	1:A:56:ARG:NH1	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB2	1:D:115:TRP:CH2	2.47	0.50
1:D:227:ALA:O	1:D:232:LEU:HD12	2.11	0.50
1:C:64:ALA:C	1:C:66:ASP:H	2.11	0.50
1:C:225:PHE:HB3	1:D:10:ILE:HG22	1.93	0.50
1:A:147:GLY:O	1:A:150:TRP:HB2	2.11	0.50
1:D:27:PHE:CD1	1:D:27:PHE:C	2.85	0.50
1:D:172:ILE:HG21	1:D:184:VAL:CG2	2.42	0.50
1:D:172:ILE:HG13	1:D:173:CYS:N	2.26	0.50
1:A:149:LEU:O	1:A:153:PHE:HB2	2.12	0.50
1:B:115:TRP:NE1	1:C:47:GLU:OE1	2.45	0.50
1:C:132:VAL:HA	1:C:187:PHE:O	2.11	0.50
1:C:131:SER:OG	1:C:203:GLN:NE2	2.41	0.50
1:B:68:LEU:O	1:B:70:ARG:N	2.45	0.49
1:B:212:PHE:CD2	1:B:228:ILE:HG21	2.47	0.49
1:D:13:ILE:HD13	1:D:53:LEU:HD21	1.94	0.49
1:D:83:PHE:CD1	1:D:83:PHE:C	2.84	0.49
1:D:124:ILE:HG23	1:D:208:LYS:NZ	2.26	0.49
1:B:137:TYR:CD2	1:B:183:TYR:HB3	2.46	0.49
1:C:7:LEU:HD22	1:C:18:LEU:CD2	2.43	0.49
1:C:225:PHE:CD1	1:D:10:ILE:HG22	2.47	0.49
1:C:108:THR:HG22	1:C:108:THR:O	2.12	0.49
1:B:42:GLN:H	1:B:45:GLN:HE21	1.60	0.49
1:D:172:ILE:CG2	1:D:184:VAL:CG2	2.91	0.49
1:B:160:ILE:HG23	1:B:160:ILE:O	2.11	0.49
1:D:254:ARG:NH2	1:D:260:ASN:OD1	2.45	0.49
1:B:214:HIS:CD2	1:B:214:HIS:C	2.85	0.49
1:C:52:ILE:O	1:C:56:ARG:HB2	2.12	0.49
1:C:73:ALA:HB2	1:C:79:ARG:NE	2.17	0.49
1:A:222:ALA:O	1:A:226:GLN:HG3	2.12	0.49
1:A:85:GLN:OE1	1:A:88:GLN:OE1	2.29	0.49
1:A:86:ARG:O	1:A:89:HIS:CB	2.52	0.49
1:B:48:GLN:NE2	1:B:75:ASP:OD2	2.24	0.49
1:D:133:VAL:HG11	1:D:195:VAL:HG23	1.94	0.49
1:C:61:PRO:O	1:C:62:LEU:HD12	2.13	0.49
1:D:86:ARG:HA	1:D:86:ARG:HE	1.77	0.49
1:D:130:PHE:CE1	1:D:204:VAL:HG11	2.48	0.49
1:A:75:ASP:OD1	1:A:75:ASP:N	2.46	0.48
1:A:78:GLN:HG2	1:D:215:LYS:O	2.13	0.48
1:B:207:GLN:HG3	1:B:209:TYR:CZ	2.47	0.48
1:C:172:ILE:O	1:C:183:TYR:HA	2.13	0.48
1:D:132:VAL:HG22	1:D:133:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:THR:C	1:C:5:GLY:N	2.64	0.48
1:B:228:ILE:O	1:B:230:SER:N	2.47	0.48
1:C:78:GLN:OE1	1:C:78:GLN:N	2.44	0.48
1:D:69:LYS:CG	1:D:70:ARG:N	2.71	0.48
1:A:250:ASP:HB2	1:A:251:GLN:OE1	2.12	0.48
1:C:241:LYS:HB2	1:C:270:TYR:CE2	2.49	0.48
1:A:57:ARG:HE	1:D:104:GLU:CG	2.26	0.48
1:B:212:PHE:CE2	1:B:228:ILE:HG21	2.49	0.48
1:C:53:LEU:HD12	1:C:57:ARG:NH2	2.29	0.48
1:A:86:ARG:HD3	1:A:86:ARG:HA	1.73	0.48
1:D:182:HIS:HD1	1:D:182:HIS:C	2.15	0.48
1:B:49:LEU:O	1:B:52:ILE:N	2.47	0.48
1:D:239:GLU:HG2	1:D:270:TYR:HD2	1.79	0.48
1:A:71:ASP:H	1:A:72:GLY:HA2	1.78	0.48
1:B:187:PHE:O	1:B:189:VAL:HG13	2.13	0.48
1:A:57:ARG:NE	1:D:104:GLU:CG	2.76	0.48
1:B:96:SER:HA	1:B:99:GLN:HG2	1.95	0.48
1:B:133:VAL:HG21	1:B:160:ILE:HD11	1.91	0.48
1:D:88:GLN:O	1:D:88:GLN:HG3	2.12	0.48
1:A:181:PHE:CG	1:A:182:HIS:N	2.81	0.47
1:B:101:LEU:O	1:B:105:LEU:HB2	2.14	0.47
1:B:149:LEU:HA	1:B:152:ARG:NH2	2.30	0.47
1:D:27:PHE:C	1:D:27:PHE:HD1	2.18	0.47
1:D:102:LEU:O	1:D:106:ASP:HB2	2.13	0.47
1:D:170:TYR:CE2	1:D:188:GLU:HB2	2.48	0.47
1:C:79:ARG:C	1:C:81:ARG:N	2.65	0.47
1:B:135:MET:HE2	1:B:153:PHE:HD1	1.79	0.47
1:B:228:ILE:HA	1:B:232:LEU:CD1	2.45	0.47
1:C:4:ILE:HG13	1:C:41:TYR:OH	2.10	0.47
1:C:62:LEU:O	1:C:64:ALA:N	2.47	0.47
1:D:132:VAL:CB	1:D:188:GLU:HA	2.44	0.47
1:A:77:PRO:HG3	1:D:115:TRP:HE3	1.79	0.47
1:C:90:THR:OG1	1:C:91:LEU:N	2.47	0.47
1:D:172:ILE:HG23	1:D:184:VAL:HG23	1.95	0.47
1:C:47:GLU:HG2	1:C:51:ARG:NH1	2.29	0.47
1:A:56:ARG:O	1:A:57:ARG:HG3	2.14	0.47
1:A:66:ASP:O	1:A:69:LYS:HB2	2.14	0.47
1:B:108:THR:C	1:B:112:LEU:CD2	2.81	0.47
1:B:205:PRO:O	1:B:207:GLN:HG2	2.15	0.47
1:B:212:PHE:CE2	1:B:228:ILE:CG2	2.97	0.47
1:B:230:SER:OG	1:B:231:HIS:ND1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:GLN:HG2	1:C:49:LEU:HD23	1.96	0.47
1:D:214:HIS:ND1	1:D:215:LYS:C	2.68	0.47
1:A:10:ILE:HD11	1:B:226:GLN:HG3	1.97	0.47
1:A:54:ALA:N	1:A:55:LEU:CB	2.73	0.47
1:A:54:ALA:HA	1:A:56:ARG:N	2.30	0.47
1:A:57:ARG:NE	1:D:104:GLU:HG3	2.30	0.47
1:A:172:ILE:HA	1:A:246:PHE:HB3	1.96	0.47
1:B:109:LEU:CA	1:B:112:LEU:HD21	2.45	0.47
1:C:73:ALA:HB1	1:C:76:ASP:HB2	1.97	0.47
1:C:168:VAL:HG13	1:C:249:TYR:O	2.15	0.47
1:A:57:ARG:HG2	1:D:104:GLU:HG3	1.96	0.47
1:B:65:ILE:HG13	1:B:66:ASP:H	1.80	0.47
1:C:12:GLU:OE2	1:C:12:GLU:HA	2.15	0.47
1:C:160:ILE:CD1	1:C:199:MET:HE1	2.44	0.47
1:C:249:TYR:CE1	1:C:263:VAL:HG11	2.50	0.47
1:A:3:THR:HG23	1:A:6:GLN:H	1.80	0.47
1:B:29:PRO:CB	1:B:41:TYR:CD1	2.98	0.47
1:D:15:THR:O	1:D:19:ARG:HG3	2.15	0.47
1:D:153:PHE:CE2	1:D:157:GLU:HA	2.49	0.47
1:B:14:SER:HG	1:B:17:THR:CB	2.20	0.47
1:C:9:ARG:HD3	1:D:225:PHE:CE2	2.50	0.47
1:C:233:LEU:HD21	1:C:267:ILE:HD11	1.96	0.47
1:C:245:ASP:HB3	1:C:268:PRO:HD3	1.97	0.47
1:D:214:HIS:CE1	1:D:215:LYS:C	2.88	0.46
1:A:115:TRP:HH2	1:D:75:ASP:HA	1.79	0.46
1:B:43:PRO:HG2	1:B:44:GLU:CD	2.36	0.46
1:B:49:LEU:C	1:B:51:ARG:H	2.18	0.46
1:C:3:THR:C	1:C:5:GLY:H	2.17	0.46
1:D:132:VAL:HG22	1:D:187:PHE:H	1.20	0.46
1:A:85:GLN:CD	1:A:88:GLN:HG2	2.35	0.46
1:A:87:HIS:C	1:A:89:HIS:N	2.68	0.46
1:B:62:LEU:HA	1:B:65:ILE:HG12	1.97	0.46
1:C:4:ILE:HD12	1:C:4:ILE:N	2.31	0.46
1:C:175:GLN:HB2	1:C:243:GLY:O	2.15	0.46
1:D:86:ARG:HA	1:D:86:ARG:NE	2.31	0.46
1:D:214:HIS:ND1	1:D:214:HIS:C	2.68	0.46
1:A:112:LEU:O	1:A:116:ARG:HB2	2.15	0.46
1:D:67:ARG:O	1:D:71:ASP:CB	2.58	0.46
1:D:217:THR:HG22	1:D:259:PRO:HA	1.98	0.46
1:A:127:ARG:NH2	1:A:188:GLU:OE2	2.49	0.46
1:C:7:LEU:CD2	1:C:18:LEU:CD2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ARG:HA	1:C:101:LEU:HD12	1.98	0.46
1:C:181:PHE:HE2	1:D:15:THR:HG23	1.76	0.46
1:C:206:ALA:C	1:C:207:GLN:CG	2.84	0.46
1:A:164:HIS:CD2	1:A:165:ASP:CG	2.89	0.46
1:C:6:GLN:C	1:C:8:ALA:N	2.69	0.46
1:C:167:GLU:CG	1:C:251:GLN:OE1	2.64	0.46
1:C:249:TYR:HE1	1:C:263:VAL:HG11	1.80	0.46
1:D:183:TYR:O	1:D:184:VAL:HG22	2.16	0.46
1:A:236:ARG:HE	1:A:236:ARG:HB3	1.62	0.46
1:B:121:HIS:ND1	1:B:122:ALA:N	2.63	0.46
1:C:84:LEU:HD12	1:C:84:LEU:HA	1.72	0.46
1:C:95:ILE:CG2	1:C:99:GLN:NE2	2.67	0.46
1:A:15:THR:O	1:A:16:LYS:C	2.53	0.45
1:A:55:LEU:HD22	1:A:55:LEU:HA	1.76	0.45
1:B:148:GLN:C	1:B:152:ARG:HH21	2.15	0.45
1:C:6:GLN:OE1	1:C:6:GLN:HA	2.16	0.45
1:C:153:PHE:O	1:C:153:PHE:CD1	2.70	0.45
1:C:231:HIS:O	1:C:235:GLU:CG	2.62	0.45
1:D:27:PHE:CD1	1:D:27:PHE:O	2.69	0.45
1:D:74:LEU:HD12	1:D:74:LEU:O	2.16	0.45
1:D:193:TRP:HA	1:D:194:PRO:HD3	1.77	0.45
1:C:110:ALA:O	1:C:113:ALA:CB	2.64	0.45
1:D:153:PHE:O	1:D:155:PRO:CA	2.60	0.45
1:A:10:ILE:HA	1:A:11:PHE:HA	1.72	0.45
1:A:214:HIS:NE2	1:A:221:ILE:HG12	2.23	0.45
1:B:251:GLN:C	1:B:253:PHE:H	2.19	0.45
1:C:9:ARG:CG	1:C:10:ILE:H	2.06	0.45
1:D:254:ARG:NH2	1:D:258:ASP:OD2	2.49	0.45
1:A:109:LEU:C	1:A:112:LEU:HD23	2.37	0.45
1:C:55:LEU:C	1:C:57:ARG:H	2.19	0.45
1:D:6:GLN:O	1:D:10:ILE:HG12	2.16	0.45
1:D:69:LYS:HZ1	1:D:70:ARG:NH1	2.14	0.45
1:A:60:VAL:HB	1:A:65:ILE:HD11	1.95	0.45
1:B:95:ILE:O	1:B:99:GLN:HG2	2.16	0.45
1:C:250:ASP:OD2	1:C:252:ARG:NH2	2.50	0.45
1:B:133:VAL:HG12	1:B:201:ARG:HG3	1.99	0.45
1:C:14:SER:HB3	1:C:17:THR:HG23	1.99	0.45
1:C:136:GLU:HB2	1:C:184:VAL:HG22	1.98	0.45
1:C:163:LYS:HD2	1:C:166:PRO:HA	1.98	0.45
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.78	0.45
1:C:160:ILE:HG22	1:C:161:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:PHE:HD1	1:D:130:PHE:H	1.64	0.45
1:D:148:GLN:O	1:D:152:ARG:HD2	2.17	0.45
1:A:42:GLN:CG	1:A:43:PRO:CD	2.85	0.45
1:A:170:TYR:N	1:A:170:TYR:CD2	2.85	0.45
1:D:3:THR:HG22	1:D:6:GLN:HG3	1.89	0.45
1:D:248:TYR:CE2	1:D:250:ASP:HB2	2.52	0.45
1:D:135:MET:HE1	1:D:153:PHE:CD1	2.49	0.45
1:D:149:LEU:C	1:D:151:GLU:H	2.20	0.45
1:A:18:LEU:O	1:A:21:TYR:N	2.50	0.44
1:A:122:ALA:O	1:A:236:ARG:NH2	2.49	0.44
1:C:150:TRP:CH2	1:C:185:ALA:HB1	2.53	0.44
1:C:225:PHE:HB3	1:D:10:ILE:CB	2.47	0.44
1:D:121:HIS:O	1:D:212:PHE:HD1	2.00	0.44
1:D:231:HIS:O	1:D:235:GLU:HG3	2.17	0.44
1:B:67:ARG:NH1	1:B:67:ARG:CG	2.80	0.44
1:D:183:TYR:C	1:D:184:VAL:CG2	2.86	0.44
1:A:98:ARG:HB2	1:D:95:ILE:HD11	2.00	0.44
1:A:110:ALA:C	1:A:112:LEU:H	2.19	0.44
1:B:112:LEU:HD23	1:B:112:LEU:N	2.17	0.44
1:C:51:ARG:O	1:C:54:ALA:HB3	2.17	0.44
1:D:152:ARG:O	1:D:155:PRO:CD	2.65	0.44
1:D:154:ILE:HD12	1:D:154:ILE:H	1.82	0.44
1:A:2:LEU:CD1	1:A:7:LEU:N	2.81	0.44
1:A:71:ASP:N	1:A:72:GLY:CA	2.81	0.44
1:A:214:HIS:O	1:A:262:GLN:HA	2.16	0.44
1:A:11:PHE:HD1	1:B:181:PHE:CE2	2.33	0.44
1:A:178:ASN:N	1:A:179:GLY:HA2	2.24	0.44
1:B:220:GLN:NE2	1:C:81:ARG:HH12	2.14	0.44
1:C:167:GLU:HG2	1:C:251:GLN:CD	2.37	0.44
1:D:212:PHE:CE2	1:D:267:ILE:HD11	2.53	0.44
1:A:6:GLN:C	1:A:8:ALA:N	2.70	0.44
1:A:105:LEU:HD21	1:D:84:LEU:CD2	2.48	0.44
1:B:4:ILE:HG12	1:B:15:THR:HG23	1.98	0.44
1:B:214:HIS:HD2	1:B:215:LYS:H	1.63	0.44
1:C:62:LEU:C	1:C:64:ALA:N	2.70	0.44
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.74	0.44
1:D:54:ALA:HA	1:D:57:ARG:HD2	2.00	0.44
1:A:7:LEU:HD23	1:A:9:ARG:CD	2.48	0.43
1:B:42:GLN:HB3	1:B:45:GLN:HG2	2.00	0.43
1:C:165:ASP:OD2	1:C:167:GLU:HB3	2.19	0.43
1:D:69:LYS:CE	1:D:70:ARG:NH1	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:PHE:HB3	1:D:154:ILE:H	1.51	0.43
1:D:228:ILE:HA	1:D:232:LEU:HD13	2.00	0.43
1:A:41:TYR:HD1	1:A:41:TYR:O	2.00	0.43
1:A:228:ILE:HA	1:A:232:LEU:HB2	1.99	0.43
1:B:18:LEU:HD11	1:B:41:TYR:CE2	2.53	0.43
1:D:3:THR:HG23	1:D:6:GLN:H	1.83	0.43
1:A:42:GLN:NE2	1:A:43:PRO:CD	2.73	0.43
1:A:75:ASP:CB	1:D:115:TRP:CH2	3.01	0.43
1:A:77:PRO:HG3	1:D:115:TRP:CE3	2.53	0.43
1:B:1:MET:SD	1:B:40:TYR:HB3	2.58	0.43
1:B:208:LYS:NZ	1:B:270:TYR:C	2.72	0.43
1:B:268:PRO:O	1:B:269:ILE:HD13	2.19	0.43
1:C:42:GLN:HB3	1:C:44:GLU:HG2	2.00	0.43
1:C:179:GLY:O	1:D:15:THR:HG21	2.18	0.43
1:D:3:THR:HG23	1:D:3:THR:O	2.18	0.43
1:D:65:ILE:C	1:D:67:ARG:N	2.69	0.43
1:A:55:LEU:C	1:A:57:ARG:N	2.69	0.43
1:A:79:ARG:O	1:A:81:ARG:N	2.51	0.43
1:A:247:GLU:OE1	1:A:249:TYR:OH	2.37	0.43
1:C:196:PRO:CG	1:C:199:MET:HE3	2.39	0.43
1:C:228:ILE:C	1:C:230:SER:H	2.21	0.43
1:A:11:PHE:O	1:A:11:PHE:CD1	2.72	0.43
1:A:110:ALA:C	1:A:112:LEU:N	2.72	0.43
1:A:147:GLY:O	1:A:150:TRP:N	2.47	0.43
1:A:217:THR:HB	1:A:257:LEU:HA	2.00	0.43
1:B:89:HIS:HA	1:B:92:ARG:HG3	1.99	0.43
1:D:86:ARG:C	1:D:88:GLN:N	2.72	0.43
1:D:96:SER:O	1:D:100:ARG:HG2	2.19	0.43
1:A:4:ILE:HG13	1:A:5:GLY:N	2.33	0.43
1:C:56:ARG:HD3	1:C:56:ARG:HA	1.91	0.43
1:D:39:ARG:H	1:D:39:ARG:HG3	1.58	0.43
1:A:52:ILE:HG23	1:A:55:LEU:HG	2.00	0.43
1:B:56:ARG:C	1:B:58:LEU:H	2.21	0.43
1:B:116:ARG:HH11	1:B:116:ARG:CG	2.28	0.43
1:B:207:GLN:HE21	1:B:241:LYS:NZ	2.17	0.43
1:C:55:LEU:C	1:C:57:ARG:N	2.72	0.43
1:D:229:TYR:HD1	1:D:233:LEU:HD11	1.84	0.43
1:A:23:ALA:C	1:A:25:GLY:H	2.18	0.42
1:D:3:THR:HG21	1:D:6:GLN:CD	2.38	0.42
1:D:144:ASP:CG	1:D:148:GLN:HB3	2.39	0.42
1:D:241:LYS:HG2	1:D:270:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ILE:C	1:B:230:SER:N	2.72	0.42
1:C:130:PHE:CZ	1:C:204:VAL:CG2	2.99	0.42
1:B:149:LEU:CA	1:B:152:ARG:HD3	2.37	0.42
1:B:172:ILE:HD13	1:B:202:PHE:HD2	1.82	0.42
1:B:245:ASP:O	1:B:246:PHE:HB3	2.19	0.42
1:C:12:GLU:OE2	1:C:12:GLU:CA	2.67	0.42
1:D:254:ARG:HH21	1:D:258:ASP:CG	2.23	0.42
1:A:6:GLN:O	1:A:8:ALA:N	2.51	0.42
1:A:78:GLN:CD	1:D:260:ASN:HA	2.39	0.42
1:A:154:ILE:N	1:A:155:PRO:HD2	2.34	0.42
1:D:105:LEU:C	1:D:107:ARG:N	2.70	0.42
1:D:122:ALA:HB2	1:D:212:PHE:CD1	2.50	0.42
1:A:181:PHE:O	1:A:182:HIS:HB2	2.20	0.42
1:C:64:ALA:C	1:C:66:ASP:N	2.72	0.42
1:D:147:GLY:H	1:D:150:TRP:H	1.67	0.42
1:B:101:LEU:HD13	1:C:58:LEU:HA	2.01	0.42
1:B:151:GLU:C	1:B:153:PHE:N	2.72	0.42
1:D:3:THR:HG21	1:D:6:GLN:CG	2.20	0.42
1:A:22:ASP:CG	1:A:23:ALA:N	2.72	0.42
1:A:71:ASP:H	1:A:72:GLY:CA	2.32	0.42
1:C:134:GLY:O	1:C:199:MET:HA	2.19	0.42
1:C:167:GLU:HG2	1:C:251:GLN:OE1	2.19	0.42
1:A:46:ILE:CG2	1:A:47:GLU:N	2.49	0.42
1:A:61:PRO:HG2	1:A:64:ALA:CB	2.50	0.42
1:B:29:PRO:HD3	1:B:39:ARG:HH22	1.84	0.42
1:B:42:GLN:H	1:B:45:GLN:NE2	2.18	0.42
1:C:157:GLU:O	1:C:163:LYS:NZ	2.53	0.42
1:C:225:PHE:HB3	1:D:10:ILE:CG2	2.49	0.42
1:C:262:GLN:HE21	1:C:262:GLN:HB2	1.58	0.42
1:D:207:GLN:OE1	1:D:209:TYR:CE1	2.70	0.42
1:B:14:SER:OG	1:B:17:THR:HB	2.19	0.42
1:B:48:GLN:O	1:B:48:GLN:CG	2.68	0.42
1:B:90:THR:O	1:B:94:GLU:HG3	2.20	0.42
1:C:206:ALA:O	1:C:207:GLN:HG3	2.20	0.42
1:D:51:ARG:HH21	1:D:75:ASP:CG	1.77	0.42
1:D:112:LEU:HD13	1:D:112:LEU:HA	1.74	0.42
1:A:78:GLN:NE2	1:D:215:LYS:HB3	2.35	0.41
1:B:27:PHE:CE2	1:B:49:LEU:HG	2.55	0.41
1:B:110:ALA:HB3	1:D:110:ALA:HB3	2.01	0.41
1:B:154:ILE:HG13	1:B:154:ILE:H	1.57	0.41
1:B:207:GLN:HG3	1:B:209:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:THR:OG1	1:B:219:PRO:HD2	2.21	0.41
1:C:153:PHE:CD1	1:C:153:PHE:C	2.89	0.41
1:A:117:ILE:HG23	1:A:232:LEU:HD11	2.02	0.41
1:C:160:ILE:H	1:C:160:ILE:HG12	1.66	0.41
1:B:67:ARG:HG2	1:B:67:ARG:O	2.20	0.41
1:D:215:LYS:HE2	1:D:262:GLN:OE1	2.20	0.41
1:D:228:ILE:O	1:D:233:LEU:HG	2.20	0.41
1:D:231:HIS:HD1	1:D:235:GLU:CD	2.23	0.41
1:C:66:ASP:O	1:C:69:LYS:HG2	2.20	0.41
1:A:111:THR:O	1:A:111:THR:CG2	2.69	0.41
1:A:224:SER:O	1:A:228:ILE:HG12	2.20	0.41
1:B:208:LYS:HZ3	1:B:269:ILE:HG22	1.86	0.41
1:D:152:ARG:H	1:D:152:ARG:HG3	1.57	0.41
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.71	0.41
1:D:65:ILE:C	1:D:67:ARG:H	2.23	0.41
1:D:183:TYR:C	1:D:184:VAL:HG23	2.41	0.41
1:B:104:GLU:CD	1:B:107:ARG:HG2	2.41	0.41
1:B:221:ILE:HA	1:B:224:SER:HB2	2.01	0.41
1:B:228:ILE:CG1	1:B:229:TYR:H	2.21	0.41
1:A:75:ASP:HB2	1:D:115:TRP:HZ3	1.81	0.41
1:A:135:MET:HB2	1:A:153:PHE:CD1	2.56	0.41
1:B:84:LEU:O	1:B:88:GLN:N	2.50	0.41
1:C:20:HIS:HD2	1:C:21:TYR:CE1	2.39	0.41
1:D:3:THR:HG21	1:D:6:GLN:NE2	2.27	0.41
1:A:22:ASP:OD1	1:A:23:ALA:N	2.54	0.41
1:A:54:ALA:CB	1:A:57:ARG:CD	2.85	0.41
1:B:29:PRO:CD	1:B:29:PRO:O	2.69	0.41
1:B:49:LEU:O	1:B:50:SER:C	2.57	0.41
1:B:56:ARG:C	1:B:58:LEU:N	2.73	0.41
1:C:71:ASP:N	1:C:72:GLY:HA2	2.22	0.41
1:C:154:ILE:O	1:C:157:GLU:HB2	2.20	0.41
1:C:159:GLU:HG2	1:C:196:PRO:HG3	2.02	0.41
1:D:200:VAL:CG2	1:D:201:ARG:H	2.32	0.41
1:A:119:ASN:HD22	1:A:119:ASN:C	2.09	0.41
1:B:18:LEU:CD1	1:B:41:TYR:CE2	3.04	0.41
1:B:58:LEU:C	1:B:60:VAL:N	2.74	0.41
1:B:145:THR:HG22	1:B:148:GLN:OE1	2.21	0.41
1:B:145:THR:O	1:B:148:GLN:HB2	2.21	0.41
1:B:214:HIS:CE1	1:B:221:ILE:HA	2.56	0.41
1:C:218:ALA:HB3	1:C:219:PRO:HD3	2.02	0.41
1:C:71:ASP:OD1	1:C:72:GLY:CA	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ILE:O	1:D:172:ILE:HG23	2.21	0.40
1:A:2:LEU:HD12	1:A:7:LEU:N	2.36	0.40
1:B:93:GLU:HA	1:B:96:SER:HB2	2.03	0.40
1:D:208:LYS:HB3	1:D:269:ILE:O	2.21	0.40
1:A:9:ARG:H	1:A:9:ARG:HD3	1.84	0.40
1:A:65:ILE:O	1:A:65:ILE:CG2	2.68	0.40
1:B:110:ALA:O	1:B:113:ALA:HB3	2.21	0.40
1:B:197:GLU:HA	1:B:198:GLY:HA2	1.48	0.40
1:B:210:ALA:HB2	1:B:269:ILE:HD11	2.03	0.40
1:C:6:GLN:OE1	1:C:6:GLN:CA	2.68	0.40
1:C:154:ILE:N	1:C:155:PRO:CD	2.85	0.40
1:C:213:THR:CG2	1:C:262:GLN:HE21	2.35	0.40
1:D:156:ARG:HE	1:D:156:ARG:HB3	1.78	0.40
1:B:68:LEU:C	1:B:70:ARG:N	2.74	0.40
1:D:183:TYR:O	1:D:184:VAL:CG2	2.70	0.40

All (7) 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:B:203:GLN:OE1	1:D:38:TYR:O[5_555]	1.36	0.84
1:A:119:ASN:ND2	1:C:164:HIS:CD2[5_445]	1.83	0.37
1:A:158:HIS:ND1	1:B:70:ARG:NH1[5_445]	1.89	0.31
1:B:203:GLN:OE1	1:D:38:TYR:C[5_555]	1.98	0.22
1:A:158:HIS:CB	1:B:70:ARG:NH1[5_445]	2.04	0.16
1:A:119:ASN:ND2	1:C:164:HIS:NE2[5_445]	2.17	0.03
1:A:158:HIS:CG	1:B:70:ARG:NH1[5_445]	2.19	0.01

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	243/291 (84%)	195 (80%)	31 (13%)	17 (7%)	1 3
1	B	246/291 (84%)	203 (82%)	33 (13%)	10 (4%)	3 11
1	C	243/291 (84%)	185 (76%)	44 (18%)	14 (6%)	1 5
1	D	246/291 (84%)	196 (80%)	29 (12%)	21 (8%)	1 2
All	All	978/1164 (84%)	779 (80%)	137 (14%)	62 (6%)	1 4

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	13	ILE
1	A	16	LYS
1	A	23	ALA
1	A	24	ILE
1	A	53	LEU
1	A	57	ARG
1	A	80	LEU
1	A	181	PHE
1	A	182	HIS
1	B	53	LEU
1	B	59	ASP
1	B	66	ASP
1	B	73	ALA
1	B	117	ILE
1	C	6	GLN
1	C	65	ILE
1	C	91	LEU
1	C	92	ARG
1	C	196	PRO
1	C	252	ARG
1	D	65	ILE
1	D	66	ASP
1	D	73	ALA
1	D	87	HIS
1	D	106	ASP
1	D	113	ALA
1	D	153	PHE
1	D	154	ILE
1	D	182	HIS
1	D	262	GLN
1	A	54	ALA
1	B	65	ILE

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Mol	Chain	Res	Type
1	B	229	TYR
1	B	252	ARG
1	C	10	ILE
1	D	114	HIS
1	D	115	TRP
1	D	120	MET
1	D	180	GLU
1	D	196	PRO
1	A	79	ARG
1	A	88	GLN
1	B	52	ILE
1	C	57	ARG
1	C	63	GLU
1	C	64	ALA
1	C	177	PRO
1	C	183	TYR
1	D	26	LEU
1	D	86	ARG
1	D	183	TYR
1	D	213	THR
1	A	15	THR
1	A	46	ILE
1	A	52	ILE
1	A	56	ARG
1	C	12	GLU
1	B	50	SER
1	C	181	PHE
1	D	97	ALA
1	D	184	VAL

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	213/245 (87%)	187 (88%)	26 (12%)	5 15
1	B	217/245 (89%)	197 (91%)	20 (9%)	9 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	213/245 (87%)	183 (86%)	30 (14%)	3 10
1	D	217/245 (89%)	177 (82%)	40 (18%)	1 5
All	All	860/980 (88%)	744 (86%)	116 (14%)	4 11

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	9	ARG
1	A	13	ILE
1	A	16	LYS
1	A	18	LEU
1	A	19	ARG
1	A	26	LEU
1	A	41	TYR
1	A	44	GLU
1	A	46	ILE
1	A	51	ARG
1	A	56	ARG
1	A	76	ASP
1	A	78	GLN
1	A	80	LEU
1	A	83	PHE
1	A	86	ARG
1	A	87	HIS
1	A	112	LEU
1	A	119	ASN
1	A	148	GLN
1	A	152	ARG
1	A	180	GLU
1	A	201	ARG
1	A	225	PHE
1	A	240	PRO
1	B	28	VAL
1	B	29	PRO
1	B	42	GLN
1	B	47	GLU
1	B	49	LEU
1	B	56	ARG
1	B	65	ILE
1	B	106	ASP

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Mol	Chain	Res	Type
1	B	107	ARG
1	B	108	THR
1	B	109	LEU
1	B	116	ARG
1	B	152	ARG
1	B	160	ILE
1	B	211	VAL
1	B	224	SER
1	B	228	ILE
1	B	245	ASP
1	B	247	GLU
1	B	253	PHE
1	C	4	ILE
1	C	7	LEU
1	C	9	ARG
1	C	12	GLU
1	C	14	SER
1	C	56	ARG
1	C	61	PRO
1	C	63	GLU
1	C	67	ARG
1	C	71	ASP
1	C	76	ASP
1	C	107	ARG
1	C	116	ARG
1	C	119	ASN
1	C	120	MET
1	C	133	VAL
1	C	135	MET
1	C	136	GLU
1	C	159	GLU
1	C	163	LYS
1	C	169	SER
1	C	188	GLU
1	C	189	VAL
1	C	199	MET
1	C	230	SER
1	C	235	GLU
1	C	241	LYS
1	C	245	ASP
1	C	251	GLN
1	C	262	GLN

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Mol	Chain	Res	Type
1	D	7	LEU
1	D	9	ARG
1	D	27	PHE
1	D	39	ARG
1	D	50	SER
1	D	56	ARG
1	D	61	PRO
1	D	62	LEU
1	D	63	GLU
1	D	67	ARG
1	D	70	ARG
1	D	71	ASP
1	D	79	ARG
1	D	81	ARG
1	D	88	GLN
1	D	92	ARG
1	D	95	ILE
1	D	96	SER
1	D	99	GLN
1	D	107	ARG
1	D	114	HIS
1	D	116	ARG
1	D	120	MET
1	D	130	PHE
1	D	133	VAL
1	D	150	TRP
1	D	156	ARG
1	D	163	LYS
1	D	172	ILE
1	D	197	GLU
1	D	201	ARG
1	D	203	GLN
1	D	205	PRO
1	D	208	LYS
1	D	211	VAL
1	D	214	HIS
1	D	230	SER
1	D	236	ARG
1	D	238	LEU
1	D	267	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	87	HIS
1	A	114	HIS
1	A	148	GLN
1	A	164	HIS
1	A	207	GLN
1	A	220	GLN
1	A	226	GLN
1	B	45	GLN
1	B	48	GLN
1	B	88	GLN
1	B	207	GLN
1	B	214	HIS
1	B	220	GLN
1	C	20	HIS
1	C	87	HIS
1	C	114	HIS
1	C	158	HIS
1	C	182	HIS
1	C	203	GLN
1	C	262	GLN
1	D	6	GLN
1	D	88	GLN
1	D	114	HIS
1	D	121	HIS
1	D	207	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	249/291 (85%)	0.36	11 (4%)	34	30	25, 55, 113, 169	0
1	B	254/291 (87%)	0.29	8 (3%)	49	44	33, 59, 93, 134	0
1	C	249/291 (85%)	0.31	12 (4%)	30	27	16, 58, 111, 160	0
1	D	254/291 (87%)	0.38	16 (6%)	20	16	39, 70, 104, 135	0
All	All	1006/1164 (86%)	0.33	47 (4%)	31	28	16, 62, 110, 169	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	181	PHE	7.0
1	C	70	ARG	6.5
1	A	44	GLU	5.2
1	C	23	ALA	5.2
1	B	182	HIS	5.1
1	B	186	GLY	4.6
1	C	15	THR	4.3
1	C	19	ARG	3.9
1	C	25	GLY	3.3
1	B	121	HIS	3.3
1	C	146	ILE	3.2
1	D	137	TYR	3.1
1	A	13	ILE	3.0
1	C	3	THR	3.0
1	D	229	TYR	3.0
1	D	100	ARG	2.9
1	A	51	ARG	2.9
1	A	82	HIS	2.9
1	A	115	TRP	2.8
1	C	18	LEU	2.8
1	D	25	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	102	LEU	2.7
1	A	4	ILE	2.7
1	D	135	MET	2.6
1	C	112	LEU	2.6
1	B	64	ALA	2.5
1	D	252	ARG	2.5
1	C	48	GLN	2.5
1	D	170	TYR	2.5
1	D	38	TYR	2.4
1	A	41	TYR	2.4
1	A	71	ASP	2.4
1	D	265	LEU	2.2
1	D	233	LEU	2.2
1	C	4	ILE	2.2
1	A	251	GLN	2.2
1	D	160	ILE	2.2
1	C	181	PHE	2.1
1	B	137	TYR	2.1
1	D	221	ILE	2.1
1	A	25	GLY	2.1
1	B	160	ILE	2.0
1	A	77	PRO	2.0
1	B	256	PRO	2.0
1	D	225	PHE	2.0
1	D	178	ASN	2.0
1	D	77	PRO	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.