



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 05:01 am GMT

PDB ID : 4A51
Title : Crystal structure of human kinesin Eg5 in complex with 1-(3-(((2-Aminoethyl)thio)diphenylmethyl)phenyl)ethanone hydrochloride
Authors : Kaan, H.Y.K.; Kozielski, F.
Deposited on : 2011-10-24
Resolution : 2.75 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

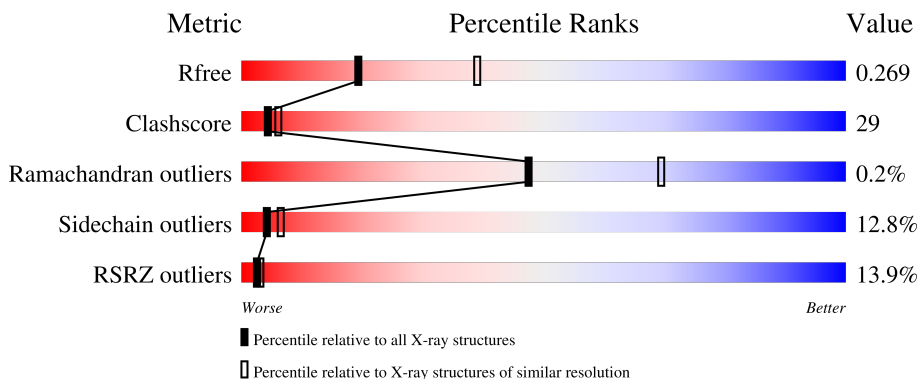
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



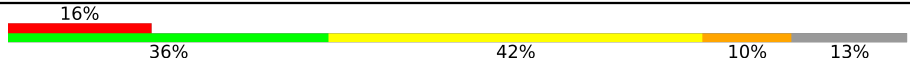
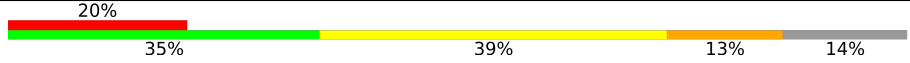
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. 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	368	 10% 50% 33% 12%
1	B	368	 11% 59% 24% 5% 12%
1	C	368	 6% 55% 28% 5% 12%
1	D	368	 7% 57% 29% 5% 12%
1	E	368	 14% 46% 36% 5% 13%

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Mol	Chain	Length	Quality of chain
1	F	368	
1	G	368	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DQ8	E	801	-	-	X	-

2 Entry composition [i](#)

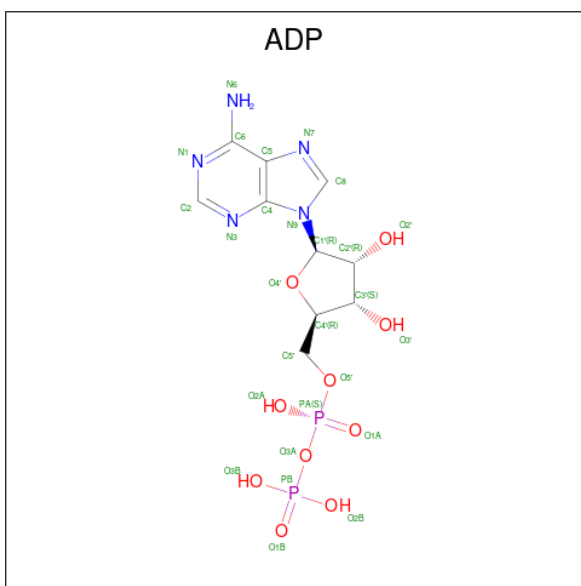
There are 7 unique types of molecules in this entry. The entry contains 18210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	Total 2522	C 1586	N 438	O 488	S 10	0	1	0
1	B	324	Total 2552	C 1602	N 446	O 494	S 10	0	1	0
1	C	325	Total 2551	C 1599	N 445	O 497	S 10	0	1	0
1	D	322	Total 2526	C 1585	N 438	O 493	S 10	0	1	0
1	E	321	Total 2504	C 1573	N 435	O 486	S 10	0	0	0
1	F	319	Total 2487	C 1559	N 433	O 486	S 9	0	1	0
1	G	318	Total 2446	C 1537	N 428	O 472	S 9	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

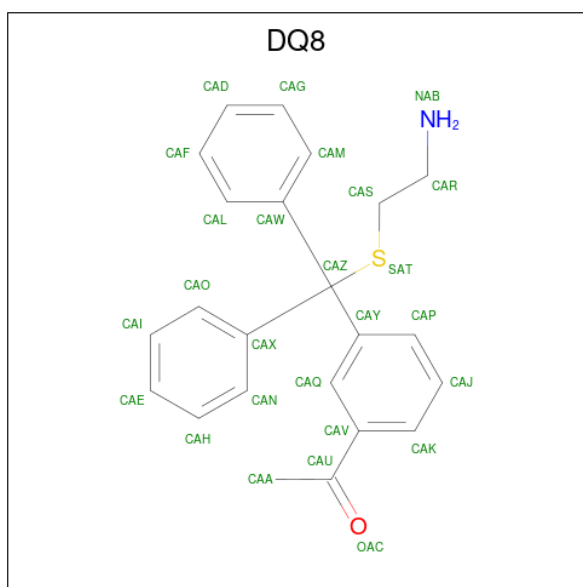


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1-(3-{{(2-aminoethyl)sulfanyl}}(diphenyl)methyl}phenyl)ethanone (three-letter code: DQ8) (formula: C₂₃H₂₃NOS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
4	A	1	26	23	1	1	1	0	0
4	B	1	26	23	1	1	1	0	0
4	C	1	26	23	1	1	1	0	0
4	D	1	26	23	1	1	1	0	0
4	E	1	26	23	1	1	1	0	0
4	F	1	26	23	1	1	1	0	0
4	G	1	26	23	1	1	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

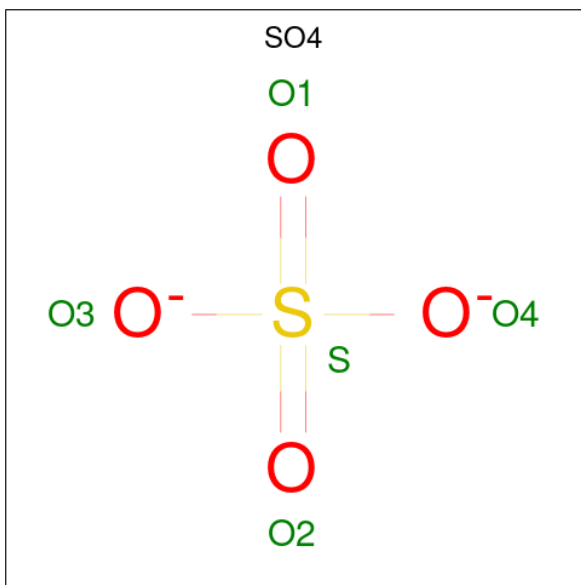
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	B	2	Total	Cl	0	0
			2	2		
5	C	3	Total	Cl	0	0
			3	3		
5	D	2	Total	Cl	0	0
			2	2		
5	E	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total O S 5 4 1	0	0

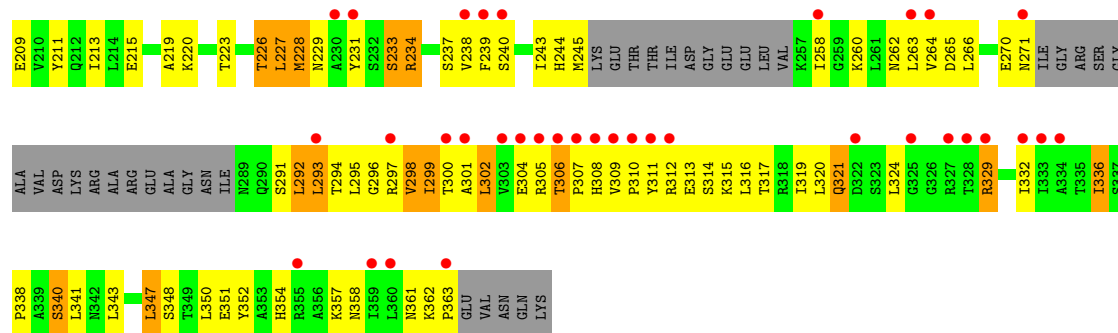
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	32	Total O 32 32	0	0
7	B	34	Total O 34 34	0	0
7	C	47	Total O 47 47	0	0
7	D	46	Total O 46 46	0	0
7	E	22	Total O 22 22	0	0
7	F	25	Total O 25 25	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	19	Total	O	0	0
			19	19		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.84Å 156.40Å 170.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.75 29.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.99-2.75) 97.4 (29.99-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.76Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.280 0.213 , 0.269	Depositor DCC
R_{free} test set	4939 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtrriage
Anisotropy	0.453	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18210	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, CL, SO4, DQ8

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	0.68	0/2563	0.83	0/3467
1	B	0.65	0/2593	0.80	1/3505 (0.0%)
1	C	0.66	0/2589	0.83	1/3503 (0.0%)
1	D	0.67	0/2566	0.80	1/3471 (0.0%)
1	E	0.53	0/2542	0.71	0/3440
1	F	0.54	0/2527	0.78	0/3421
1	G	0.52	0/2483	0.75	2/3364 (0.1%)
All	All	0.61	0/17863	0.79	5/24171 (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	B	0	1
1	C	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ASN	N-CA-C	-6.89	92.40	111.00
1	G	57	LEU	CA-CB-CG	6.63	130.54	115.30
1	D	263	LEU	CA-CB-CG	-5.99	101.53	115.30
1	B	241	VAL	CB-CA-C	-5.68	100.60	111.40
1	G	57	LEU	N-CA-C	5.36	125.47	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	GLU	Peptide
1	C	189	ARG	Peptide
1	F	304	GLU	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	2522	0	2550	138	0
1	B	2552	0	2584	78	0
1	C	2551	0	2563	117	0
1	D	2526	0	2539	88	0
1	E	2504	0	2520	139	0
1	F	2487	0	2494	222	0
1	G	2446	0	2442	232	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	4	0
2	D	27	0	12	5	0
2	E	27	0	12	5	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	26	0	23	7	0
4	B	26	0	23	8	0
4	C	26	0	23	2	0
4	D	26	0	23	4	0
4	E	26	0	23	9	0
4	F	26	0	23	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	26	0	23	7	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	3	0	0	0	0
5	D	2	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	D	5	0	0	0	0
7	A	32	0	0	2	0
7	B	34	0	0	0	0
7	C	47	0	0	2	0
7	D	46	0	0	2	0
7	E	22	0	0	1	0
7	F	25	0	0	1	0
7	G	19	0	0	0	0
All	All	18210	0	17937	1040	0

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 29.

All (1040) 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:E:82:TYR:CE2	1:E:86:VAL:HG21	1.82	1.12
1:F:89:ILE:HD12	1:F:101:ILE:HD11	1.23	1.12
1:A:141:HIS:O	1:A:207:LYS:NZ	1.83	1.11
1:F:136:ILE:HD13	1:F:263:LEU:HD12	1.29	1.09
1:F:171:LEU:HD12	1:F:220:LYS:HB3	1.34	1.09
1:E:215:GLU:HA	4:E:801:DQ8:HAH	1.31	1.08
1:C:206:ASN:ND2	1:C:208:ASP:HB2	1.69	1.06
1:G:181:ARG:HG2	1:G:181:ARG:HH11	1.15	1.05
2:F:601:ADP:H5'1	2:F:601:ADP:H8	1.19	1.05
2:D:601:ADP:H5'1	2:D:601:ADP:H8	1.19	1.05
1:E:92:GLU:OE1	1:E:92:GLU:N	1.88	1.04
1:F:86:VAL:HA	1:F:89:ILE:HD13	1.42	1.02
1:F:89:ILE:CD1	1:F:101:ILE:HD11	1.92	1.00
1:A:144:PHE:CD2	1:A:207:LYS:HD2	1.97	1.00
1:A:145:GLU:H	1:A:207:LYS:HZ3	1.03	0.99
1:D:31:ALA:O	1:D:34:LYS:HG3	1.62	0.98
1:A:192:ARG:NH1	1:A:322:ASP:OD1	1.96	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:TYR:CE1	1:G:86:VAL:HG21	1.98	0.98
1:D:255:LEU:HD12	1:D:256:VAL:H	1.26	0.97
1:A:144:PHE:HD2	1:A:207:LYS:HD2	1.28	0.97
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.46	0.96
1:E:306:THR:HG22	1:E:307:PRO:HD2	1.45	0.96
1:G:160:LEU:H	1:G:172:LEU:HD12	1.30	0.96
1:G:155:SER:OG	1:G:244:HIS:HB2	1.66	0.95
1:F:306:THR:HG22	1:F:307:PRO:HD2	1.50	0.94
1:C:306:THR:HG23	1:C:307:PRO:HD2	1.47	0.93
1:G:40:ILE:CD1	1:G:340:SER:HA	1.98	0.92
1:A:51:SER:HB2	1:A:65:THR:OG1	1.68	0.92
2:D:601:ADP:H5'1	2:D:601:ADP:C8	2.03	0.92
2:F:601:ADP:H5'1	2:F:601:ADP:C8	2.04	0.92
1:C:33:ARG:HD2	1:G:228:MET:HE1	1.50	0.91
1:A:306:THR:OG1	1:A:307:PRO:HD2	1.70	0.91
1:G:196:ILE:HD11	1:G:199:LEU:HB2	1.51	0.90
1:G:205:HIS:O	1:G:206:ASN:ND2	2.04	0.89
1:A:63:ARG:HH11	1:A:63:ARG:CG	1.86	0.89
1:A:264:VAL:HG21	1:A:320:LEU:HD11	1.56	0.87
1:D:102:PHE:CE1	1:D:320:LEU:HD13	2.09	0.87
1:G:56:GLY:C	1:G:58:ALA:HB3	1.92	0.87
1:G:181:ARG:HH11	1:G:181:ARG:CG	1.88	0.86
1:C:126:THR:HG23	1:C:129:GLU:HG2	1.57	0.86
1:B:162:GLU:OE1	1:B:231:TYR:OH	1.94	0.86
1:F:135:ILE:HG22	1:F:263:LEU:HD13	1.56	0.86
1:F:136:ILE:HD12	1:F:239:PHE:CD2	2.11	0.85
1:G:262:ASN:HD22	1:G:320:LEU:HD22	1.42	0.84
1:D:152:THR:OG1	1:D:246:LYS:O	1.95	0.84
1:E:215:GLU:CA	4:E:801:DQ8:HAH	2.08	0.84
1:F:215:GLU:HA	4:F:801:DQ8:HAH	1.58	0.84
1:F:94:ILE:HD11	1:F:147:LEU:HD21	1.60	0.84
1:E:82:TYR:CZ	1:E:86:VAL:HG21	2.13	0.83
1:F:230:ALA:HB3	1:F:234:ARG:HD2	1.61	0.83
1:F:82:TYR:O	1:F:86:VAL:HG13	1.78	0.83
1:F:172:LEU:HD23	1:F:216:LYS:HZ1	1.45	0.82
1:A:63:ARG:HH11	1:A:63:ARG:HG2	1.44	0.82
1:F:156:VAL:HG13	1:F:204:VAL:HG13	1.61	0.82
2:C:601:ADP:H5'1	2:C:601:ADP:H8	1.44	0.82
1:A:144:PHE:HE1	1:A:156:VAL:HG11	1.45	0.81
1:F:323:SER:O	1:F:330:THR:OG1	1.98	0.81
1:C:356:ALA:O	1:C:359:ILE:HG12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:244:HIS:HA	1:G:258:ILE:HG23	1.61	0.81
1:A:102:PHE:HB3	1:A:264:VAL:HB	1.60	0.81
1:F:158:VAL:HG21	1:F:213:ILE:HD11	1.63	0.81
1:C:206:ASN:HD22	1:C:208:ASP:HB2	1.45	0.81
1:D:87:CYS:HB2	1:D:88:PRO:HD3	1.63	0.80
1:F:136:ILE:HD13	1:F:263:LEU:CD1	2.11	0.80
1:D:299:ILE:HG23	1:D:359:ILE:HD11	1.63	0.80
1:F:158:VAL:HB	1:F:239:PHE:HE1	1.46	0.80
1:E:102:PHE:HB3	1:E:264:VAL:HB	1.62	0.80
1:F:170:ASP:HB2	1:F:182:LEU:HD11	1.64	0.80
1:B:160:LEU:HD13	1:B:239:PHE:HD2	1.46	0.80
1:E:300:THR:HG23	1:E:355:ARG:HH12	1.48	0.79
1:F:115:MET:O	1:F:136:ILE:HG12	1.81	0.79
1:F:322:ASP:O	1:F:328:THR:HG22	1.82	0.79
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.65	0.79
1:E:43:CYS:HB3	1:E:71:VAL:CG1	2.13	0.79
1:E:90:LEU:HD11	1:E:143:ILE:HD11	1.63	0.79
1:E:161:LEU:HD12	1:E:161:LEU:C	2.02	0.79
1:D:255:LEU:HD12	1:D:256:VAL:N	1.98	0.79
1:G:181:ARG:HG2	1:G:181:ARG:NH1	1.91	0.79
1:B:355:ARG:HB2	1:B:355:ARG:NH1	1.97	0.78
1:F:136:ILE:HB	1:F:137:PRO:HD3	1.63	0.78
1:G:82:TYR:CD1	1:G:86:VAL:HG21	2.18	0.78
1:F:86:VAL:HA	1:F:89:ILE:CD1	2.13	0.77
1:F:98:ASN:O	1:F:328:THR:OG1	1.99	0.77
1:G:262:ASN:HD22	1:G:320:LEU:CD2	1.97	0.77
1:E:306:THR:CG2	1:E:307:PRO:HD2	2.14	0.77
1:G:40:ILE:HD11	1:G:340:SER:HA	1.66	0.77
1:G:228:MET:HA	1:G:228:MET:HE2	1.64	0.77
1:G:347:LEU:HD12	1:G:348:SER:H	1.50	0.77
1:D:88:PRO:O	1:D:92:GLU:HG3	1.84	0.77
1:G:244:HIS:O	1:G:245:MET:HG3	1.85	0.77
1:E:86:VAL:CG2	1:E:87:CYS:N	2.48	0.77
1:G:156:VAL:HG12	1:G:204:VAL:O	1.85	0.76
1:G:312:ARG:O	1:G:313:GLU:HG2	1.84	0.76
1:C:119:ARG:HD3	1:C:211:TYR:OH	1.85	0.76
1:F:90:LEU:HD11	1:F:143:ILE:CD1	2.15	0.76
1:G:196:ILE:CD1	1:G:199:LEU:HB2	2.15	0.76
1:D:64:LYS:HE2	1:D:66:TYR:OH	1.86	0.76
1:F:49:GLU:HG2	1:F:67:THR:HG22	1.68	0.76
1:D:190:ASN:OD1	1:D:192:ARG:N	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:VAL:HG23	1:E:204:VAL:HB	1.68	0.75
1:G:311:TYR:CG	1:G:321:GLN:HG3	2.21	0.75
1:F:100:THR:HG22	1:F:262:ASN:HB2	1.66	0.75
1:E:218:ALA:O	1:E:222:THR:HG23	1.87	0.75
2:C:601:ADP:H5'1	2:C:601:ADP:C8	2.20	0.75
1:B:247:GLU:N	1:B:247:GLU:OE1	2.20	0.75
1:D:102:PHE:CZ	1:D:320:LEU:HD13	2.20	0.75
1:D:120:SER:HB3	1:D:121:PRO:HD2	1.67	0.75
1:F:270:GLU:HG2	1:F:271:ASN:OD1	1.86	0.75
1:G:41:VAL:CG1	1:G:338:PRO:HA	2.15	0.75
1:G:184:MET:SD	1:G:194:VAL:HG11	2.27	0.75
1:F:43:CYS:HB3	1:F:71:VAL:CG1	2.18	0.74
1:G:177:ASP:H	1:G:180:GLU:HG3	1.50	0.74
1:F:306:THR:CG2	1:F:307:PRO:HD2	2.17	0.74
1:B:178:VAL:HG13	1:B:220:LYS:HG2	1.69	0.74
1:G:90:LEU:HD11	1:G:143:ILE:HD11	1.70	0.74
1:A:66:TYR:HE2	1:A:351:GLU:OE1	1.70	0.74
1:B:355:ARG:HB2	1:B:355:ARG:HH11	1.52	0.74
1:C:207:LYS:NZ	1:G:123:GLU:HG2	2.03	0.74
1:F:323:SER:HA	1:F:328:THR:CG2	2.17	0.74
1:A:54:THR:HG21	1:A:64:LYS:HG3	1.70	0.74
5:D:1363:CL:CL	7:D:2037:HOH:O	2.43	0.74
1:B:92:GLU:OE2	1:B:329:ARG:NH1	2.20	0.74
1:G:56:GLY:O	1:G:58:ALA:HB3	1.88	0.73
1:G:312:ARG:HG2	1:G:313:GLU:H	1.52	0.73
1:A:255:LEU:HD12	1:A:256:VAL:N	2.04	0.73
1:G:170:ASP:OD2	1:G:200:GLU:HB2	1.88	0.73
1:F:19:ILE:HG23	1:F:359:ILE:O	1.89	0.73
1:G:162:GLU:HG3	1:G:171:LEU:HD13	1.70	0.73
1:G:347:LEU:HD12	1:G:348:SER:N	2.04	0.73
1:A:152:THR:HG22	1:A:153:GLU:H	1.54	0.72
1:D:26:ARG:HG3	1:D:26:ARG:HH11	1.55	0.72
1:G:104:TYR:HB2	1:G:266:LEU:HD12	1.71	0.72
1:G:26:ARG:NH1	1:G:29:ASN:HD22	1.87	0.72
1:A:294:THR:HG22	1:A:317:THR:HG21	1.71	0.72
1:A:142:GLN:OE1	1:A:146:LYS:NZ	2.22	0.72
1:A:99:CYS:O	1:A:261:LEU:HD12	1.90	0.72
1:D:247:GLU:HG3	1:D:255:LEU:O	1.90	0.72
1:E:299:ILE:O	1:E:303:VAL:HG23	1.89	0.72
1:F:148:THR:O	1:F:151:GLY:N	2.21	0.71
1:G:270:GLU:HG2	1:G:271:ASN:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HD12	1:A:256:VAL:H	1.53	0.71
1:B:102:PHE:CE1	1:B:332:ILE:HG12	2.26	0.71
1:F:78:GLN:HG2	1:F:133:ALA:O	1.89	0.71
1:F:310:PRO:HB3	1:F:313:GLU:OE2	1.90	0.71
1:B:178:VAL:CG1	1:B:220:LYS:HG2	2.20	0.71
1:C:186:ASP:OD1	7:C:2030:HOH:O	2.08	0.71
1:G:270:GLU:OE1	1:G:270:GLU:N	2.22	0.71
1:C:186:ASP:OD2	1:C:312:ARG:NH2	2.23	0.71
1:A:144:PHE:CE1	1:A:156:VAL:HG11	2.25	0.71
1:D:54:THR:HG21	1:D:64:LYS:HG3	1.73	0.71
1:B:247:GLU:OE1	1:B:255:LEU:O	2.09	0.71
1:F:90:LEU:HD11	1:F:143:ILE:HD13	1.70	0.71
1:F:157:LYS:HG3	1:F:242:THR:HG23	1.73	0.71
1:C:126:THR:OG1	1:C:128:GLU:OE1	2.09	0.70
1:E:92:GLU:O	1:E:97:TYR:HB2	1.91	0.70
1:B:160:LEU:HD13	1:B:239:PHE:CD2	2.25	0.70
1:F:323:SER:HA	1:F:328:THR:HG23	1.72	0.70
2:D:601:ADP:H8	2:D:601:ADP:C5'	2.00	0.70
1:F:103:ALA:HB1	1:F:111:LYS:HG2	1.74	0.70
1:C:270:GLU:HG2	1:C:271:ASN:N	2.07	0.70
1:D:163:ILE:HG12	1:D:168:LEU:HD12	1.72	0.70
2:C:601:ADP:H8	2:C:601:ADP:C5'	2.04	0.70
1:F:90:LEU:O	1:F:93:VAL:HG13	1.92	0.69
1:B:18:ASN:OD1	1:B:18:ASN:N	2.25	0.69
1:E:139:THR:O	1:E:143:ILE:HG12	1.92	0.69
1:F:136:ILE:CD1	1:F:263:LEU:HD12	2.17	0.69
1:G:362:LYS:HB3	1:G:363:PRO:HD2	1.73	0.69
1:G:152:THR:OG1	1:G:153:GLU:N	2.24	0.69
1:E:82:TYR:HA	1:E:86:VAL:HG13	1.74	0.69
1:F:90:LEU:O	1:F:90:LEU:HD12	1.92	0.69
1:A:141:HIS:O	1:A:207:LYS:CE	2.40	0.69
1:F:98:ASN:OD1	1:F:260:LYS:HB3	1.92	0.69
1:C:87:CYS:HB2	1:C:88:PRO:HD3	1.74	0.69
1:C:302:LEU:HB3	1:C:359:ILE:HG22	1.75	0.69
1:E:170:ASP:CG	1:E:173:ASN:HB2	2.13	0.69
1:G:147:LEU:HD21	1:G:245:MET:HE1	1.73	0.69
1:G:192:ARG:O	1:G:321:GLN:NE2	2.25	0.68
1:A:59:ASP:C	1:A:59:ASP:OD1	2.30	0.68
1:D:247:GLU:OE1	1:D:255:LEU:HB3	1.93	0.68
1:E:161:LEU:HD12	1:E:161:LEU:O	1.93	0.68
1:F:244:HIS:CD2	1:F:258:ILE:HG22	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:PHE:CE2	1:F:207:LYS:N	2.62	0.68
1:C:361:ASN:O	1:C:363:PRO:HD3	1.93	0.68
1:F:82:TYR:HA	1:F:86:VAL:CG1	2.24	0.68
1:C:362:LYS:H	1:C:362:LYS:HD3	1.59	0.68
1:C:362:LYS:HD3	1:C:362:LYS:N	2.08	0.68
1:F:238:VAL:O	1:F:238:VAL:HG22	1.94	0.68
4:B:801:DQ8:HAO	4:B:801:DQ8:HAS2	1.75	0.67
1:E:86:VAL:HG22	1:E:87:CYS:N	2.09	0.67
2:E:601:ADP:C5'	2:E:601:ADP:H8	2.07	0.67
1:G:134:GLY:O	1:G:137:PRO:HD2	1.94	0.67
1:G:315:LYS:O	1:G:319:ILE:HD12	1.94	0.67
1:A:330:THR:HG22	1:A:331:SER:N	2.08	0.67
1:B:361:ASN:O	1:B:363:PRO:HD3	1.94	0.67
1:D:30:LEU:HD12	1:D:33:ARG:NH2	2.09	0.67
1:G:105:GLY:O	1:G:111:LYS:HE3	1.94	0.67
1:G:160:LEU:N	1:G:172:LEU:HD12	2.08	0.67
1:C:306:THR:CG2	1:C:307:PRO:HD2	2.20	0.67
1:F:141:HIS:C	1:F:141:HIS:HD1	1.97	0.67
1:G:111:LYS:NZ	2:G:601:ADP:O2B	2.28	0.67
1:G:161:LEU:C	1:G:161:LEU:HD12	2.15	0.67
1:G:295:LEU:O	1:G:298:VAL:HG12	1.95	0.67
1:E:82:TYR:CZ	1:E:86:VAL:CG2	2.78	0.67
1:E:147:LEU:HD21	1:E:245:MET:SD	2.34	0.67
1:G:111:LYS:NZ	1:G:111:LYS:HB2	2.10	0.67
1:A:62:SER:O	1:A:63:ARG:HG2	1.94	0.67
1:D:311:TYR:CD1	1:D:321:GLN:HG3	2.29	0.67
1:E:246:LYS:HA	1:E:256:VAL:HA	1.77	0.67
1:A:66:TYR:CE2	1:A:351:GLU:OE1	2.48	0.66
1:C:29:ASN:O	1:C:33:ARG:HG3	1.95	0.66
1:G:40:ILE:O	1:G:40:ILE:HG22	1.95	0.66
1:A:82:TYR:CD1	1:A:86:VAL:HB	2.30	0.66
1:C:54:THR:HG21	1:C:64:LYS:HG3	1.75	0.66
1:F:211:TYR:O	1:F:211:TYR:CD1	2.48	0.66
4:B:801:DQ8:HAS2	4:B:801:DQ8:CAO	2.26	0.66
1:B:157:LYS:NZ	1:B:201:GLU:OE1	2.18	0.66
1:G:298:VAL:HG23	1:G:310:PRO:HB3	1.77	0.66
1:C:360:LEU:HD12	1:C:360:LEU:H	1.61	0.66
1:E:82:TYR:O	1:E:86:VAL:HG13	1.95	0.66
1:E:298:VAL:HG22	1:E:309:VAL:HG12	1.78	0.66
1:A:327:ARG:O	1:A:363:PRO:HA	1.95	0.66
1:E:106:GLN:OE1	1:E:345:GLU:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HA	1:A:244:HIS:O	1.96	0.65
1:E:28:PHE:CE1	1:E:338:PRO:HG2	2.31	0.65
1:F:162:GLU:OE2	1:F:237:SER:HB3	1.97	0.65
1:G:57:LEU:N	1:G:58:ALA:O	2.30	0.65
1:C:62:SER:O	1:C:63:ARG:HD2	1.95	0.65
1:F:102:PHE:HB3	1:F:264:VAL:CG1	2.26	0.65
1:C:19:ILE:CD1	1:C:359:ILE:HG13	2.25	0.65
1:F:124:GLU:HG2	1:F:125:TYR:CE1	2.31	0.65
1:B:102:PHE:HE1	1:B:332:ILE:CD1	2.09	0.65
1:G:209:GLU:O	1:G:213:ILE:HD13	1.97	0.65
1:A:98:ASN:O	1:A:328:THR:HG22	1.96	0.64
1:D:311:TYR:CG	1:D:321:GLN:HG3	2.32	0.64
2:E:601:ADP:C8	2:E:601:ADP:H5'1	2.32	0.64
1:D:196:ILE:HD11	1:D:319:ILE:HD11	1.80	0.64
2:E:601:ADP:H8	2:E:601:ADP:H5'1	1.62	0.64
1:F:86:VAL:O	1:F:89:ILE:HG12	1.97	0.64
1:G:317:THR:O	1:G:321:GLN:N	2.30	0.64
1:G:43:CYS:O	1:G:45:PRO:HD3	1.98	0.64
1:G:92:GLU:HG3	1:G:329:ARG:HD2	1.80	0.64
1:B:192:ARG:HB2	1:B:321:GLN:CD	2.17	0.64
1:F:68:PHE:HA	1:F:357:LYS:NZ	2.13	0.64
1:F:136:ILE:HD12	1:F:239:PHE:HD2	1.62	0.64
1:A:100:THR:OG1	1:A:323:SER:OG	2.10	0.64
1:E:43:CYS:HB3	1:E:71:VAL:HG11	1.80	0.64
1:A:306:THR:OG1	1:A:307:PRO:CD	2.46	0.64
1:B:69:ASP:O	1:B:70:MET:HG3	1.97	0.64
1:E:143:ILE:HD12	1:E:243:ILE:HD11	1.80	0.63
1:F:82:TYR:CD2	1:F:86:VAL:HG11	2.33	0.63
1:F:136:ILE:O	1:F:139:THR:HG22	1.97	0.63
1:F:162:GLU:HG3	1:F:171:LEU:CD2	2.28	0.63
1:G:161:LEU:HD12	1:G:162:GLU:N	2.13	0.63
1:G:270:GLU:HG2	1:G:271:ASN:N	2.11	0.63
1:B:87:CYS:HB2	1:B:88:PRO:HD3	1.80	0.63
1:F:102:PHE:HB3	1:F:264:VAL:HG12	1.79	0.63
1:F:161:LEU:C	1:F:161:LEU:HD12	2.19	0.63
1:E:86:VAL:HG22	1:E:87:CYS:H	1.61	0.63
4:E:801:DQ8:HAS1	4:E:801:DQ8:CAQ	2.28	0.63
1:C:178:VAL:HG13	1:C:220:LYS:HG3	1.81	0.63
1:F:82:TYR:CD2	1:F:138:ARG:HB2	2.34	0.63
1:D:306:THR:HG23	1:D:307:PRO:HD2	1.80	0.63
1:G:53:ARG:NH2	1:G:57:LEU:HA	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:PHE:CE1	1:G:332:ILE:HG12	2.34	0.63
1:F:28:PHE:CE1	1:F:338:PRO:HG2	2.34	0.63
4:F:801:DQ8:CAL	4:F:801:DQ8:HAP	2.28	0.63
1:A:178:VAL:CG1	1:A:220:LYS:HG2	2.29	0.63
1:G:228:MET:O	1:G:229:ASN:CG	2.36	0.63
1:E:143:ILE:HD12	1:E:243:ILE:CD1	2.29	0.62
1:G:82:TYR:CE1	1:G:86:VAL:CG2	2.80	0.62
1:C:262:ASN:O	1:C:263:LEU:HD23	1.99	0.62
4:C:801:DQ8:CAQ	4:C:801:DQ8:HAS1	2.30	0.62
1:D:190:ASN:OD1	1:D:191:LYS:N	2.32	0.62
1:E:156:VAL:HG12	1:E:243:ILE:HG12	1.79	0.62
1:B:352:TYR:HA	1:B:355:ARG:NH1	2.15	0.62
1:E:168:LEU:HD21	1:E:315:LYS:HD2	1.81	0.62
1:F:20:GLN:NE2	1:F:85:VAL:HG23	2.14	0.62
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.33	0.62
1:C:365:VAL:O	1:C:366:ASN:HB2	1.98	0.62
1:D:306:THR:CG2	1:D:307:PRO:HD2	2.30	0.62
1:E:82:TYR:HA	1:E:86:VAL:CG1	2.29	0.62
1:E:120:SER:OG	1:E:132:LEU:HD23	1.99	0.62
1:E:154:PHE:O	1:E:154:PHE:CD1	2.52	0.62
1:G:306:THR:HG22	1:G:307:PRO:HD2	1.80	0.62
1:A:178:VAL:HG13	1:A:220:LYS:CG	2.30	0.62
1:F:172:LEU:HD23	1:F:216:LYS:NZ	2.14	0.62
1:G:175:SER:O	1:G:176:SER:HB2	2.00	0.62
1:A:209:GLU:O	1:A:213:ILE:HG13	2.00	0.61
1:C:42:GLU:HA	1:C:42:GLU:OE1	2.00	0.61
1:F:306:THR:CB	1:F:307:PRO:HD2	2.28	0.61
1:C:206:ASN:N	1:C:206:ASN:OD1	2.33	0.61
1:F:18:ASN:OD1	1:F:360:LEU:HB3	1.99	0.61
1:F:158:VAL:HB	1:F:239:PHE:CE1	2.31	0.61
1:G:170:ASP:CG	1:G:173:ASN:HB2	2.21	0.61
1:A:145:GLU:N	1:A:207:LYS:HZ3	1.87	0.61
1:C:129:GLU:OE1	1:G:211:TYR:OH	2.16	0.61
1:E:54:THR:HG21	1:E:64:LYS:HD2	1.83	0.61
1:E:270:GLU:O	1:E:271:ASN:HB2	1.99	0.61
1:G:44:ASP:OD1	1:G:47:ARG:HB3	2.01	0.61
1:D:22:VAL:CG1	1:D:70:MET:HB2	2.30	0.61
1:G:21:VAL:CG1	1:G:357:LYS:HB3	2.30	0.61
1:C:27:PRO:HG2	1:G:227:LEU:HD21	1.81	0.61
1:D:143:ILE:HD13	1:D:243:ILE:HD11	1.81	0.61
1:E:309:VAL:HB	1:E:311:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HG12	1:A:263:LEU:HD12	1.83	0.61
1:F:184:MET:SD	1:F:318:ARG:HD3	2.41	0.61
2:D:601:ADP:C8	2:D:601:ADP:C5'	2.81	0.60
1:E:119:ARG:HD3	1:E:211:TYR:HE1	1.65	0.60
1:E:119:ARG:HG2	4:E:801:DQ8:HAO	1.82	0.60
1:F:204:VAL:HG21	1:F:210:VAL:HG23	1.83	0.60
1:A:308:HIS:ND1	7:A:2026:HOH:O	2.32	0.60
4:A:801:DQ8:CAQ	4:A:801:DQ8:HAS1	2.31	0.60
4:B:801:DQ8:HAO	4:B:801:DQ8:CAS	2.29	0.60
1:D:22:VAL:HG12	1:D:70:MET:HB2	1.83	0.60
1:A:189:ARG:O	1:A:190:ASN:HB2	2.01	0.60
1:E:90:LEU:HD11	1:E:143:ILE:CD1	2.30	0.60
1:F:29:ASN:OD1	1:F:32:GLU:HB2	2.02	0.60
1:G:53:ARG:HH21	1:G:57:LEU:HA	1.67	0.60
1:G:139:THR:O	1:G:143:ILE:HG12	2.01	0.60
1:B:130:ASP:OD1	1:B:131:PRO:HD2	2.01	0.60
1:C:25:CYS:O	1:C:74:ALA:HA	2.01	0.60
1:C:207:LYS:HZ1	1:G:123:GLU:HG2	1.66	0.60
1:F:132:LEU:HD12	1:F:132:LEU:O	2.01	0.60
1:G:362:LYS:CB	1:G:363:PRO:HD2	2.31	0.60
2:E:601:ADP:C5'	2:E:601:ADP:C8	2.84	0.60
1:F:100:THR:HG22	1:F:262:ASN:CB	2.31	0.60
1:E:328:THR:O	1:E:361:ASN:ND2	2.35	0.60
1:F:100:THR:CG2	1:F:262:ASN:HB2	2.32	0.60
1:F:162:GLU:HG3	1:F:171:LEU:HD23	1.82	0.60
1:E:40:ILE:HD12	1:E:343:LEU:HD13	1.84	0.60
1:E:82:TYR:CD2	1:E:86:VAL:HG21	2.35	0.60
1:F:43:CYS:HB3	1:F:71:VAL:HG12	1.82	0.60
1:G:196:ILE:HD11	1:G:199:LEU:CB	2.29	0.60
1:C:245:MET:HE3	1:C:257:LYS:HE3	1.84	0.60
1:E:136:ILE:HG12	1:E:263:LEU:HD12	1.84	0.60
1:F:18:ASN:HA	1:F:360:LEU:CB	2.31	0.60
1:G:196:ILE:CG1	1:G:199:LEU:HB2	2.32	0.60
1:G:47:ARG:O	1:G:47:ARG:HG3	2.00	0.59
1:C:293:LEU:HD21	1:C:297:ARG:NH2	2.17	0.59
1:G:26:ARG:NH1	1:G:29:ASN:ND2	2.49	0.59
1:E:92:GLU:H	1:E:92:GLU:CD	1.98	0.59
1:E:309:VAL:HG12	1:E:310:PRO:HD2	1.85	0.59
1:A:202:ILE:HG21	1:A:213:ILE:HD13	1.85	0.59
1:C:161:LEU:HD12	1:C:161:LEU:C	2.22	0.59
1:F:216:LYS:HZ3	1:F:217:GLY:N	1.98	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:GLN:O	1:G:81:VAL:HG23	2.02	0.59
1:A:141:HIS:ND1	1:A:141:HIS:C	2.55	0.59
1:B:89:ILE:HD13	1:B:101:ILE:HD11	1.85	0.59
1:E:120:SER:HB3	1:E:121:PRO:HD2	1.84	0.59
1:F:140:LEU:O	1:F:143:ILE:HG22	2.02	0.59
1:B:129:GLU:HA	1:B:129:GLU:OE1	2.03	0.59
1:B:154:PHE:HA	1:B:244:HIS:O	2.03	0.59
1:F:311:TYR:CD1	1:F:321:GLN:HG3	2.38	0.59
1:G:233:SER:OG	1:G:234:ARG:HD2	2.03	0.59
1:C:238:VAL:HG22	1:C:264:VAL:HG22	1.83	0.59
1:B:126:THR:HG23	1:B:129:GLU:HB2	1.84	0.59
1:C:75:SER:O	1:C:77:LYS:HD2	2.03	0.59
1:E:244:HIS:ND1	1:E:258:ILE:HG23	2.18	0.59
1:F:150:ASN:O	1:F:152:THR:HG23	2.03	0.59
1:G:314:SER:OG	1:G:317:THR:OG1	2.13	0.59
1:B:168:LEU:HD12	1:B:168:LEU:N	2.17	0.58
1:C:72:PHE:CD1	1:C:76:THR:HG21	2.38	0.58
1:F:128:GLU:O	1:F:129:GLU:OE2	2.21	0.58
1:G:296:GLY:O	1:G:300:THR:HG23	2.03	0.58
1:G:311:TYR:CD1	1:G:321:GLN:HG3	2.38	0.58
1:F:18:ASN:HA	1:F:360:LEU:HB3	1.84	0.58
1:B:111:LYS:HB2	1:B:111:LYS:NZ	2.19	0.58
1:F:141:HIS:C	1:F:141:HIS:ND1	2.56	0.58
1:G:116:GLU:HG2	4:G:801:DQ8:CAK	2.34	0.58
1:D:102:PHE:CE1	1:D:320:LEU:CD1	2.86	0.58
1:E:187:ASP:HB2	1:E:195:ILE:HG23	1.85	0.58
1:G:312:ARG:HG2	1:G:313:GLU:N	2.17	0.58
1:C:118:GLU:OE1	1:G:226:THR:CG2	2.51	0.58
1:E:288:ILE:N	7:E:2015:HOH:O	2.36	0.58
1:A:63:ARG:HH11	1:A:63:ARG:HG3	1.68	0.58
1:A:145:GLU:H	1:A:207:LYS:NZ	1.88	0.58
1:F:238:VAL:O	1:F:238:VAL:CG2	2.51	0.58
1:G:29:ASN:OD1	1:G:31:ALA:HB3	2.03	0.58
1:G:147:LEU:HD21	1:G:245:MET:CE	2.34	0.58
1:F:89:ILE:HG12	1:F:90:LEU:N	2.18	0.58
1:E:91:ASP:O	1:E:94:ILE:HB	2.04	0.57
1:F:102:PHE:CE1	1:F:332:ILE:HG12	2.39	0.57
1:E:154:PHE:HA	1:E:244:HIS:O	2.05	0.57
1:B:102:PHE:HE1	1:B:332:ILE:HD11	1.69	0.57
1:G:111:LYS:HB2	2:G:601:ADP:O2B	2.03	0.57
1:C:88:PRO:O	1:C:92:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:SER:OG	1:E:130:ASP:OD1	2.22	0.57
1:F:244:HIS:NE2	1:F:258:ILE:HG22	2.20	0.57
1:G:168:LEU:HD13	1:G:168:LEU:N	2.19	0.57
1:F:110:GLY:HA2	2:F:601:ADP:O2A	2.05	0.57
1:F:141:HIS:ND1	1:F:141:HIS:O	2.37	0.57
1:G:91:ASP:O	1:G:94:ILE:HG22	2.03	0.57
1:A:178:VAL:HG13	1:A:220:LYS:HG2	1.86	0.57
1:B:207:LYS:HD2	1:B:207:LYS:O	2.04	0.57
1:E:143:ILE:HG22	1:E:143:ILE:O	2.03	0.57
1:E:210:VAL:O	1:E:213:ILE:HG22	2.04	0.57
1:A:82:TYR:CE1	1:A:86:VAL:HB	2.39	0.57
1:E:103:ALA:HB1	1:E:111:LYS:CG	2.34	0.57
1:F:361:ASN:OD1	1:F:361:ASN:N	2.38	0.57
1:G:40:ILE:HD12	1:G:340:SER:HA	1.81	0.57
1:B:94:ILE:CD1	1:B:146:LYS:HE3	2.35	0.57
1:A:137:PRO:HG3	4:A:801:DQ8:HAP	1.87	0.57
1:B:20:GLN:OE1	1:B:70:MET:CE	2.53	0.57
1:B:288:ILE:HG13	1:B:289:ASN:N	2.20	0.57
1:C:327:ARG:HG2	1:C:362:LYS:O	2.05	0.57
1:F:158:VAL:HG21	1:F:213:ILE:CD1	2.35	0.57
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.04	0.56
1:D:130:ASP:OD1	1:D:131:PRO:HD2	2.05	0.56
4:F:801:DQ8:CAL	4:F:801:DQ8:CAP	2.78	0.56
1:C:126:THR:HG23	1:C:129:GLU:CG	2.30	0.56
1:C:207:LYS:HZ3	1:G:123:GLU:HG2	1.71	0.56
1:A:144:PHE:HB2	1:A:207:LYS:HZ2	1.70	0.56
1:G:82:TYR:CD1	1:G:86:VAL:CG2	2.88	0.56
1:G:107:THR:HB	1:G:270:GLU:OE2	2.05	0.56
1:A:230:ALA:HB3	1:A:234:ARG:NE	2.20	0.56
1:E:152:THR:HG22	1:E:153:GLU:H	1.70	0.56
1:F:190:ASN:OD1	1:F:191:LYS:N	2.38	0.56
1:G:44:ASP:OD1	1:G:46:VAL:HG23	2.06	0.56
1:G:155:SER:CB	1:G:244:HIS:HB2	2.35	0.56
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.71	0.56
1:A:330:THR:CG2	1:A:331:SER:N	2.69	0.56
1:D:92:GLU:O	1:D:97:TYR:HB2	2.06	0.56
1:D:247:GLU:OE2	1:D:257:LYS:HE3	2.05	0.56
1:F:19:ILE:HG21	1:F:359:ILE:HG22	1.87	0.56
1:G:21:VAL:HG11	1:G:357:LYS:HB3	1.87	0.56
1:G:170:ASP:C	1:G:170:ASP:OD1	2.43	0.56
1:E:299:ILE:HG23	1:E:359:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:GLN:O	1:G:20:GLN:HG3	2.05	0.56
1:D:26:ARG:NH2	1:D:32:GLU:OE2	2.36	0.56
1:F:139:THR:O	1:F:143:ILE:HB	2.05	0.56
1:G:136:ILE:HG12	1:G:263:LEU:HD13	1.88	0.56
1:G:186:ASP:OD1	1:G:186:ASP:N	2.39	0.56
1:A:127:TRP:CE2	1:A:128:GLU:HG3	2.40	0.56
1:C:288:ILE:HD12	1:C:288:ILE:H	1.72	0.56
1:F:144:PHE:HE2	1:F:207:LYS:N	2.02	0.56
1:A:69:ASP:O	1:A:70:MET:HG3	2.07	0.55
1:B:91:ASP:O	1:B:95:MET:HG2	2.07	0.55
1:D:18:ASN:N	1:D:361:ASN:H	2.04	0.55
1:D:186:ASP:OD2	1:D:312:ARG:NH2	2.39	0.55
1:G:295:LEU:O	1:G:299:ILE:HG12	2.06	0.55
1:E:87:CYS:SG	1:E:88:PRO:HD3	2.47	0.55
1:E:323:SER:HA	1:E:328:THR:HB	1.88	0.55
1:A:51:SER:HB2	1:A:65:THR:HG1	1.68	0.55
1:C:118:GLU:OE1	1:G:226:THR:HG21	2.07	0.55
4:D:801:DQ8:CAQ	4:D:801:DQ8:HAS1	2.36	0.55
1:E:161:LEU:C	1:E:161:LEU:CD1	2.72	0.55
1:G:158:VAL:HA	1:G:240:SER:O	2.07	0.55
1:A:289:ASN:O	1:A:293:LEU:HD13	2.07	0.55
1:D:34:LYS:HD2	1:D:35:ALA:N	2.22	0.55
1:G:98:ASN:HD22	1:G:98:ASN:H	1.53	0.55
1:G:312:ARG:CG	1:G:313:GLU:H	2.18	0.55
1:E:343:LEU:HD11	1:E:347:LEU:HD11	1.88	0.55
1:A:44:ASP:OD2	1:A:47:ARG:HD2	2.07	0.55
4:B:801:DQ8:HAS1	4:B:801:DQ8:CAQ	2.36	0.55
1:G:69:ASP:O	1:G:70:MET:HG2	2.07	0.55
1:E:310:PRO:HB2	1:E:313:GLU:HG3	1.87	0.55
1:F:230:ALA:CB	1:F:234:ARG:HD2	2.34	0.55
1:G:19:ILE:O	1:G:19:ILE:HG13	2.06	0.55
1:D:293:LEU:HD12	1:D:297:ARG:CZ	2.37	0.54
1:E:323:SER:O	1:E:330:THR:HG21	2.07	0.54
1:F:82:TYR:CE2	1:F:138:ARG:HB2	2.42	0.54
1:G:41:VAL:HG11	1:G:338:PRO:HA	1.86	0.54
1:C:89:ILE:O	1:C:93:VAL:HG23	2.07	0.54
1:D:26:ARG:NE	1:D:108:GLY:O	2.41	0.54
1:A:141:HIS:O	1:A:141:HIS:ND1	2.39	0.54
1:A:162:GLU:OE1	1:A:231:TYR:OH	2.04	0.54
1:F:19:ILE:HG22	1:F:360:LEU:HA	1.88	0.54
1:F:135:ILE:O	1:F:139:THR:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:VAL:HG13	1:B:220:LYS:CG	2.37	0.54
1:D:162:GLU:OE1	1:D:231:TYR:OH	2.13	0.54
1:F:325:GLY:HA2	1:F:360:LEU:O	2.07	0.54
1:A:132:LEU:HD23	1:A:132:LEU:N	2.21	0.54
1:A:288:ILE:HG23	1:A:289:ASN:H	1.71	0.54
1:D:90:LEU:HD22	1:D:139:THR:HG23	1.88	0.54
1:F:120:SER:OG	1:F:130:ASP:OD1	2.25	0.54
1:F:134:GLY:O	1:F:137:PRO:HD2	2.07	0.54
1:F:44:ASP:OD1	1:F:47:ARG:HG3	2.08	0.54
1:F:157:LYS:HB3	1:F:203:THR:HG22	1.89	0.54
1:G:136:ILE:HG12	1:G:263:LEU:CD1	2.37	0.54
1:G:362:LYS:HB3	1:G:363:PRO:CD	2.38	0.54
1:D:115:MET:O	1:D:136:ILE:HG13	2.07	0.54
1:F:114:THR:O	1:F:134:GLY:HA3	2.07	0.54
1:C:186:ASP:OD1	1:C:186:ASP:N	2.36	0.54
1:E:168:LEU:HB2	1:E:182:LEU:HB2	1.90	0.54
1:G:137:PRO:HB3	4:G:801:DQ8:CAF	2.38	0.54
1:G:177:ASP:O	1:G:179:SER:N	2.41	0.54
1:G:361:ASN:C	1:G:362:LYS:HD2	2.29	0.54
1:A:103:ALA:HB1	1:A:111:LYS:HB3	1.88	0.54
1:D:126:THR:HG23	1:D:129:GLU:HB2	1.90	0.54
1:F:91:ASP:O	1:F:94:ILE:HG22	2.08	0.54
1:F:143:ILE:HG12	1:F:243:ILE:HD11	1.88	0.54
1:F:185:PHE:O	1:F:194:VAL:HG12	2.08	0.54
1:E:170:ASP:HB2	1:E:182:LEU:HD11	1.90	0.53
1:G:215:GLU:HB2	4:G:801:DQ8:HAH	1.90	0.53
1:B:204:VAL:HG22	1:B:213:ILE:CD1	2.39	0.53
1:E:137:PRO:HD3	4:E:801:DQ8:HAJ	1.90	0.53
1:D:67:THR:O	1:D:357:LYS:HE2	2.08	0.53
1:F:54:THR:HG21	1:F:64:LYS:HG3	1.90	0.53
1:G:102:PHE:HB2	1:G:264:VAL:HG22	1.89	0.53
1:A:120:SER:OG	1:A:130:ASP:OD1	2.27	0.53
1:E:59:ASP:OD1	1:E:59:ASP:C	2.46	0.53
1:G:155:SER:HG	1:G:244:HIS:HB2	1.72	0.53
2:C:601:ADP:C8	2:C:601:ADP:C5'	2.85	0.53
1:F:100:THR:OG1	1:F:323:SER:OG	2.09	0.53
1:G:82:TYR:O	1:G:86:VAL:HG22	2.09	0.53
1:A:63:ARG:HG2	1:A:63:ARG:NH1	2.20	0.53
1:C:121:PRO:HG2	7:C:2023:HOH:O	2.07	0.53
1:D:26:ARG:HG3	1:D:26:ARG:NH1	2.22	0.53
1:E:352:TYR:O	1:E:355:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:PHE:CE2	1:G:206:ASN:C	2.82	0.53
1:G:156:VAL:CG1	1:G:204:VAL:O	2.56	0.53
1:A:130:ASP:OD1	1:A:131:PRO:HD2	2.08	0.53
1:B:206:ASN:OD1	1:B:208:ASP:HB2	2.09	0.53
1:C:23:VAL:HG11	1:C:50:VAL:HG21	1.89	0.53
1:C:150:ASN:OD1	1:C:152:THR:HG22	2.09	0.53
1:F:82:TYR:O	1:F:86:VAL:CG1	2.56	0.53
1:D:190:ASN:OD1	1:D:190:ASN:C	2.47	0.53
1:E:301:ALA:HB3	1:E:309:VAL:HG13	1.90	0.53
1:C:142:GLN:O	1:C:143:ILE:C	2.47	0.52
1:F:327:ARG:O	1:F:363:PRO:HA	2.09	0.52
1:F:163:ILE:HG12	1:F:168:LEU:HD23	1.91	0.52
1:G:56:GLY:O	1:G:57:LEU:HD13	2.09	0.52
1:D:102:PHE:HE1	1:D:320:LEU:HD13	1.70	0.52
1:E:125:TYR:CD1	1:E:125:TYR:N	2.78	0.52
1:G:40:ILE:HG22	1:G:52:VAL:HG13	1.91	0.52
1:B:184:MET:HE2	1:B:319:ILE:HG12	1.91	0.52
1:A:144:PHE:HB2	1:A:207:LYS:NZ	2.25	0.52
1:B:144:PHE:HZ	1:B:204:VAL:HG12	1.74	0.52
1:E:28:PHE:CD1	1:E:338:PRO:HG2	2.44	0.52
1:E:51:SER:OG	1:E:63:ARG:HD2	2.10	0.52
1:G:30:LEU:O	1:G:34:LYS:HE2	2.10	0.52
1:G:90:LEU:O	1:G:94:ILE:HB	2.09	0.52
1:A:63:ARG:CG	1:A:63:ARG:NH1	2.55	0.52
1:B:190:ASN:OD1	1:B:191:LYS:N	2.42	0.52
1:F:154:PHE:N	1:F:154:PHE:HD1	2.07	0.52
1:F:270:GLU:CG	1:F:271:ASN:OD1	2.57	0.52
1:B:94:ILE:HD12	1:B:146:LYS:HE3	1.91	0.52
1:F:221:ARG:O	1:F:224:ALA:N	2.42	0.52
1:C:365:VAL:O	1:C:366:ASN:CB	2.58	0.52
1:F:90:LEU:O	1:F:93:VAL:CG1	2.57	0.52
1:F:154:PHE:N	1:F:154:PHE:CD1	2.77	0.52
1:G:83:ARG:HA	1:G:87:CYS:SG	2.50	0.52
1:G:123:GLU:O	1:G:125:TYR:N	2.41	0.52
1:A:98:ASN:CB	1:A:328:THR:HG23	2.39	0.52
1:F:196:ILE:HB	1:F:199:LEU:HB2	1.91	0.52
1:G:166:GLU:HG3	1:G:315:LYS:CG	2.40	0.52
1:D:64:LYS:CE	1:D:66:TYR:OH	2.57	0.52
1:A:141:HIS:O	1:A:207:LYS:HE3	2.10	0.51
1:C:159:SER:HB2	1:C:199:LEU:HD11	1.92	0.51
4:B:801:DQ8:CAO	4:B:801:DQ8:CAS	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:ILE:CD1	1:G:343:LEU:HB2	2.40	0.51
1:G:354:HIS:CE1	1:G:358:ASN:HA	2.46	0.51
1:C:341:LEU:O	1:C:341:LEU:HD22	2.10	0.51
1:D:30:LEU:CD1	1:D:33:ARG:HH21	2.24	0.51
1:A:188:PRO:HD3	1:A:195:ILE:HD12	1.93	0.51
1:C:137:PRO:HD3	4:C:801:DQ8:HAJ	1.92	0.51
1:F:82:TYR:HA	1:F:86:VAL:HG12	1.93	0.51
1:A:109:THR:O	1:A:335:THR:CG2	2.59	0.51
1:E:86:VAL:HG23	1:E:87:CYS:N	2.24	0.51
1:G:244:HIS:C	1:G:245:MET:HG3	2.30	0.51
1:A:210:VAL:O	1:A:211:TYR:C	2.48	0.51
1:D:25:CYS:O	1:D:74:ALA:HA	2.10	0.51
1:F:89:ILE:HD12	1:F:101:ILE:CD1	2.16	0.51
1:A:23:VAL:HG21	1:A:68:PHE:CE2	2.46	0.51
1:E:103:ALA:CB	1:E:111:LYS:HG2	2.41	0.51
1:E:234:ARG:HD3	1:E:288:ILE:CG2	2.41	0.51
1:G:98:ASN:HD22	1:G:98:ASN:N	2.09	0.51
1:A:289:ASN:OD1	1:A:289:ASN:N	2.38	0.51
1:E:264:VAL:HG21	1:E:320:LEU:HD21	1.92	0.51
1:G:238:VAL:HG22	1:G:264:VAL:HB	1.92	0.51
1:E:29:ASN:ND2	1:E:32:GLU:OE1	2.42	0.51
4:A:801:DQ8:CAQ	4:A:801:DQ8:CAS	2.89	0.51
1:D:143:ILE:CD1	1:D:243:ILE:HD11	2.40	0.51
1:E:306:THR:HG22	1:E:307:PRO:CD	2.30	0.51
1:F:310:PRO:HB3	1:F:313:GLU:HG3	1.92	0.51
1:G:98:ASN:CB	1:G:260:LYS:HB3	2.41	0.50
1:G:41:VAL:HG13	1:G:338:PRO:HA	1.90	0.50
1:F:211:TYR:O	1:F:215:GLU:HB2	2.11	0.50
1:G:72:PHE:HB3	1:G:76:THR:OG1	2.12	0.50
1:G:124:GLU:HG2	1:G:125:TYR:CD2	2.46	0.50
1:C:365:VAL:HG12	1:C:366:ASN:N	2.24	0.50
1:D:26:ARG:HG3	1:D:27:PRO:O	2.11	0.50
1:E:127:TRP:CD1	1:E:211:TYR:HB2	2.46	0.50
1:E:126:THR:HG22	1:E:129:GLU:OE1	2.11	0.50
1:E:261:LEU:HD21	1:E:263:LEU:HD21	1.92	0.50
1:F:59:ASP:OD1	1:F:59:ASP:O	2.30	0.50
1:F:190:ASN:OD1	1:F:192:ARG:N	2.45	0.50
1:G:56:GLY:O	1:G:57:LEU:CD1	2.60	0.50
1:F:102:PHE:CB	1:F:264:VAL:HG13	2.42	0.50
1:F:119:ARG:HG2	4:F:801:DQ8:CAM	2.42	0.50
1:G:104:TYR:CD1	1:G:104:TYR:C	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ASP:OD1	1:C:265:ASP:C	2.50	0.50
1:G:181:ARG:CG	1:G:181:ARG:NH1	2.57	0.50
1:A:144:PHE:HD2	1:A:207:LYS:CD	2.12	0.50
1:C:102:PHE:HB3	1:C:264:VAL:HB	1.93	0.50
1:E:82:TYR:CA	1:E:86:VAL:HG13	2.42	0.50
1:F:320:LEU:O	1:F:323:SER:N	2.43	0.50
4:G:801:DQ8:CAO	4:G:801:DQ8:HAS2	2.42	0.50
1:E:234:ARG:HD3	1:E:288:ILE:HG21	1.92	0.49
1:F:265:ASP:OD1	1:F:265:ASP:C	2.50	0.49
1:C:19:ILE:HD13	1:C:359:ILE:HG13	1.91	0.49
1:D:212:GLN:CD	1:D:212:GLN:H	2.15	0.49
1:E:102:PHE:CB	1:E:264:VAL:HB	2.39	0.49
1:E:140:LEU:HD21	1:E:241:VAL:HG22	1.94	0.49
1:G:37:ALA:HB1	1:G:340:SER:OG	2.11	0.49
1:C:353:ALA:O	1:C:356:ALA:HB3	2.12	0.49
1:G:86:VAL:HG11	1:G:135:ILE:HG23	1.93	0.49
1:A:178:VAL:HG13	1:A:220:LYS:HG3	1.93	0.49
1:B:186:ASP:OD2	1:B:312:ARG:NH2	2.45	0.49
1:G:170:ASP:OD2	1:G:173:ASN:HB2	2.11	0.49
1:B:167:GLU:OE1	1:B:181:ARG:NE	2.43	0.49
1:F:154:PHE:HD1	1:F:154:PHE:H	1.61	0.49
1:G:123:GLU:C	1:G:125:TYR:H	2.13	0.49
1:A:187:ASP:OD1	1:A:188:PRO:HD2	2.12	0.49
1:B:205:HIS:N	1:B:209:GLU:OE1	2.32	0.49
1:E:29:ASN:ND2	1:E:32:GLU:HB2	2.28	0.49
1:G:111:LYS:HB2	1:G:111:LYS:HZ3	1.77	0.49
1:G:228:MET:HE2	1:G:228:MET:CA	2.38	0.49
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.95	0.49
1:F:215:GLU:CA	4:F:801:DQ8:HAH	2.36	0.49
1:G:111:LYS:HB2	1:G:111:LYS:HZ2	1.78	0.49
1:G:231:TYR:O	1:G:234:ARG:N	2.31	0.49
1:A:271:ASN:O	7:A:2025:HOH:O	2.20	0.49
1:C:162:GLU:OE1	1:C:231:TYR:OH	2.29	0.49
1:C:309:VAL:HB	1:C:311:TYR:CE2	2.48	0.49
1:G:295:LEU:O	1:G:295:LEU:HD12	2.12	0.49
1:G:354:HIS:CE1	1:G:358:ASN:OD1	2.66	0.49
1:A:40:ILE:HD13	1:A:343:LEU:HB2	1.95	0.48
1:D:161:LEU:C	1:D:161:LEU:HD12	2.34	0.48
1:F:173:ASN:OD1	1:F:174:PRO:HD2	2.13	0.48
1:G:26:ARG:HD2	1:G:27:PRO:O	2.12	0.48
1:G:160:LEU:H	1:G:172:LEU:CD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:TYR:CB	1:G:321:GLN:HG3	2.43	0.48
1:D:119:ARG:HA	1:D:130:ASP:OD2	2.12	0.48
1:G:295:LEU:HD12	1:G:298:VAL:HG12	1.95	0.48
1:C:262:ASN:C	1:C:263:LEU:HD23	2.32	0.48
1:E:170:ASP:OD2	1:E:173:ASN:HB2	2.13	0.48
1:F:40:ILE:HD13	1:F:340:SER:HA	1.94	0.48
1:F:309:VAL:HG13	1:F:311:TYR:CE2	2.47	0.48
1:G:167:GLU:HB2	1:G:169:PHE:CE1	2.48	0.48
1:B:291:SER:HA	1:B:314:SER:HB2	1.95	0.48
1:C:143:ILE:HD13	1:C:243:ILE:HD11	1.94	0.48
1:E:82:TYR:CD2	1:E:86:VAL:HG11	2.48	0.48
1:E:134:GLY:O	1:E:137:PRO:HD2	2.13	0.48
1:F:264:VAL:HG11	1:F:320:LEU:HD21	1.95	0.48
1:F:311:TYR:CE1	1:F:321:GLN:HG3	2.48	0.48
1:G:137:PRO:HB3	4:G:801:DQ8:HAF	1.94	0.48
1:D:139:THR:HG21	1:D:261:LEU:HD23	1.94	0.48
1:F:136:ILE:HG23	1:F:239:PHE:CE2	2.49	0.48
1:G:361:ASN:O	1:G:362:LYS:HD2	2.13	0.48
1:A:119:ARG:HD3	4:A:801:DQ8:CAG	2.44	0.48
1:A:123:GLU:O	1:A:125:TYR:N	2.46	0.48
1:E:163:ILE:HG12	1:E:168:LEU:CD1	2.43	0.48
1:A:178:VAL:CG1	1:A:220:LYS:CG	2.90	0.48
1:C:77:LYS:HG2	1:G:219:ALA:HB1	1.94	0.48
1:C:308:HIS:O	1:C:308:HIS:ND1	2.46	0.48
1:F:239:PHE:CD1	1:F:239:PHE:C	2.86	0.48
1:G:102:PHE:CB	1:G:264:VAL:HG22	2.43	0.48
1:D:171:LEU:HD13	1:D:221:ARG:HB2	1.96	0.48
1:E:25:CYS:HB2	1:E:336:ILE:CG1	2.43	0.48
1:G:311:TYR:HB2	1:G:321:GLN:HG3	1.96	0.48
1:C:33:ARG:CD	1:G:228:MET:HE1	2.33	0.48
1:E:90:LEU:HD12	1:E:90:LEU:O	2.14	0.48
1:F:49:GLU:HG2	1:F:67:THR:CG2	2.42	0.48
1:F:68:PHE:HA	1:F:357:LYS:HZ2	1.78	0.48
1:G:40:ILE:O	1:G:40:ILE:CG2	2.61	0.48
1:B:29:ASN:OD1	1:B:31:ALA:HB3	2.14	0.48
1:C:293:LEU:HD21	1:C:297:ARG:HH22	1.78	0.48
1:G:147:LEU:HD11	1:G:245:MET:CE	2.44	0.48
1:G:298:VAL:O	1:G:302:LEU:HD12	2.14	0.48
1:A:158:VAL:HG12	1:A:241:VAL:HG22	1.96	0.47
1:C:360:LEU:HD12	1:C:360:LEU:N	2.27	0.47
1:F:140:LEU:O	1:F:143:ILE:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:VAL:HG22	1:G:239:PHE:CE1	2.48	0.47
1:G:170:ASP:OD1	1:G:172:LEU:N	2.47	0.47
1:A:288:ILE:HG23	1:A:289:ASN:OD1	2.14	0.47
1:B:102:PHE:CD1	1:B:332:ILE:HG12	2.49	0.47
1:C:144:PHE:O	1:C:146:LYS:N	2.48	0.47
1:E:49:GLU:HG2	1:E:67:THR:CG2	2.44	0.47
1:G:26:ARG:HH12	1:G:29:ASN:ND2	2.11	0.47
1:G:35:ALA:CB	1:G:341:LEU:HD11	2.45	0.47
1:G:102:PHE:HB2	1:G:264:VAL:O	2.14	0.47
1:C:320:LEU:O	1:C:323:SER:HB2	2.14	0.47
1:E:323:SER:HB3	1:E:330:THR:HG21	1.94	0.47
1:C:135:ILE:HG22	1:C:263:LEU:HD13	1.95	0.47
1:E:245:MET:O	1:E:257:LYS:N	2.44	0.47
1:E:300:THR:CG2	1:E:355:ARG:HH12	2.21	0.47
1:F:19:ILE:CG2	1:F:359:ILE:O	2.62	0.47
1:F:161:LEU:HD12	1:F:161:LEU:O	2.14	0.47
1:F:345:GLU:OE1	1:F:345:GLU:HA	2.14	0.47
1:B:162:GLU:OE2	1:B:221:ARG:NE	2.46	0.47
1:D:196:ILE:CD1	1:D:319:ILE:HD11	2.44	0.47
1:E:103:ALA:HB1	1:E:111:LYS:HG2	1.97	0.47
1:G:77:LYS:O	1:G:80:ASP:HB2	2.14	0.47
1:A:98:ASN:HB2	1:A:328:THR:HG23	1.96	0.47
1:B:192:ARG:HD2	1:B:322:ASP:OD1	2.15	0.47
1:C:178:VAL:CG1	1:C:220:LYS:HG3	2.43	0.47
1:D:90:LEU:O	1:D:90:LEU:HD12	2.14	0.47
1:D:142:GLN:O	1:D:146:LYS:HB2	2.15	0.47
1:D:163:ILE:HG12	1:D:168:LEU:CD1	2.42	0.47
2:E:601:ADP:H8	2:E:601:ADP:H5'2	1.79	0.47
1:F:128:GLU:OE1	1:F:128:GLU:HA	2.13	0.47
1:F:135:ILE:CG2	1:F:263:LEU:HD13	2.38	0.47
1:F:156:VAL:CG1	1:F:204:VAL:HG13	2.38	0.47
1:F:301:ALA:O	1:F:305:ARG:HA	2.14	0.47
1:G:98:ASN:HB3	1:G:260:LYS:HB3	1.95	0.47
1:G:311:TYR:CG	1:G:321:GLN:CG	2.97	0.47
1:B:144:PHE:CZ	1:B:204:VAL:HG12	2.50	0.47
1:F:271:ASN:O	7:F:2020:HOH:O	2.20	0.47
1:G:166:GLU:HG3	1:G:315:LYS:HG2	1.95	0.47
1:G:262:ASN:ND2	1:G:320:LEU:CD2	2.74	0.47
1:A:123:GLU:C	1:A:125:TYR:H	2.19	0.47
1:C:309:VAL:O	1:C:311:TYR:N	2.45	0.47
1:E:128:GLU:HG2	1:E:141:HIS:ND1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:THR:CG2	1:E:153:GLU:H	2.26	0.47
1:B:40:ILE:HD13	1:B:340:SER:HA	1.97	0.47
1:C:161:LEU:HD12	1:C:161:LEU:O	2.13	0.47
1:C:264:VAL:HG21	1:C:320:LEU:HD21	1.97	0.47
1:E:86:VAL:O	1:E:90:LEU:N	2.46	0.47
1:G:53:ARG:NH2	1:G:57:LEU:CA	2.78	0.47
1:G:308:HIS:O	1:G:310:PRO:O	2.32	0.47
1:G:343:LEU:O	1:G:347:LEU:HG	2.14	0.47
1:D:162:GLU:OE1	1:D:231:TYR:CE2	2.68	0.46
1:D:197:LYS:NZ	1:F:58:ALA:O	2.45	0.46
1:E:89:ILE:O	1:E:93:VAL:HG23	2.15	0.46
1:E:173:ASN:CG	1:E:174:PRO:HD2	2.35	0.46
1:F:68:PHE:HA	1:F:357:LYS:CE	2.44	0.46
1:F:101:ILE:HA	1:F:331:SER:O	2.14	0.46
1:G:20:GLN:HB2	1:G:69:ASP:OD2	2.15	0.46
1:C:72:PHE:HB3	1:C:76:THR:HG21	1.97	0.46
1:F:317:THR:O	1:F:321:GLN:N	2.48	0.46
1:G:293:LEU:HA	1:G:352:TYR:HE2	1.80	0.46
4:G:801:DQ8:HAA1	4:G:801:DQ8:HAK	1.61	0.46
1:C:128:GLU:OE2	1:C:207:LYS:HE3	2.15	0.46
1:E:178:VAL:O	1:E:178:VAL:HG22	2.16	0.46
1:G:123:GLU:HA	1:G:123:GLU:OE1	2.15	0.46
1:A:156:VAL:HG13	1:A:156:VAL:O	2.15	0.46
1:E:152:THR:HG22	1:E:153:GLU:N	2.29	0.46
1:E:158:VAL:HA	1:E:240:SER:O	2.15	0.46
1:F:89:ILE:HG12	1:F:90:LEU:H	1.80	0.46
1:F:102:PHE:HD1	1:F:102:PHE:O	1.97	0.46
1:A:30:LEU:CD2	1:A:33:ARG:HD2	2.46	0.46
1:F:59:ASP:OD1	1:F:59:ASP:C	2.53	0.46
1:F:293:LEU:CD2	1:F:297:ARG:HH21	2.29	0.46
1:G:136:ILE:CG1	1:G:263:LEU:HD13	2.46	0.46
1:G:177:ASP:N	1:G:180:GLU:HG3	2.26	0.46
1:G:347:LEU:O	1:G:351:GLU:N	2.44	0.46
1:A:293:LEU:H	1:A:293:LEU:CD1	2.29	0.46
1:B:139:THR:O	1:B:143:ILE:HG13	2.15	0.46
1:E:103:ALA:HB1	1:E:111:LYS:HG3	1.97	0.46
1:F:91:ASP:OD1	1:F:146:LYS:NZ	2.48	0.46
1:A:19:ILE:HG22	1:A:361:ASN:OD1	2.15	0.46
1:E:142:GLN:O	1:E:146:LYS:HB2	2.15	0.46
1:A:104:TYR:CE2	1:A:352:TYR:CE1	3.04	0.46
1:C:306:THR:CG2	1:C:307:PRO:CD	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:801:DQ8:CAL	4:D:801:DQ8:CAP	2.94	0.46
1:E:154:PHE:CD1	1:E:154:PHE:C	2.89	0.46
1:F:94:ILE:HD11	1:F:147:LEU:CD2	2.38	0.46
1:F:299:ILE:HA	1:F:359:ILE:HD11	1.98	0.46
1:C:149:ASP:N	1:C:149:ASP:OD1	2.50	0.45
1:C:308:HIS:O	1:C:308:HIS:CG	2.68	0.45
1:C:327:ARG:HB3	1:C:363:PRO:HA	1.98	0.45
1:D:30:LEU:CD1	1:D:33:ARG:NH2	2.76	0.45
1:G:40:ILE:HD12	1:G:343:LEU:HB2	1.99	0.45
1:D:40:ILE:O	1:D:52:VAL:HA	2.15	0.45
4:E:801:DQ8:CAQ	4:E:801:DQ8:HAN	2.46	0.45
1:F:28:PHE:CD1	1:F:338:PRO:HG2	2.50	0.45
1:G:26:ARG:CZ	1:G:29:ASN:HD22	2.28	0.45
1:G:293:LEU:CD2	1:G:297:ARG:HE	2.30	0.45
1:B:79:ILE:O	1:B:83:ARG:HB2	2.17	0.45
1:E:289:ASN:O	1:E:293:LEU:HB2	2.17	0.45
1:F:49:GLU:CG	1:F:67:THR:HG22	2.44	0.45
1:G:40:ILE:HD11	1:G:340:SER:CA	2.42	0.45
1:A:40:ILE:HD12	1:A:52:VAL:CG1	2.47	0.45
1:C:92:GLU:O	1:C:97:TYR:HB2	2.17	0.45
1:D:120:SER:HB3	1:D:121:PRO:CD	2.40	0.45
1:F:293:LEU:HD22	1:F:297:ARG:HH21	1.79	0.45
1:A:144:PHE:CB	1:A:207:LYS:HZ2	2.29	0.45
4:A:801:DQ8:HAP	4:A:801:DQ8:CAL	2.46	0.45
1:B:106:GLN:NE2	1:B:345:GLU:HG3	2.32	0.45
1:B:130:ASP:OD1	1:B:131:PRO:CD	2.64	0.45
1:C:163:ILE:HG12	1:C:168:LEU:HD23	1.97	0.45
1:D:18:ASN:HB2	1:D:360:LEU:HD23	1.98	0.45
1:G:73:GLY:O	1:G:75:SER:N	2.49	0.45
1:G:190:ASN:O	1:G:192:ARG:N	2.50	0.45
1:C:146:LYS:HB2	1:C:146:LYS:HE2	1.70	0.45
1:C:173:ASN:ND2	1:E:57:LEU:HD22	2.32	0.45
1:C:187:ASP:HA	1:C:188:PRO:HD3	1.88	0.45
1:G:132:LEU:HD23	1:G:132:LEU:HA	1.87	0.45
1:G:309:VAL:N	1:G:310:PRO:HD2	2.32	0.45
1:D:322:ASP:OD1	1:D:322:ASP:N	2.47	0.45
1:G:196:ILE:C	1:G:196:ILE:HD12	2.37	0.45
1:G:308:HIS:C	1:G:310:PRO:HD2	2.37	0.45
1:F:25:CYS:O	1:F:74:ALA:HA	2.17	0.45
1:F:82:TYR:CE2	1:F:86:VAL:HG21	2.51	0.45
1:F:123:GLU:C	1:F:123:GLU:CD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:HIS:O	1:F:206:ASN:HB3	2.17	0.45
1:G:87:CYS:HB2	1:G:88:PRO:HD3	1.98	0.45
1:G:310:PRO:HB2	1:G:311:TYR:CD1	2.52	0.45
1:A:78:GLN:NE2	1:A:113:PHE:CE1	2.85	0.45
1:B:82:TYR:CD1	1:B:86:VAL:HB	2.51	0.45
1:B:162:GLU:CD	1:B:171:LEU:HD11	2.36	0.45
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.75	0.45
1:E:294:THR:O	1:E:295:LEU:C	2.54	0.45
1:F:144:PHE:O	1:F:147:LEU:N	2.50	0.45
1:A:98:ASN:C	1:A:328:THR:HG22	2.36	0.45
1:A:106:GLN:NE2	1:A:345:GLU:HG2	2.32	0.45
1:A:136:ILE:HG13	1:A:263:LEU:HD13	1.99	0.45
1:B:92:GLU:O	1:B:97:TYR:HB2	2.17	0.45
1:D:18:ASN:HA	1:D:360:LEU:HA	1.98	0.45
1:G:302:LEU:CD1	1:G:324:LEU:HD23	2.47	0.45
1:B:149:ASP:OD1	1:B:149:ASP:N	2.50	0.44
4:E:801:DQ8:CAL	4:E:801:DQ8:CAP	2.92	0.44
1:A:202:ILE:HG21	1:A:213:ILE:CD1	2.46	0.44
1:B:152:THR:HA	1:B:246:LYS:O	2.17	0.44
1:F:118:GLU:O	4:F:801:DQ8:HAG	2.17	0.44
1:F:308:HIS:O	1:F:308:HIS:CG	2.68	0.44
1:A:123:GLU:HB2	1:A:124:GLU:H	1.44	0.44
1:A:288:ILE:HG13	1:A:289:ASN:N	2.32	0.44
4:A:801:DQ8:CAS	4:A:801:DQ8:HAQ	2.48	0.44
1:C:39:SER:HA	1:C:338:PRO:O	2.17	0.44
1:F:23:VAL:HA	1:F:334:ALA:O	2.18	0.44
1:G:299:ILE:HG12	1:G:299:ILE:H	1.61	0.44
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.32	0.44
1:A:152:THR:HG22	1:A:153:GLU:N	2.29	0.44
1:E:239:PHE:CD1	1:E:239:PHE:C	2.91	0.44
1:C:190:ASN:OD1	1:C:190:ASN:C	2.55	0.44
1:C:266:LEU:HD22	1:C:316:LEU:HD21	1.99	0.44
1:F:241:VAL:HG12	1:F:261:LEU:HB3	1.99	0.44
1:G:20:GLN:O	1:G:20:GLN:CG	2.64	0.44
1:A:90:LEU:O	1:A:93:VAL:HG22	2.18	0.44
1:A:192:ARG:HH21	1:A:327:ARG:NH1	2.15	0.44
1:F:72:PHE:HB3	1:F:76:THR:HG21	1.99	0.44
1:F:144:PHE:CE1	1:F:156:VAL:HG11	2.52	0.44
1:G:18:ASN:N	1:G:18:ASN:OD1	2.50	0.44
1:G:205:HIS:O	1:G:206:ASN:CB	2.66	0.44
1:G:293:LEU:O	1:G:297:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ARG:O	1:B:363:PRO:HA	2.18	0.44
1:E:77:LYS:O	1:E:80:ASP:HB2	2.18	0.44
1:F:27:PRO:HB3	1:F:74:ALA:HB1	2.00	0.44
1:F:63:ARG:HH11	1:F:63:ARG:HG3	1.82	0.44
1:G:59:ASP:OD1	1:G:61:SER:O	2.36	0.44
1:B:157:LYS:HB2	1:B:157:LYS:HE3	1.77	0.44
1:F:132:LEU:H	1:F:132:LEU:HG	1.63	0.44
1:F:135:ILE:HD12	1:F:135:ILE:N	2.33	0.44
1:F:309:VAL:HG13	1:F:311:TYR:CD2	2.53	0.44
1:G:57:LEU:HD22	1:G:57:LEU:O	2.17	0.44
1:A:168:LEU:HD21	1:A:315:LYS:HD2	1.99	0.43
1:C:100:THR:HG22	1:C:101:ILE:N	2.32	0.43
1:G:53:ARG:HH21	1:G:57:LEU:CA	2.30	0.43
1:G:199:LEU:HD13	1:G:200:GLU:N	2.33	0.43
1:G:295:LEU:HD12	1:G:298:VAL:CG1	2.48	0.43
1:A:153:GLU:HG3	1:A:246:LYS:HE2	2.00	0.43
1:C:302:LEU:CB	1:C:359:ILE:HG22	2.45	0.43
1:E:205:HIS:O	1:E:206:ASN:HB3	2.18	0.43
1:F:19:ILE:CG2	1:F:360:LEU:HA	2.47	0.43
1:F:168:LEU:HB2	1:F:182:LEU:HB2	1.99	0.43
1:F:178:VAL:HG22	1:F:178:VAL:O	2.18	0.43
1:F:309:VAL:O	1:F:311:TYR:N	2.51	0.43
1:A:63:ARG:HG3	1:A:63:ARG:NH1	2.29	0.43
1:A:311:TYR:CE1	1:A:321:GLN:HG3	2.53	0.43
1:A:98:ASN:HB3	1:A:328:THR:HG23	2.00	0.43
1:B:264:VAL:HG21	1:B:320:LEU:HD11	1.99	0.43
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.53	0.43
1:B:327:ARG:HG3	1:B:362:LYS:O	2.18	0.43
1:C:270:GLU:HG2	1:C:271:ASN:H	1.83	0.43
1:C:322:ASP:O	1:C:328:THR:HB	2.19	0.43
1:E:158:VAL:HG13	1:E:204:VAL:HG21	2.00	0.43
1:F:128:GLU:OE2	1:F:141:HIS:NE2	2.51	0.43
1:F:144:PHE:CE2	1:F:206:ASN:C	2.92	0.43
1:A:109:THR:OG1	1:A:335:THR:HG22	2.18	0.43
1:B:116:GLU:HG2	4:B:801:DQ8:CAK	2.48	0.43
1:F:146:LYS:HE3	1:F:146:LYS:HB3	1.66	0.43
1:C:23:VAL:HG21	1:C:68:PHE:CE2	2.53	0.43
1:C:306:THR:HG23	1:C:307:PRO:CD	2.33	0.43
1:E:106:GLN:HE22	1:E:342:ASN:HB3	1.84	0.43
1:E:156:VAL:CG2	1:E:204:VAL:O	2.67	0.43
1:F:309:VAL:HA	1:F:310:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:VAL:O	1:E:89:ILE:N	2.51	0.43
1:G:196:ILE:O	1:G:196:ILE:HG13	2.18	0.43
1:A:202:ILE:HD12	1:A:202:ILE:N	2.34	0.43
4:A:801:DQ8:CAL	4:A:801:DQ8:CAP	2.95	0.43
1:B:293:LEU:HD11	1:B:297:ARG:NH1	2.34	0.43
1:C:19:ILE:HD11	1:C:359:ILE:HG13	1.98	0.43
1:G:124:GLU:HG2	1:G:125:TYR:CE2	2.54	0.43
1:G:293:LEU:HD21	1:G:297:ARG:HH21	1.84	0.43
4:E:801:DQ8:HAK	4:E:801:DQ8:HAA1	1.83	0.43
1:F:91:ASP:O	1:F:94:ILE:N	2.52	0.43
1:A:99:CYS:O	1:A:261:LEU:CD1	2.65	0.43
1:A:230:ALA:O	1:A:234:ARG:HB2	2.19	0.43
1:D:26:ARG:NH1	1:D:26:ARG:CG	2.81	0.43
1:E:202:ILE:HG13	1:E:213:ILE:HD11	2.00	0.43
1:F:102:PHE:HB3	1:F:264:VAL:HG13	1.98	0.43
1:A:168:LEU:HD22	1:A:168:LEU:N	2.34	0.42
1:C:210:VAL:HG12	1:C:211:TYR:N	2.34	0.42
1:E:49:GLU:HG2	1:E:67:THR:HG22	2.01	0.42
1:E:170:ASP:C	1:E:170:ASP:OD1	2.57	0.42
1:F:216:LYS:NZ	1:F:217:GLY:N	2.66	0.42
1:F:307:PRO:O	1:F:308:HIS:C	2.57	0.42
1:G:79:ILE:HG12	1:G:83:ARG:CZ	2.49	0.42
1:G:102:PHE:CZ	1:G:295:LEU:HD21	2.54	0.42
1:E:156:VAL:CG2	1:E:204:VAL:HB	2.46	0.42
1:F:113:PHE:CD1	1:F:113:PHE:C	2.91	0.42
1:F:221:ARG:O	1:F:222:THR:C	2.56	0.42
1:G:231:TYR:H	1:G:231:TYR:HD1	1.63	0.42
1:A:47:ARG:HG3	1:A:47:ARG:HH11	1.84	0.42
1:D:26:ARG:HD3	1:D:109:THR:HA	2.00	0.42
1:G:43:CYS:HB3	1:G:71:VAL:CG1	2.49	0.42
1:G:196:ILE:HG12	1:G:199:LEU:HD23	2.00	0.42
1:A:126:THR:O	1:A:127:TRP:C	2.57	0.42
1:B:357:LYS:HE2	1:B:357:LYS:HB3	1.77	0.42
1:C:165:ASN:O	1:C:166:GLU:HB2	2.19	0.42
1:E:162:GLU:HG3	1:E:171:LEU:HD21	2.02	0.42
1:G:78:GLN:O	1:G:81:VAL:CG2	2.68	0.42
1:C:59:ASP:C	1:C:59:ASP:OD1	2.58	0.42
1:F:123:GLU:OE1	1:F:124:GLU:N	2.52	0.42
1:G:91:ASP:HA	1:G:94:ILE:HG22	2.01	0.42
1:G:169:PHE:CD1	1:G:169:PHE:N	2.87	0.42
1:G:336:ILE:HA	1:G:336:ILE:HD13	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HE1	1:A:156:VAL:CG1	2.23	0.42
1:C:143:ILE:CD1	1:C:243:ILE:HD11	2.49	0.42
1:D:236:HIS:HE2	1:D:291:SER:HB3	1.85	0.42
1:B:303:VAL:CG2	1:B:304:GLU:HG3	2.50	0.42
1:D:64:LYS:HE2	1:D:66:TYR:CZ	2.53	0.42
1:F:102:PHE:O	1:F:102:PHE:CD1	2.72	0.42
1:B:102:PHE:CE1	1:B:332:ILE:CG1	2.98	0.42
1:B:362:LYS:HA	1:B:363:PRO:HD3	1.82	0.42
1:C:170:ASP:OD2	1:C:199:LEU:HA	2.20	0.42
1:C:212:GLN:HE21	1:C:212:GLN:HB2	1.68	0.42
1:E:93:VAL:O	1:E:259:GLY:HA3	2.20	0.42
1:F:306:THR:CB	1:F:307:PRO:CD	2.96	0.42
4:F:801:DQ8:HAK	4:F:801:DQ8:HAA1	1.77	0.42
1:G:78:GLN:HB2	1:G:138:ARG:NH2	2.35	0.42
1:A:33:ARG:HG2	1:A:33:ARG:NH1	2.34	0.42
1:A:309:VAL:HB	1:A:311:TYR:CE2	2.55	0.42
1:E:26:ARG:H	1:E:26:ARG:HG3	1.65	0.42
1:E:72:PHE:CD2	1:E:76:THR:HG21	2.55	0.42
1:E:195:ILE:HG13	1:E:195:ILE:O	2.20	0.42
1:E:292:LEU:HD12	1:E:292:LEU:HA	1.77	0.42
1:G:149:ASP:OD1	1:G:149:ASP:N	2.44	0.42
1:G:155:SER:HB2	1:G:244:HIS:ND1	2.35	0.42
1:D:134:GLY:O	1:D:138:ARG:HG3	2.20	0.41
1:D:158:VAL:HA	1:D:240:SER:O	2.19	0.41
1:D:214:LEU:HD13	4:D:801:DQ8:CAJ	2.50	0.41
1:F:23:VAL:HG21	1:F:68:PHE:CE2	2.54	0.41
1:F:159:SER:HA	1:F:172:LEU:HD12	2.02	0.41
1:A:136:ILE:HB	1:A:137:PRO:HD3	2.02	0.41
1:C:33:ARG:NH1	1:G:179:SER:OG	2.54	0.41
1:C:357:LYS:H	1:C:357:LYS:HG3	1.66	0.41
1:C:362:LYS:N	1:C:362:LYS:CD	2.79	0.41
1:F:143:ILE:HD12	1:F:143:ILE:HA	1.87	0.41
1:F:350:LEU:HD23	1:F:350:LEU:HA	1.82	0.41
1:G:160:LEU:HD22	4:G:801:DQ8:HAA2	2.02	0.41
1:G:182:LEU:HD12	1:G:182:LEU:HA	1.58	0.41
1:A:144:PHE:O	1:A:147:LEU:N	2.53	0.41
1:A:322:ASP:O	1:A:328:THR:OG1	2.37	0.41
1:D:162:GLU:HG2	1:D:237:SER:HB3	2.03	0.41
1:E:293:LEU:HD23	1:E:297:ARG:NH1	2.35	0.41
1:E:294:THR:HG22	1:E:317:THR:HG21	2.01	0.41
1:F:161:LEU:C	1:F:161:LEU:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HB2	1:A:207:LYS:CD	2.51	0.41
1:A:320:LEU:HA	1:A:320:LEU:HD23	1.66	0.41
1:C:261:LEU:HG	1:C:263:LEU:HD21	2.03	0.41
1:F:90:LEU:HD12	1:F:90:LEU:C	2.37	0.41
1:F:144:PHE:HE1	1:F:156:VAL:HG11	1.84	0.41
1:G:161:LEU:CD1	1:G:162:GLU:N	2.82	0.41
1:A:94:ILE:O	1:A:94:ILE:HG22	2.21	0.41
1:B:247:GLU:CD	1:B:255:LEU:O	2.59	0.41
4:B:801:DQ8:HAK	4:B:801:DQ8:HAA1	1.87	0.41
1:D:77:LYS:HD2	1:D:77:LYS:HA	1.82	0.41
1:G:271:ASN:OD1	1:G:271:ASN:O	2.38	0.41
1:G:305:ARG:HD3	1:G:306:THR:N	2.36	0.41
1:G:312:ARG:CG	1:G:313:GLU:N	2.79	0.41
1:A:64:LYS:HE2	1:A:64:LYS:HB3	1.88	0.41
1:A:330:THR:CG2	1:A:331:SER:H	2.33	0.41
1:B:92:GLU:OE2	1:B:329:ARG:CZ	2.68	0.41
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.77	0.41
1:D:51:SER:HB2	1:D:65:THR:OG1	2.21	0.41
1:D:64:LYS:HE3	1:D:64:LYS:HB3	1.63	0.41
1:E:61:SER:O	1:F:64:LYS:HA	2.21	0.41
1:F:124:GLU:O	1:F:125:TYR:CD1	2.73	0.41
1:A:120:SER:HA	1:A:121:PRO:HD3	1.94	0.41
4:B:801:DQ8:HAS1	4:B:801:DQ8:HAQ	2.01	0.41
1:C:119:ARG:HA	1:C:130:ASP:OD2	2.21	0.41
1:C:206:ASN:HD21	1:C:208:ASP:HB2	1.75	0.41
1:C:292:LEU:HD12	1:C:292:LEU:HA	1.76	0.41
1:D:212:GLN:CD	1:D:212:GLN:N	2.74	0.41
4:E:801:DQ8:HAS1	4:E:801:DQ8:HAQ	2.00	0.41
1:F:93:VAL:O	1:F:96:GLY:N	2.40	0.41
1:F:127:TRP:O	1:F:127:TRP:CE3	2.74	0.41
1:F:222:THR:O	1:F:226:THR:HG23	2.20	0.41
1:A:166:GLU:OE2	1:A:291:SER:OG	2.29	0.41
1:B:102:PHE:CE1	1:B:332:ILE:CD1	2.97	0.41
1:B:143:ILE:HD13	1:B:243:ILE:HD11	2.01	0.41
1:C:309:VAL:HG11	1:C:311:TYR:CZ	2.56	0.41
1:F:171:LEU:HA	1:F:171:LEU:HD13	1.77	0.41
1:F:263:LEU:N	1:F:263:LEU:HD23	2.36	0.41
1:F:266:LEU:HD22	1:F:316:LEU:HD21	2.03	0.41
1:F:291:SER:HB3	1:F:316:LEU:HB3	2.03	0.41
1:A:126:THR:O	1:A:129:GLU:N	2.54	0.41
1:C:82:TYR:CD1	1:C:86:VAL:HB	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ARG:HA	1:D:87:CYS:SG	2.61	0.41
1:D:123:GLU:O	1:D:125:TYR:N	2.54	0.41
1:D:168:LEU:HB2	1:D:182:LEU:HB2	2.03	0.41
1:G:144:PHE:HE2	1:G:206:ASN:O	2.03	0.41
1:G:162:GLU:OE2	1:G:231:TYR:OH	2.37	0.41
1:A:20:GLN:O	1:A:331:SER:HA	2.21	0.40
1:B:288:ILE:HD12	1:B:288:ILE:O	2.20	0.40
1:D:120:SER:N	1:D:130:ASP:OD2	2.43	0.40
1:F:69:ASP:O	1:F:70:MET:HG3	2.21	0.40
1:G:237:SER:HB3	1:G:265:ASP:HB3	2.03	0.40
1:D:127:TRP:CE2	1:D:128:GLU:HG3	2.56	0.40
1:E:59:ASP:OD2	1:F:64:LYS:NZ	2.55	0.40
1:F:234:ARG:HD3	1:F:288:ILE:HD11	2.02	0.40
1:G:292:LEU:HD12	1:G:292:LEU:HA	1.73	0.40
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.80	0.40
1:C:266:LEU:CD2	1:C:316:LEU:HD21	2.52	0.40
1:D:229:ASN:O	1:D:230:ALA:HB3	2.21	0.40
1:F:82:TYR:C	1:F:82:TYR:CD1	2.95	0.40
1:F:112:THR:HG22	1:F:113:PHE:N	2.36	0.40
1:F:242:THR:HB	1:F:260:LYS:HG3	2.03	0.40
1:A:86:VAL:O	1:A:89:ILE:N	2.54	0.40
1:A:93:VAL:HG11	1:A:261:LEU:HB2	2.02	0.40
1:A:103:ALA:HB1	1:A:111:LYS:CB	2.51	0.40
1:A:192:ARG:NH2	1:A:327:ARG:HG3	2.37	0.40
1:B:312:ARG:HA	1:B:312:ARG:HD3	1.86	0.40
1:D:111:LYS:HB2	2:D:601:ADP:O2B	2.20	0.40
1:E:143:ILE:HG23	1:E:243:ILE:HD13	2.04	0.40
1:F:199:LEU:HD12	1:F:200:GLU:N	2.37	0.40
1:A:114:THR:O	1:A:135:ILE:HG13	2.22	0.40
1:B:18:ASN:HA	1:B:360:LEU:HA	2.03	0.40
1:C:293:LEU:CD2	1:C:297:ARG:NH2	2.85	0.40
1:C:308:HIS:HB3	7:D:2024:HOH:O	2.21	0.40
1:D:137:PRO:HD3	4:D:801:DQ8:HAJ	2.02	0.40
1:E:130:ASP:OD1	1:E:131:PRO:HD2	2.22	0.40
1:F:136:ILE:CG2	1:F:239:PHE:CE2	3.05	0.40
1:F:184:MET:CE	1:F:319:ILE:HG13	2.52	0.40
1:F:243:ILE:N	1:F:259:GLY:O	2.44	0.40
1:G:301:ALA:HA	1:G:304:GLU:O	2.22	0.40

There are no symmetry-related clashes.

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	317/368 (86%)	300 (95%)	17 (5%)	0	100	100
1	B	319/368 (87%)	308 (97%)	11 (3%)	0	100	100
1	C	320/368 (87%)	302 (94%)	17 (5%)	1 (0%)	41	60
1	D	317/368 (86%)	303 (96%)	14 (4%)	0	100	100
1	E	315/368 (86%)	300 (95%)	15 (5%)	0	100	100
1	F	314/368 (85%)	286 (91%)	27 (9%)	1 (0%)	41	60
1	G	312/368 (85%)	277 (89%)	33 (11%)	2 (1%)	25	42
All	All	2214/2576 (86%)	2076 (94%)	134 (6%)	4 (0%)	47	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	206	ASN
1	G	97	TYR
1	C	190	ASN
1	F	307	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	284/322 (88%)	256 (90%)	28 (10%)	8	13
1	B	288/322 (89%)	260 (90%)	28 (10%)	8	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	287/322 (89%)	255 (89%)	32 (11%)	6	10
1	D	284/322 (88%)	262 (92%)	22 (8%)	13	22
1	E	281/322 (87%)	248 (88%)	33 (12%)	5	8
1	F	279/322 (87%)	233 (84%)	46 (16%)	2	3
1	G	269/322 (84%)	206 (77%)	63 (23%)	1	1
All	All	1972/2254 (88%)	1720 (87%)	252 (13%)	4	6

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	51	SER
1	A	63	ARG
1	A	111	LYS
1	A	126	THR
1	A	142	GLN
1	A	161	LEU
1	A	178	VAL
1	A	182	LEU
1	A	189	ARG
1	A	197	LYS
1	A	208	ASP
1	A	220	LYS
1	A	227	LEU
1	A	237	SER
1	A	240	SER
1	A	255	LEU
1	A	289	ASN
1	A	291	SER
1	A	298	VAL
1	A	306	THR
1	A	328	THR
1	A	341	LEU
1	A	343	LEU
1	A	348	SER
1	A	351	GLU
1	A	357	LYS
1	A	360	LEU
1	B	18	ASN
1	B	19	ILE

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Mol	Chain	Res	Type
1	B	20	GLN
1	B	64	LYS
1	B	102	PHE
1	B	111	LYS
1	B	119	ARG
1	B	123	GLU
1	B	126	THR
1	B	128	GLU
1	B	141	HIS
1	B	161	LEU
1	B	178	VAL
1	B	184	MET
1	B	207	LYS
1	B	220	LYS
1	B	227	LEU
1	B	233	SER
1	B	237	SER
1	B	247	GLU
1	B	255	LEU
1	B	288	ILE
1	B	289	ASN
1	B	291	SER
1	B	327	ARG
1	B	341	LEU
1	B	355	ARG
1	B	360	LEU
1	C	30	LEU
1	C	34	LYS
1	C	67	THR
1	C	94	ILE
1	C	119	ARG
1	C	126	THR
1	C	129	GLU
1	C	145[A]	GLU
1	C	145[B]	GLU
1	C	149	ASP
1	C	161	LEU
1	C	162	GLU
1	C	168	LEU
1	C	178	VAL
1	C	186	ASP
1	C	189	ARG

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Mol	Chain	Res	Type
1	C	190	ASN
1	C	203	THR
1	C	206	ASN
1	C	207	LYS
1	C	212	GLN
1	C	227	LEU
1	C	234	ARG
1	C	308	HIS
1	C	320	LEU
1	C	324	LEU
1	C	337	SER
1	C	340	SER
1	C	341	LEU
1	C	359	ILE
1	C	360	LEU
1	C	362	LYS
1	D	19	ILE
1	D	36	SER
1	D	64	LYS
1	D	79	ILE
1	D	90	LEU
1	D	93	VAL
1	D	126	THR
1	D	168	LEU
1	D	206	ASN
1	D	207	LYS
1	D	220	LYS
1	D	227	LEU
1	D	229	ASN
1	D	232	SER
1	D	237	SER
1	D	291	SER
1	D	293	LEU
1	D	303	VAL
1	D	309	VAL
1	D	337	SER
1	D	341	LEU
1	D	351	GLU
1	E	19	ILE
1	E	20	GLN
1	E	26	ARG
1	E	33	ARG

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Mol	Chain	Res	Type
1	E	36	SER
1	E	59	ASP
1	E	84	SER
1	E	92	GLU
1	E	97	TYR
1	E	111	LYS
1	E	125	TYR
1	E	142	GLN
1	E	145	GLU
1	E	147	LEU
1	E	152	THR
1	E	154	PHE
1	E	184	MET
1	E	185	PHE
1	E	191	LYS
1	E	195	ILE
1	E	202	ILE
1	E	212	GLN
1	E	216	LYS
1	E	222	THR
1	E	227	LEU
1	E	237	SER
1	E	258	ILE
1	E	288	ILE
1	E	293	LEU
1	E	312	ARG
1	E	348	SER
1	E	355	ARG
1	E	361	ASN
1	F	19	ILE
1	F	20	GLN
1	F	26	ARG
1	F	32	GLU
1	F	36	SER
1	F	51	SER
1	F	79	ILE
1	F	86	VAL
1	F	89	ILE
1	F	90	LEU
1	F	102	PHE
1	F	112	THR
1	F	115	MET

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Mol	Chain	Res	Type
1	F	120	SER
1	F	123	GLU
1	F	132	LEU
1	F	141	HIS
1	F	148	THR
1	F	154	PHE
1	F	168	LEU
1	F	171	LEU
1	F	181	ARG
1	F	194	VAL
1	F	195	ILE
1	F	204	VAL
1	F	213	ILE
1	F	216	LYS
1	F	220	LYS
1	F	227	LEU
1	F	239	PHE
1	F	242	THR
1	F	243	ILE
1	F	244	HIS
1	F	257	LYS
1	F	265	ASP
1	F	271	ASN
1	F	293	LEU
1	F	306	THR
1	F	308	HIS
1	F	312	ARG
1	F	323	SER
1	F	341	LEU
1	F	351	GLU
1	F	352	TYR
1	F	360	LEU
1	F	361	ASN
1	G	18	ASN
1	G	21	VAL
1	G	34	LYS
1	G	39	SER
1	G	41	VAL
1	G	44	ASP
1	G	47	ARG
1	G	53	ARG
1	G	57	LEU

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Mol	Chain	Res	Type
1	G	67	THR
1	G	69	ASP
1	G	79	ILE
1	G	81	VAL
1	G	86	VAL
1	G	89	ILE
1	G	98	ASN
1	G	100	THR
1	G	102	PHE
1	G	104	TYR
1	G	107	THR
1	G	122	ASN
1	G	128	GLU
1	G	149	ASP
1	G	155	SER
1	G	158	VAL
1	G	159	SER
1	G	161	LEU
1	G	166	GLU
1	G	168	LEU
1	G	181	ARG
1	G	182	LEU
1	G	184	MET
1	G	185	PHE
1	G	186	ASP
1	G	189	ARG
1	G	190	ASN
1	G	196	ILE
1	G	199	LEU
1	G	200	GLU
1	G	205	HIS
1	G	220	LYS
1	G	223	THR
1	G	226	THR
1	G	227	LEU
1	G	228	MET
1	G	233	SER
1	G	234	ARG
1	G	243	ILE
1	G	291	SER
1	G	292	LEU
1	G	293	LEU

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Mol	Chain	Res	Type
1	G	294	THR
1	G	298	VAL
1	G	299	ILE
1	G	302	LEU
1	G	306	THR
1	G	316	LEU
1	G	321	GLN
1	G	329	ARG
1	G	336	ILE
1	G	340	SER
1	G	347	LEU
1	G	350	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	20	GLN
1	G	18	ASN
1	G	262	ASN
1	G	354	HIS
1	G	358	ASN

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](#)

Of 36 ligands modelled in this entry, 21 are monoatomic - leaving 15 for Mogul analysis.

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$
4	DQ8	E	801	-	28,28,28	0.69	1 (3%)	38,38,38	1.07	4 (10%)
6	SO4	D	1362	-	4,4,4	0.21	0	6,6,6	0.38	0
4	DQ8	D	801	-	28,28,28	0.99	2 (7%)	38,38,38	1.32	5 (13%)
2	ADP	F	601	3	24,29,29	1.05	1 (4%)	29,45,45	1.58	6 (20%)
4	DQ8	A	801	-	28,28,28	0.86	1 (3%)	38,38,38	1.08	2 (5%)
2	ADP	A	601	3	24,29,29	1.12	2 (8%)	29,45,45	1.58	6 (20%)
2	ADP	G	601	3	24,29,29	1.12	3 (12%)	29,45,45	1.73	5 (17%)
4	DQ8	C	801	-	28,28,28	0.77	0	38,38,38	1.26	6 (15%)
4	DQ8	F	801	-	28,28,28	0.77	1 (3%)	38,38,38	1.08	3 (7%)
4	DQ8	G	801	-	28,28,28	0.93	2 (7%)	38,38,38	1.24	5 (13%)
2	ADP	E	601	3	24,29,29	1.07	1 (4%)	29,45,45	1.57	5 (17%)
2	ADP	D	601	3	24,29,29	1.05	1 (4%)	29,45,45	1.48	4 (13%)
2	ADP	B	601	3	24,29,29	1.07	1 (4%)	29,45,45	1.60	8 (27%)
2	ADP	C	601	3	24,29,29	1.21	2 (8%)	29,45,45	1.83	9 (31%)
4	DQ8	B	801	-	28,28,28	0.66	0	38,38,38	1.02	2 (5%)

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
4	DQ8	E	801	-	-	1/27/27/27	0/3/3/3
4	DQ8	D	801	-	-	2/27/27/27	0/3/3/3
2	ADP	F	601	3	-	1/12/32/32	0/3/3/3
4	DQ8	A	801	-	-	0/27/27/27	0/3/3/3
2	ADP	A	601	3	-	2/12/32/32	0/3/3/3
2	ADP	G	601	3	-	1/12/32/32	0/3/3/3
4	DQ8	C	801	-	-	2/27/27/27	0/3/3/3
4	DQ8	F	801	-	-	0/27/27/27	0/3/3/3
4	DQ8	G	801	-	-	2/27/27/27	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	E	601	3	-	5/12/32/32	0/3/3/3
2	ADP	D	601	3	-	2/12/32/32	0/3/3/3
2	ADP	B	601	3	-	2/12/32/32	0/3/3/3
2	ADP	C	601	3	-	3/12/32/32	0/3/3/3
4	DQ8	B	801	-	-	2/27/27/27	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ADP	C2'-C1'	-3.04	1.49	1.53
2	A	601	ADP	C2'-C1'	-2.84	1.49	1.53
2	G	601	ADP	C5-C4	2.75	1.48	1.40
2	F	601	ADP	C5-C4	2.72	1.48	1.40
2	C	601	ADP	C5-C4	2.56	1.47	1.40
4	A	801	DQ8	CAS-SAT	2.48	1.86	1.81
2	B	601	ADP	C2'-C1'	-2.48	1.50	1.53
2	D	601	ADP	O4'-C1'	2.47	1.44	1.41
2	E	601	ADP	C5-C4	2.45	1.47	1.40
4	D	801	DQ8	CAZ-SAT	-2.42	1.83	1.86
4	G	801	DQ8	CAZ-CAW	-2.39	1.50	1.54
2	A	601	ADP	C5-C4	2.35	1.47	1.40
2	G	601	ADP	O4'-C1'	2.30	1.44	1.41
4	D	801	DQ8	CAS-SAT	2.29	1.86	1.81
4	F	801	DQ8	CAS-SAT	2.28	1.86	1.81
2	G	601	ADP	C2-N3	2.23	1.35	1.32
4	E	801	DQ8	CAS-SAT	2.11	1.86	1.81
4	G	801	DQ8	CAS-SAT	2.03	1.85	1.81

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	ADP	PA-O3A-PB	-4.61	117.02	132.83
2	G	601	ADP	C5'-C4'-C3'	-4.52	98.25	115.18
2	C	601	ADP	PA-O3A-PB	-3.83	119.67	132.83
2	E	601	ADP	N3-C2-N1	-3.67	122.94	128.68
2	A	601	ADP	C4-C5-N7	-3.40	105.85	109.40
2	C	601	ADP	N3-C2-N1	-3.26	123.58	128.68
2	G	601	ADP	PA-O3A-PB	-3.18	121.92	132.83
2	E	601	ADP	PA-O3A-PB	-3.17	121.94	132.83
2	D	601	ADP	N6-C6-N1	3.16	125.13	118.57
2	C	601	ADP	O2'-C2'-C1'	-3.13	99.29	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	PA-O3A-PB	-3.11	122.16	132.83
2	B	601	ADP	O3B-PB-O1B	3.04	122.58	110.68
2	C	601	ADP	C2-N1-C6	3.03	123.94	118.75
2	B	601	ADP	C3'-C2'-C1'	3.00	105.49	100.98
2	G	601	ADP	N3-C2-N1	-2.98	124.02	128.68
2	F	601	ADP	O3B-PB-O2B	2.92	118.80	107.64
4	D	801	DQ8	CAH-CAN-CAX	-2.88	117.73	120.76
2	C	601	ADP	O3B-PB-O2B	2.87	118.59	107.64
4	G	801	DQ8	CAR-CAS-SAT	2.86	118.05	110.04
2	B	601	ADP	N3-C2-N1	-2.85	124.22	128.68
2	D	601	ADP	C5'-C4'-C3'	-2.84	104.55	115.18
2	F	601	ADP	C3'-C2'-C1'	2.77	105.15	100.98
4	G	801	DQ8	CAP-CAY-CAZ	-2.76	115.75	121.05
2	A	601	ADP	PA-O3A-PB	-2.73	123.47	132.83
2	E	601	ADP	C2-N1-C6	2.70	123.38	118.75
2	B	601	ADP	C4-C5-N7	-2.68	106.60	109.40
4	D	801	DQ8	CAK-CAV-CAQ	2.68	122.41	119.24
2	F	601	ADP	C4-C5-N7	-2.67	106.61	109.40
4	C	801	DQ8	CAG-CAM-CAW	-2.66	117.96	120.76
4	E	801	DQ8	CAX-CAZ-CAY	2.60	118.08	111.07
2	A	601	ADP	O3B-PB-O1B	2.59	120.83	110.68
2	A	601	ADP	N3-C2-N1	-2.57	124.67	128.68
2	A	601	ADP	O2A-PA-O1A	2.54	124.78	112.24
4	B	801	DQ8	CAX-CAZ-CAY	2.50	117.82	111.07
4	C	801	DQ8	CAJ-CAK-CAV	-2.48	117.41	120.34
4	C	801	DQ8	CAW-CAZ-CAX	-2.48	104.39	111.07
2	G	601	ADP	N6-C6-N1	2.47	123.71	118.57
2	G	601	ADP	O3B-PB-O2B	2.42	116.90	107.64
4	E	801	DQ8	CAW-CAZ-CAY	-2.42	104.55	111.07
2	C	601	ADP	C5'-C4'-C3'	-2.41	106.16	115.18
4	G	801	DQ8	CAK-CAV-CAU	-2.40	115.28	120.86
4	F	801	DQ8	CAO-CAX-CAZ	-2.34	116.55	121.05
4	C	801	DQ8	CAX-CAZ-CAY	2.32	117.33	111.07
2	B	601	ADP	O3B-PB-O3A	-2.30	96.92	104.64
4	C	801	DQ8	CAQ-CAV-CAU	-2.30	115.06	120.00
2	F	601	ADP	N3-C2-N1	-2.29	125.10	128.68
2	B	601	ADP	PA-O3A-PB	-2.27	125.04	132.83
4	G	801	DQ8	CAX-CAZ-CAY	2.27	117.19	111.07
2	B	601	ADP	O4'-C1'-C2'	-2.26	103.62	106.93
4	E	801	DQ8	CAK-CAV-CAQ	2.22	121.87	119.24
4	D	801	DQ8	CAX-CAZ-CAY	2.21	117.04	111.07
4	F	801	DQ8	CAR-CAS-SAT	2.19	116.18	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	801	DQ8	CAQ-CAY-CAZ	2.19	124.40	120.72
2	C	601	ADP	C3'-C2'-C1'	2.18	104.26	100.98
4	C	801	DQ8	CAM-CAW-CAL	2.16	121.19	117.97
2	C	601	ADP	C4-C5-N7	-2.15	107.16	109.40
4	F	801	DQ8	CAH-CAN-CAX	-2.15	118.50	120.76
4	B	801	DQ8	CAK-CAV-CAQ	2.14	121.77	119.24
2	D	601	ADP	N3-C2-N1	-2.14	125.34	128.68
4	E	801	DQ8	CAR-CAS-SAT	2.13	116.01	110.04
2	E	601	ADP	O3B-PB-O2B	2.12	115.75	107.64
4	A	801	DQ8	CAX-CAZ-CAY	2.12	116.79	111.07
2	F	601	ADP	C2-N1-C6	2.08	122.32	118.75
4	A	801	DQ8	CAQ-CAV-CAU	-2.07	115.56	120.00
2	C	601	ADP	C1'-N9-C4	-2.06	123.02	126.64
4	D	801	DQ8	CAQ-CAV-CAU	-2.05	115.59	120.00
4	D	801	DQ8	CAS-SAT-CAZ	2.05	106.70	103.53
2	A	601	ADP	O2B-PB-O3A	2.01	111.38	104.64
2	B	601	ADP	O2A-PA-O1A	2.01	122.18	112.24
2	E	601	ADP	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	C5'-O5'-PA-O2A
2	E	601	ADP	C3'-C4'-C5'-O5'
2	F	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	PA-O3A-PB-O1B
2	C	601	ADP	PA-O3A-PB-O2B
2	G	601	ADP	PA-O3A-PB-O2B
2	E	601	ADP	O4'-C4'-C5'-O5'
2	E	601	ADP	C5'-O5'-PA-O1A
2	C	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	C3'-C4'-C5'-O5'
4	G	801	DQ8	CAQ-CAY-CAZ-SAT
4	B	801	DQ8	CAQ-CAY-CAZ-SAT
4	C	801	DQ8	CAQ-CAY-CAZ-SAT
4	D	801	DQ8	CAQ-CAY-CAZ-SAT
4	B	801	DQ8	CAP-CAY-CAZ-SAT
4	C	801	DQ8	CAP-CAY-CAZ-SAT
4	E	801	DQ8	CAQ-CAY-CAZ-SAT
4	D	801	DQ8	CAP-CAY-CAZ-SAT

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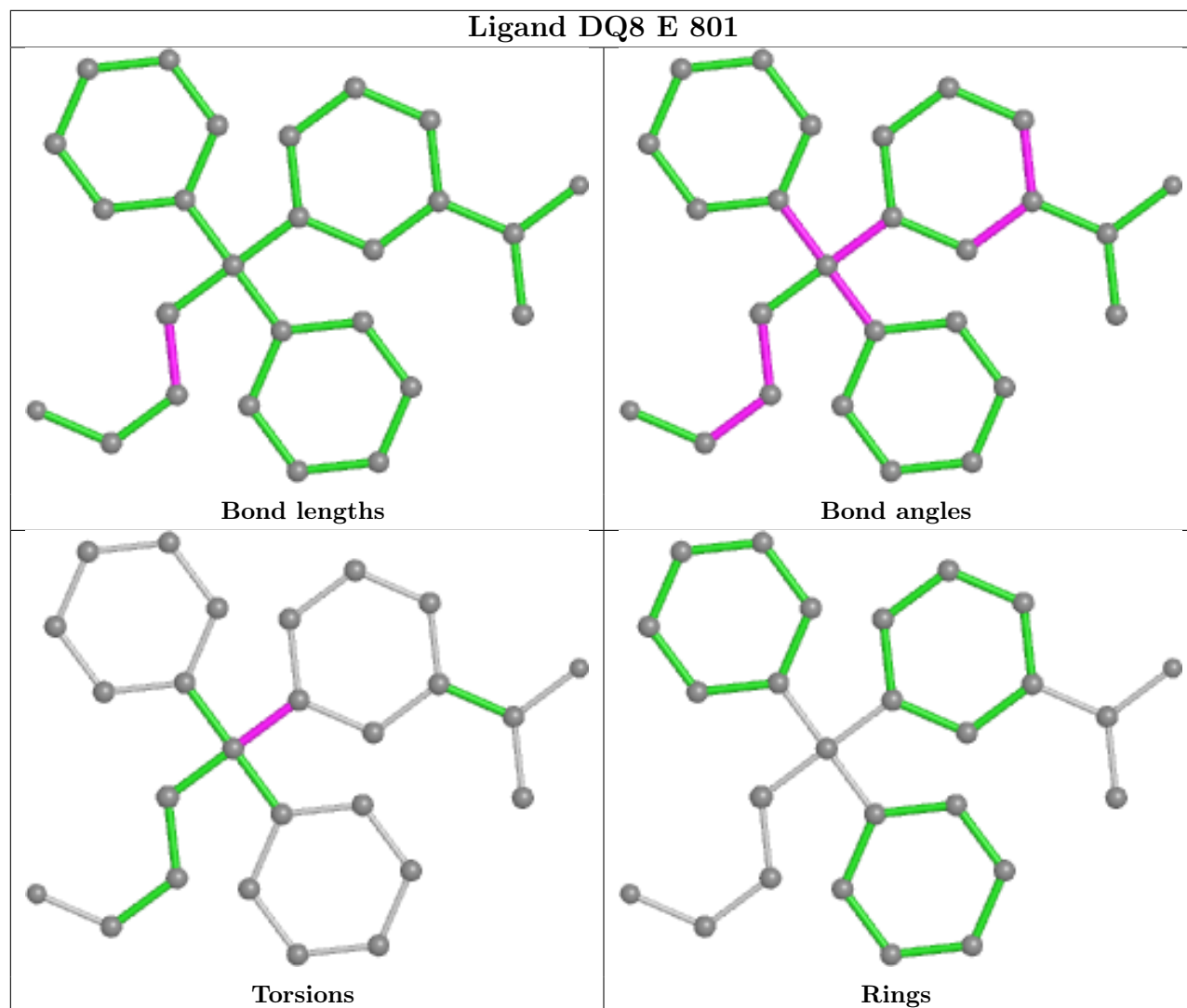
Mol	Chain	Res	Type	Atoms
4	G	801	DQ8	CAP-CAY-CAZ-SAT
2	A	601	ADP	PA-O3A-PB-O2B
2	A	601	ADP	PA-O3A-PB-O3B
2	B	601	ADP	PA-O3A-PB-O3B
2	E	601	ADP	C5'-O5'-PA-O3A
2	D	601	ADP	O4'-C4'-C5'-O5'

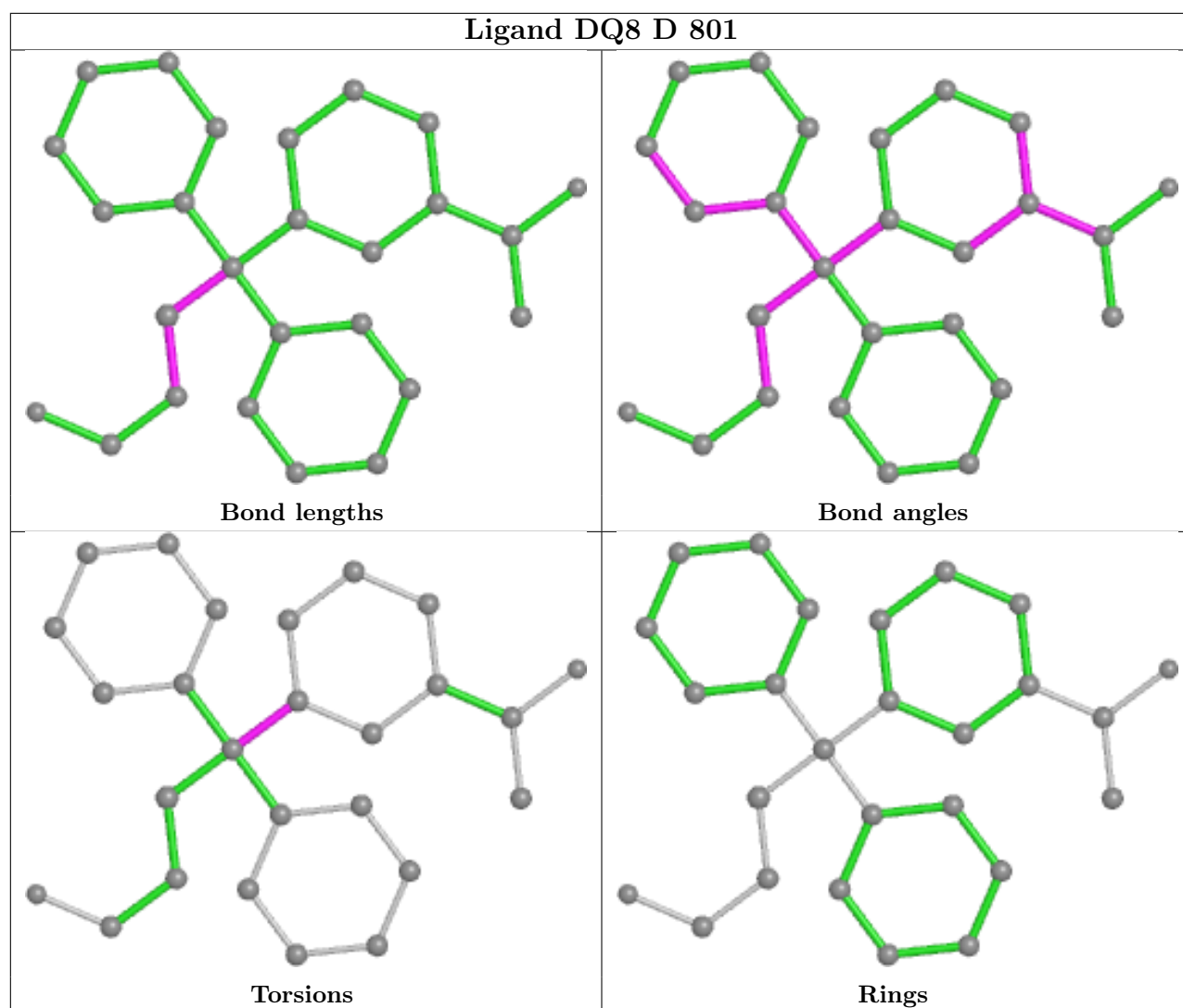
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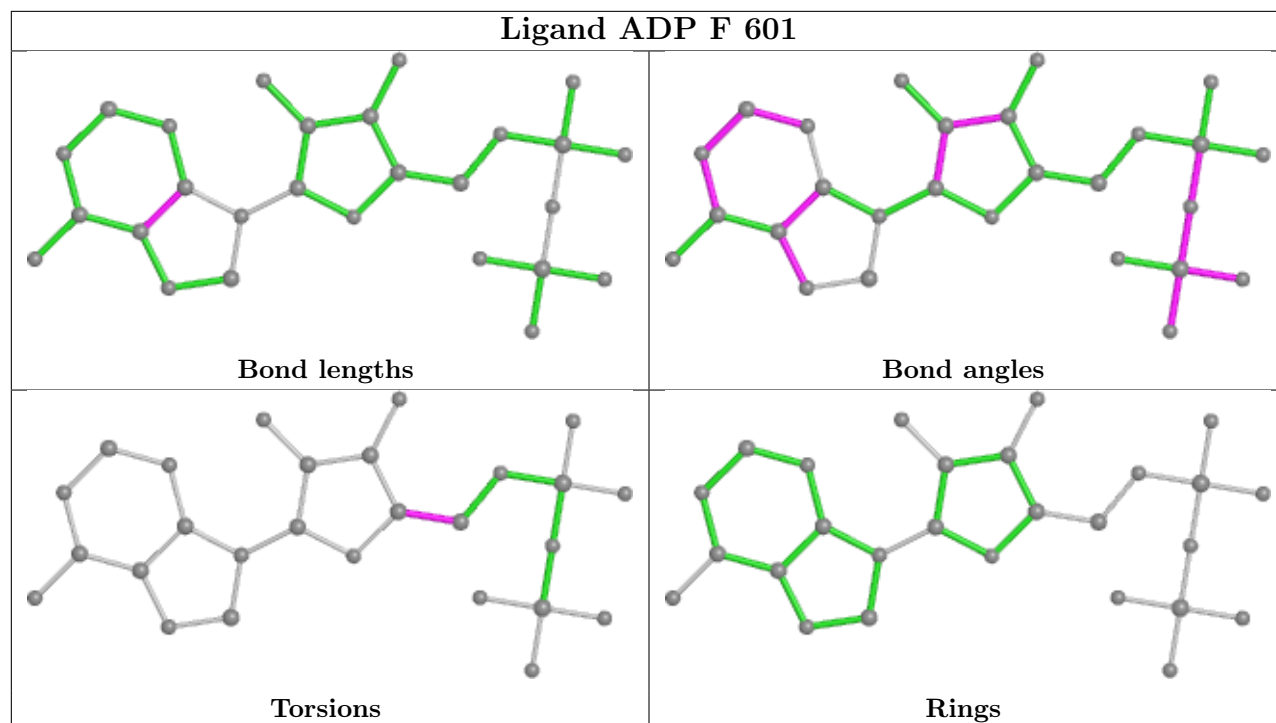
12 monomers are involved in 63 short contacts:

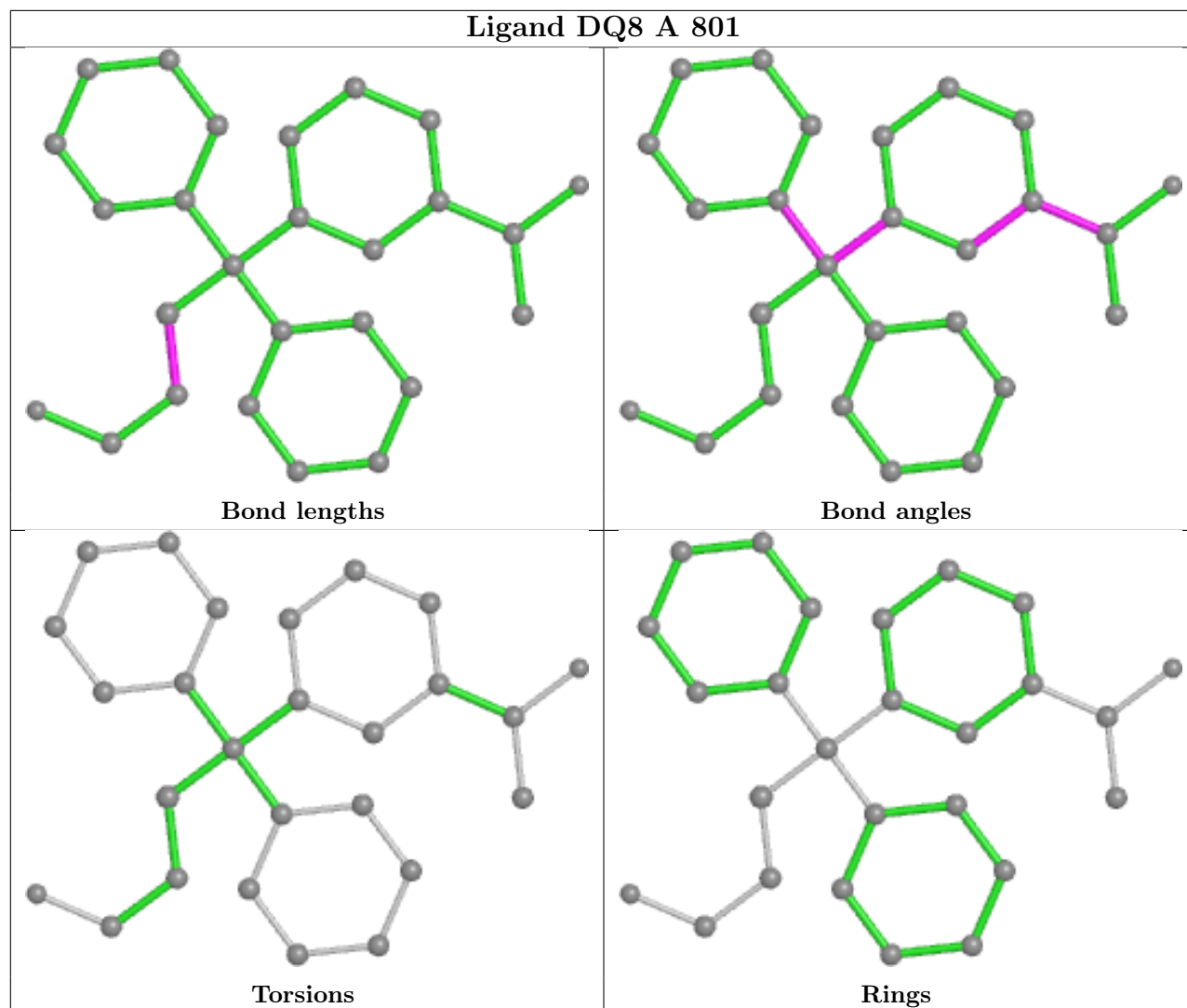
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	801	DQ8	9	0
4	D	801	DQ8	4	0
2	F	601	ADP	3	0
4	A	801	DQ8	7	0
2	G	601	ADP	2	0
4	C	801	DQ8	2	0
4	F	801	DQ8	7	0
4	G	801	DQ8	7	0
2	E	601	ADP	5	0
2	D	601	ADP	5	0
2	C	601	ADP	4	0
4	B	801	DQ8	8	0

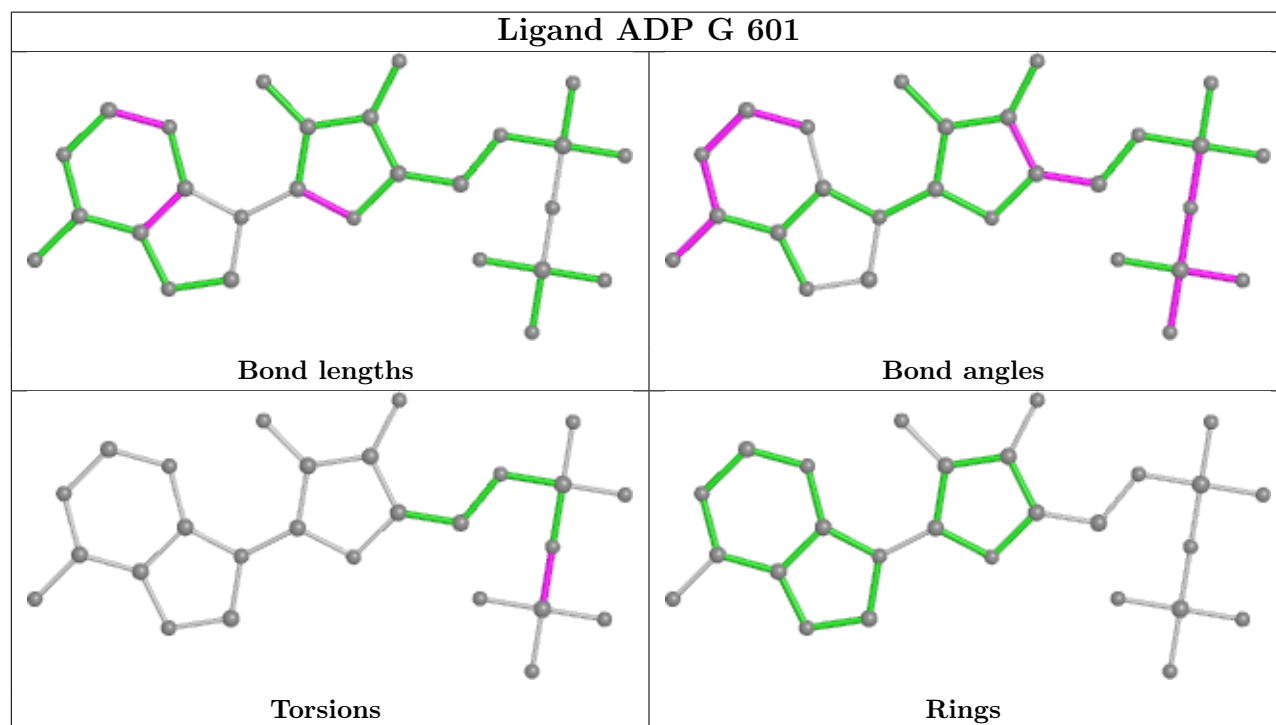
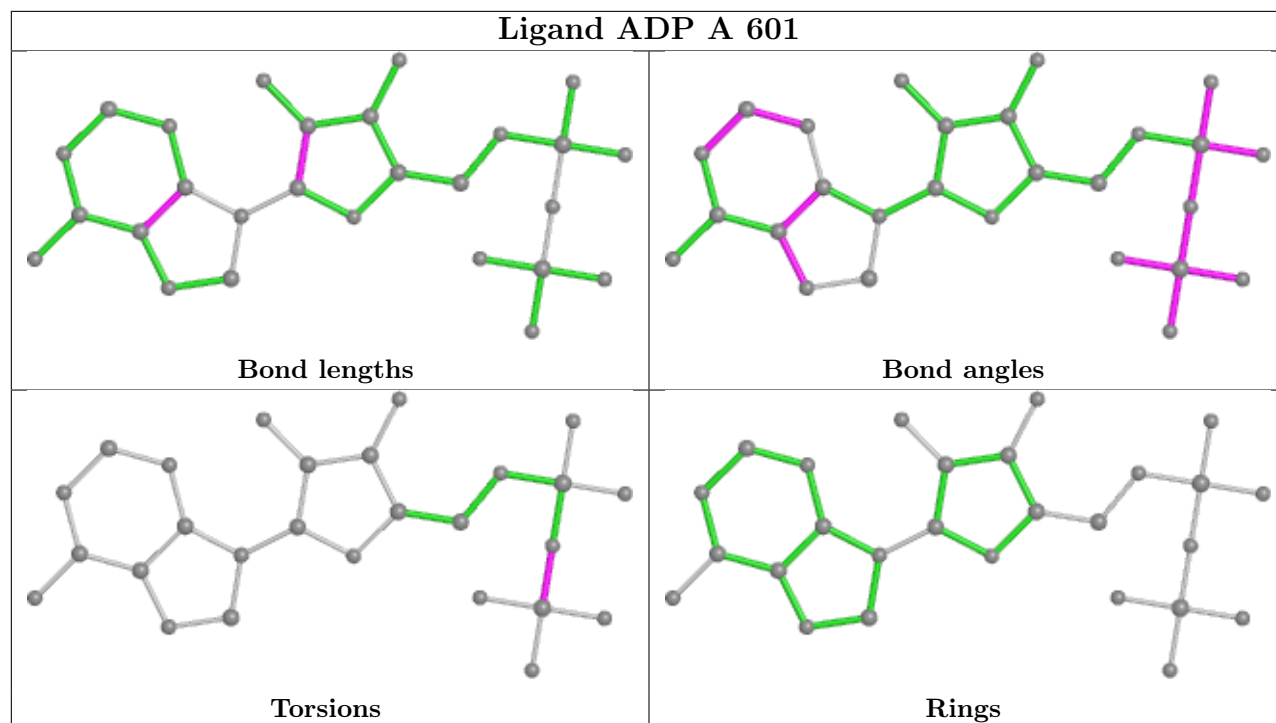
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

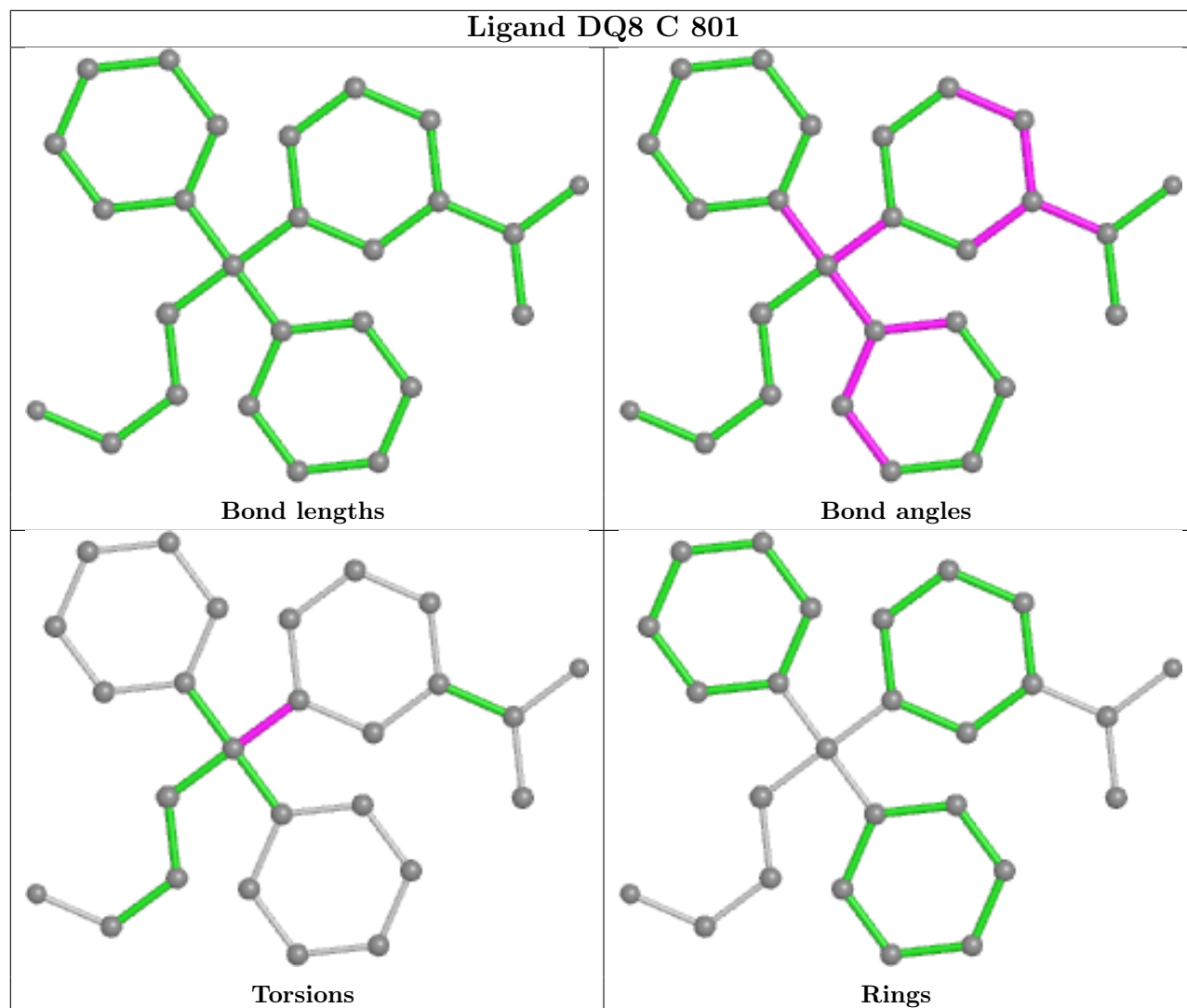


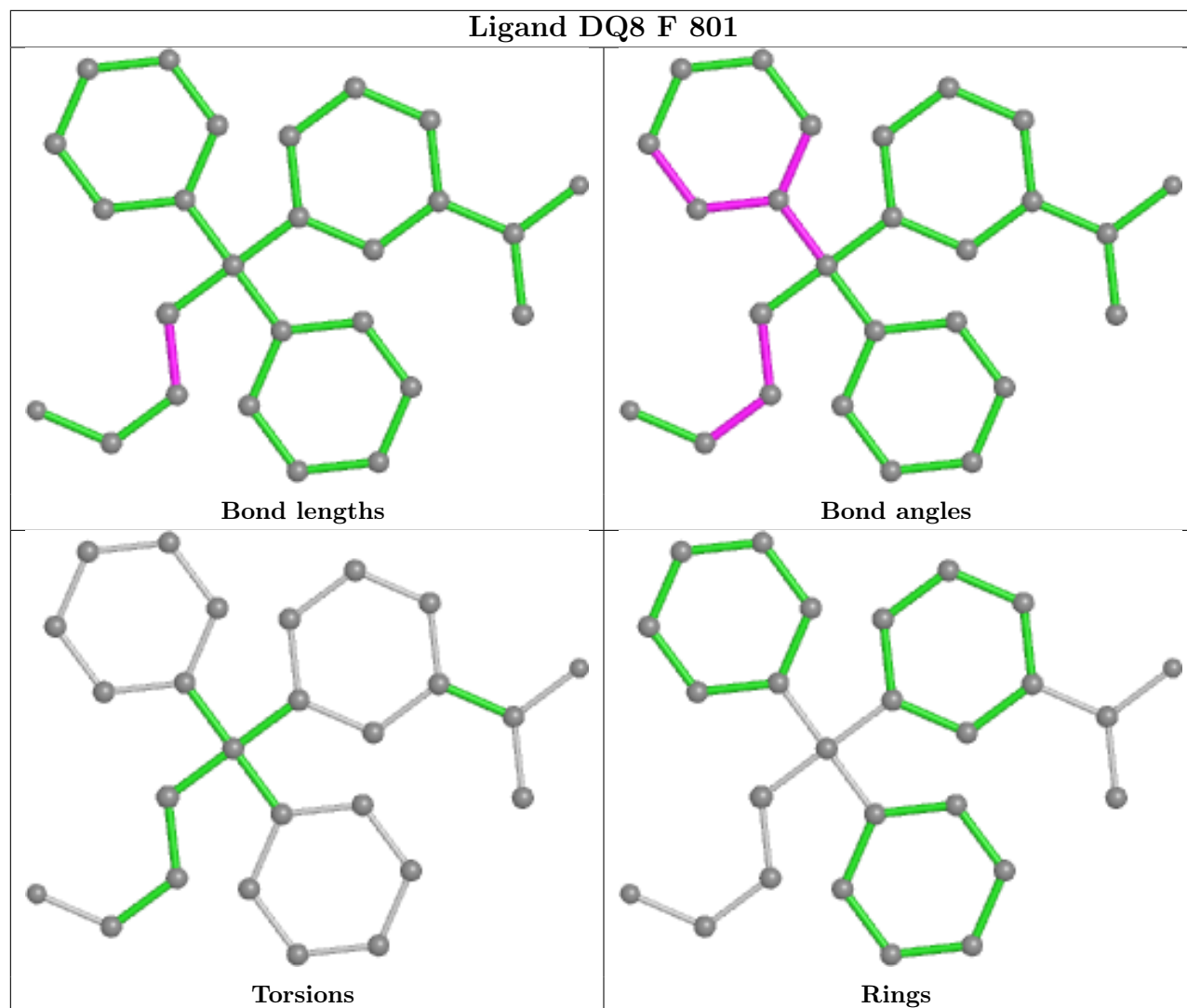


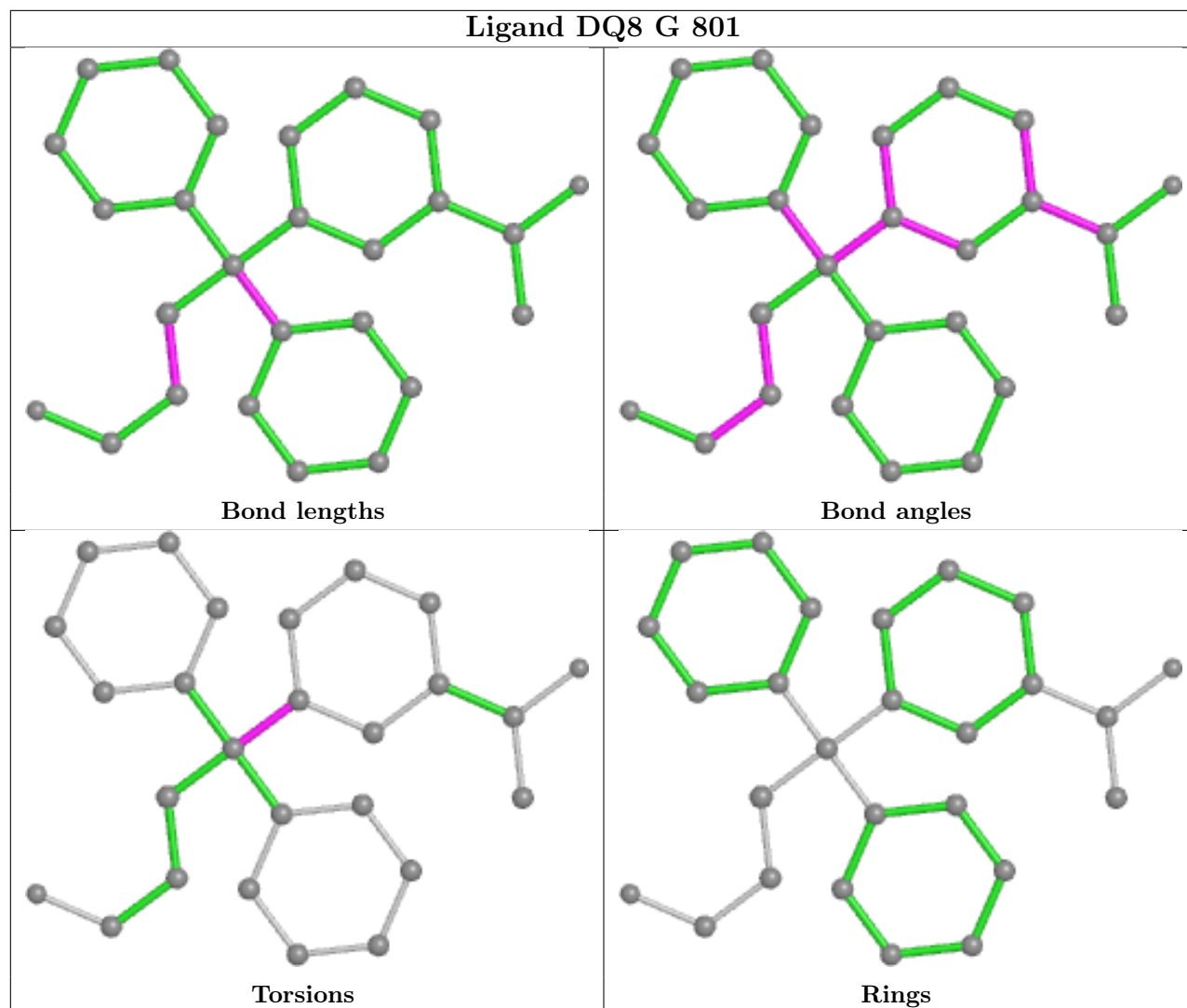


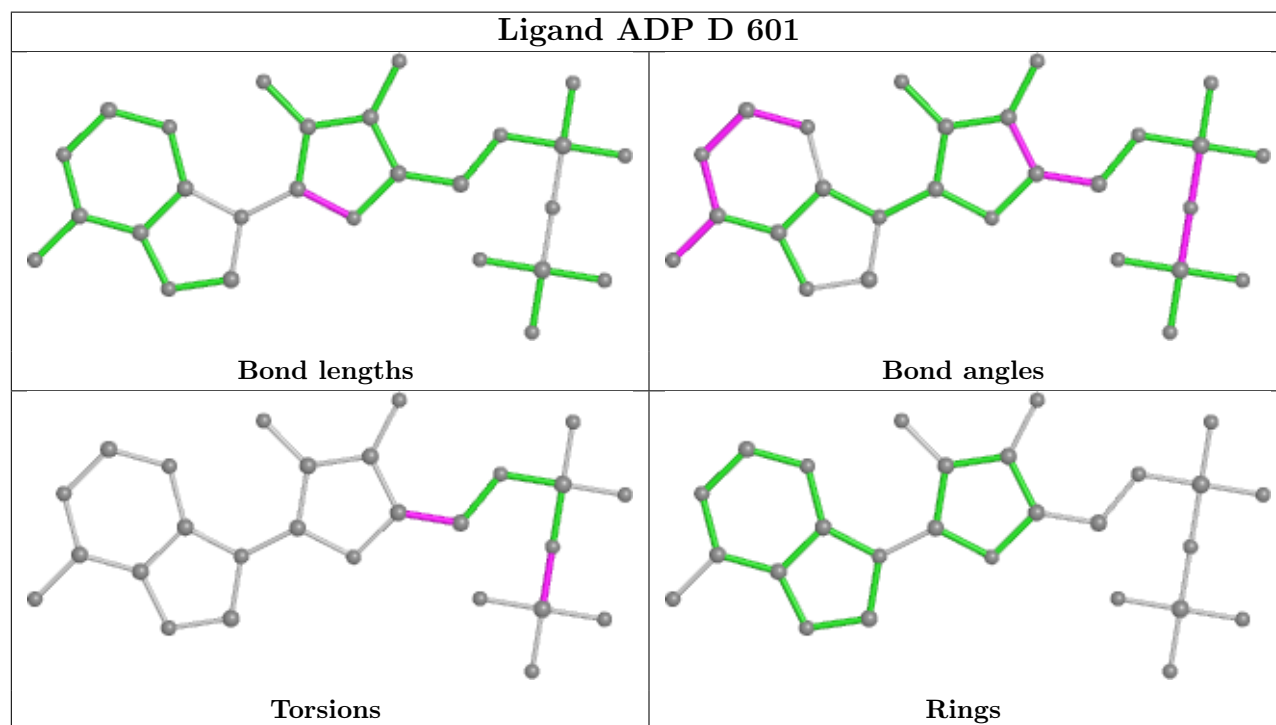
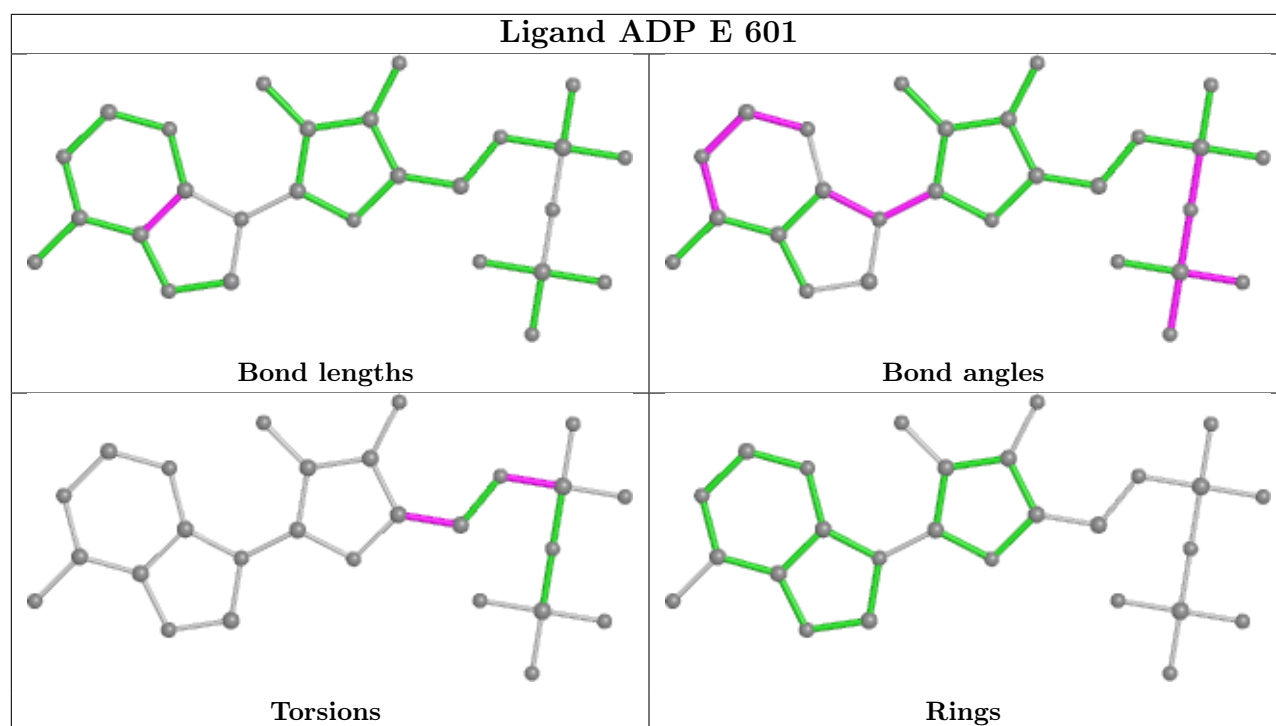


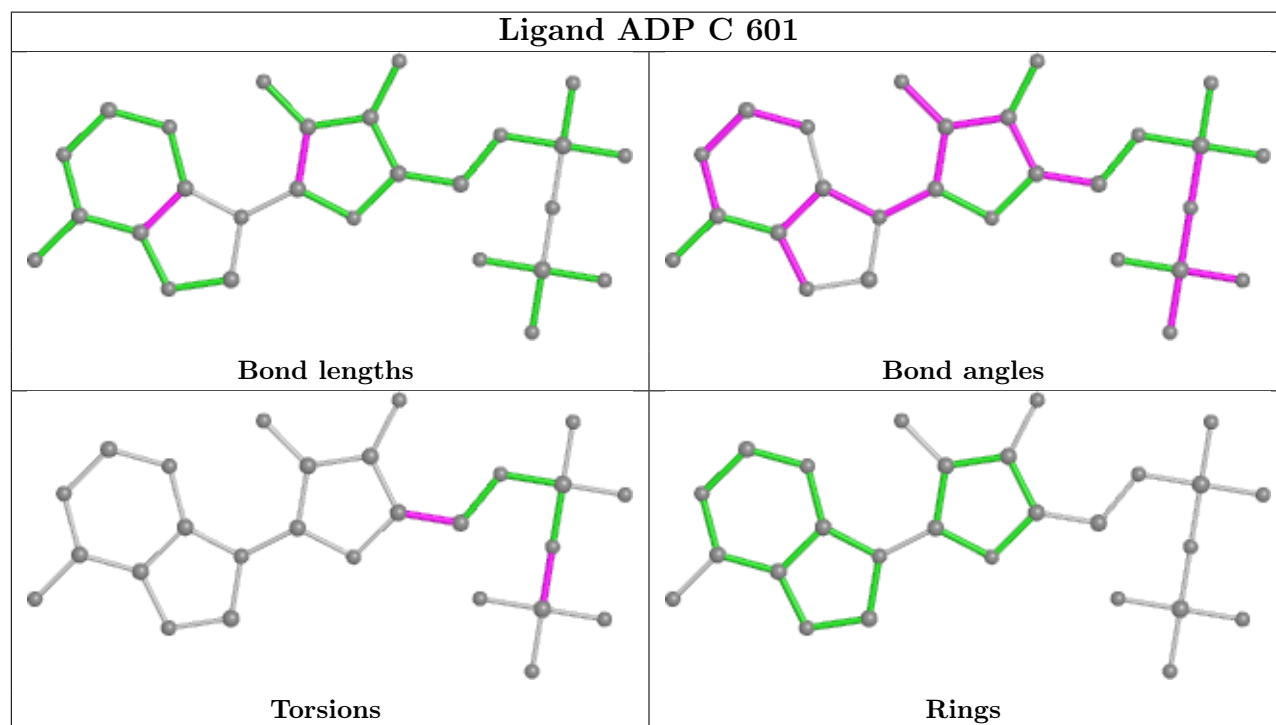
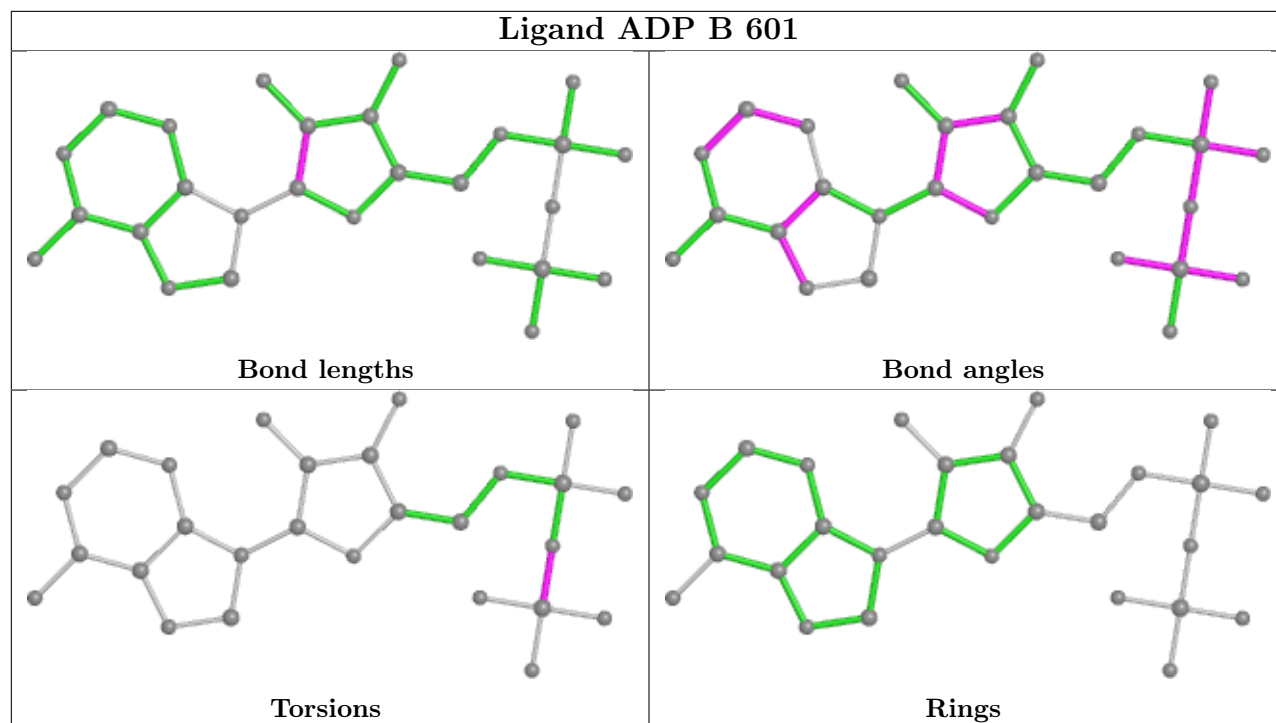


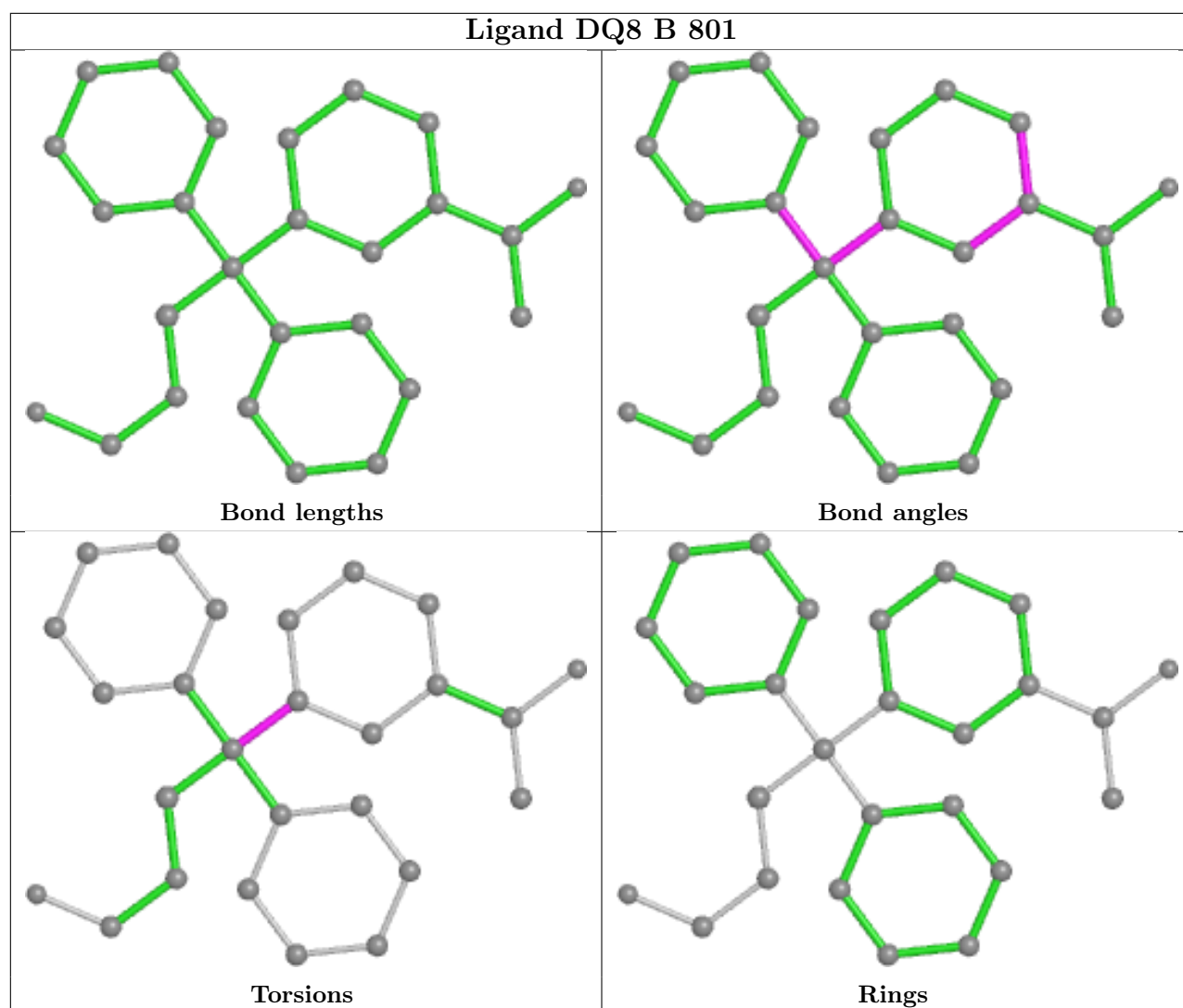












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	322/368 (87%)	0.50	38 (11%) 4 5	33, 54, 90, 112	0
1	B	324/368 (88%)	0.54	41 (12%) 3 4	34, 53, 92, 104	0
1	C	325/368 (88%)	0.26	23 (7%) 16 19	28, 50, 86, 113	0
1	D	322/368 (87%)	0.37	27 (8%) 11 13	28, 50, 92, 114	0
1	E	321/368 (87%)	0.70	51 (15%) 1 2	42, 67, 99, 119	0
1	F	319/368 (86%)	0.77	59 (18%) 1 1	41, 71, 106, 117	0
1	G	318/368 (86%)	1.08	73 (22%) 0 0	46, 81, 122, 140	0
All	All	2251/2576 (87%)	0.60	312 (13%) 2 3	28, 61, 105, 140	0

All (312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	309	VAL	8.6
1	G	308	HIS	8.2
1	G	58	ALA	7.4
1	E	149	ASP	6.9
1	G	359	ILE	6.7
1	G	102	PHE	6.5
1	D	256	VAL	6.5
1	G	307	PRO	6.4
1	A	256	VAL	6.3
1	B	152	THR	5.9
1	F	363	PRO	5.9
1	A	149	ASP	5.7
1	F	148	THR	5.6
1	D	255	LEU	5.6
1	C	364	GLU	5.5
1	G	67	THR	5.4
1	E	263	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	149	ASP	5.4
1	G	193	GLY	5.3
1	G	191	LYS	5.3
1	G	325	GLY	5.3
1	B	129	GLU	5.1
1	E	150	ASN	5.1
1	G	363	PRO	5.1
1	A	101	ILE	5.0
1	C	365	VAL	5.0
1	E	186	ASP	5.0
1	B	255	LEU	5.0
1	B	151	GLY	5.0
1	B	149	ASP	4.9
1	A	102	PHE	4.9
1	G	190	ASN	4.9
1	G	264	VAL	4.9
1	G	188	PRO	4.7
1	A	264	VAL	4.7
1	F	102	PHE	4.7
1	A	188	PRO	4.7
1	E	153	GLU	4.6
1	G	332	ILE	4.5
1	B	102	PHE	4.5
1	B	148	THR	4.4
1	F	263	LEU	4.4
1	F	301	ALA	4.4
1	G	303	VAL	4.4
1	E	360	LEU	4.3
1	B	264	VAL	4.3
1	G	56	GLY	4.3
1	B	189	ARG	4.3
1	G	45	PRO	4.2
1	A	257	LYS	4.2
1	A	238	VAL	4.2
1	E	239	PHE	4.2
1	G	263	LEU	4.2
1	B	238	VAL	4.2
1	C	237	SER	4.1
1	F	155	SER	4.1
1	F	238	VAL	4.0
1	B	361	ASN	4.0
1	F	101	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	153	GLU	4.0
1	G	192	ARG	4.0
1	G	328	THR	4.0
1	A	263	LEU	4.0
1	G	63	ARG	3.9
1	E	245	MET	3.9
1	F	308	HIS	3.9
1	G	329	ARG	3.9
1	G	334	ALA	3.9
1	B	124	GLU	3.8
1	E	332	ILE	3.8
1	G	238	VAL	3.8
1	F	360	LEU	3.8
1	G	57	LEU	3.8
1	G	103	ALA	3.8
1	G	304	GLU	3.8
1	G	115	MET	3.8
1	B	147	LEU	3.7
1	G	327	ARG	3.7
1	C	238	VAL	3.7
1	G	305	ARG	3.7
1	G	333	ILE	3.7
1	D	358	ASN	3.7
1	E	262	ASN	3.7
1	E	102	PHE	3.7
1	F	262	ASN	3.6
1	F	193	GLY	3.6
1	E	101	ILE	3.6
1	E	122	ASN	3.6
1	G	306	THR	3.6
1	B	332	ILE	3.6
1	G	310	PRO	3.6
1	B	150	ASN	3.6
1	E	185	PHE	3.6
1	F	326	GLY	3.6
1	A	360	LEU	3.6
1	B	333	ILE	3.6
1	C	153	GLU	3.6
1	B	103	ALA	3.5
1	G	360	LEU	3.5
1	B	101	ILE	3.5
1	F	332	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	362	LYS	3.5
1	D	264	VAL	3.5
1	C	363	PRO	3.5
1	A	255	LEU	3.5
1	D	258	ILE	3.5
1	E	256	VAL	3.4
1	D	263	LEU	3.4
1	A	189	ARG	3.4
1	G	44	ASP	3.4
1	E	307	PRO	3.4
1	B	360	LEU	3.4
1	D	303	VAL	3.4
1	B	303	VAL	3.4
1	D	152	THR	3.4
1	E	238	VAL	3.4
1	F	362	LYS	3.4
1	E	309	VAL	3.4
1	F	100	THR	3.3
1	E	257	LYS	3.3
1	A	239	PHE	3.3
1	F	239	PHE	3.3
1	F	327	ARG	3.3
1	F	264	VAL	3.3
1	A	125	TYR	3.3
1	B	100	THR	3.3
1	A	100	THR	3.3
1	B	240	SER	3.3
1	A	258	ILE	3.3
1	G	92	GLU	3.3
1	G	47	ARG	3.3
1	F	122	ASN	3.2
1	G	55	GLY	3.2
1	D	254	GLU	3.2
1	F	153[A]	GLU	3.2
1	B	192	ARG	3.2
1	E	131	PRO	3.2
1	B	17	LYS	3.2
1	D	257	LYS	3.2
1	F	93	VAL	3.2
1	E	264	VAL	3.2
1	G	99	CYS	3.2
1	F	307	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	129	GLU	3.1
1	E	305	ARG	3.1
1	F	312	ARG	3.1
1	A	152	THR	3.1
1	E	126	THR	3.1
1	G	23	VAL	3.1
1	A	240	SER	3.1
1	C	263	LEU	3.1
1	D	151	GLY	3.1
1	E	300	THR	3.1
1	F	95	MET	3.1
1	G	48	LYS	3.1
1	E	333	ILE	3.0
1	A	103	ALA	3.0
1	E	301	ALA	3.0
1	A	359	ILE	3.0
1	E	100	THR	3.0
1	G	46	VAL	3.0
1	A	333	ILE	3.0
1	A	262	ASN	3.0
1	G	185	PHE	3.0
1	F	288	ILE	3.0
1	F	103	ALA	3.0
1	B	363	PRO	3.0
1	C	288	ILE	3.0
1	C	152	THR	3.0
1	G	293	LEU	3.0
1	G	101	ILE	2.9
1	A	304	GLU	2.9
1	E	129	GLU	2.9
1	F	45	PRO	2.9
1	C	122	ASN	2.9
1	C	366	ASN	2.9
1	D	262	ASN	2.9
1	F	18	ASN	2.9
1	C	151	GLY	2.9
1	B	263	LEU	2.9
1	C	101	ILE	2.9
1	E	151	GLY	2.9
1	G	239	PHE	2.9
1	C	258	ILE	2.9
1	C	362	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	153	GLU	2.8
1	G	151	GLY	2.8
1	F	189	ARG	2.8
1	G	322	ASP	2.8
1	E	190	ASN	2.8
1	D	238	VAL	2.8
1	F	154	PHE	2.8
1	G	240	SER	2.8
1	G	59	ASP	2.8
1	G	136	ILE	2.8
1	A	129	GLU	2.8
1	B	331	SER	2.8
1	E	240	SER	2.8
1	D	240	SER	2.7
1	D	288	ILE	2.7
1	G	152	THR	2.7
1	A	191	LYS	2.7
1	G	311	TYR	2.7
1	G	258	ILE	2.7
1	G	149	ASP	2.7
1	B	262	ASN	2.7
1	A	246	LYS	2.7
1	F	237	SER	2.7
1	F	304	GLU	2.7
1	F	161	LEU	2.7
1	G	154	PHE	2.7
1	E	246	LYS	2.7
1	B	239	PHE	2.6
1	E	152	THR	2.6
1	F	257	LYS	2.6
1	F	30	LEU	2.6
1	E	135	ILE	2.6
1	A	151	GLY	2.6
1	F	331	SER	2.6
1	G	189	ARG	2.6
1	D	237	SER	2.6
1	B	237	SER	2.6
1	A	148	THR	2.5
1	D	148	THR	2.5
1	A	303	VAL	2.5
1	C	256	VAL	2.5
1	E	293	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	153	GLU	2.5
1	D	246	LYS	2.5
1	F	131	PRO	2.5
1	F	192	ARG	2.5
1	B	261	LEU	2.5
1	A	332	ILE	2.5
1	D	360	LEU	2.5
1	E	191	LYS	2.5
1	C	161	LEU	2.5
1	F	333	ILE	2.5
1	A	331	SER	2.4
1	G	301	ALA	2.4
1	B	312	ARG	2.4
1	G	355	ARG	2.4
1	E	361	ASN	2.4
1	E	97	TYR	2.4
1	B	191	LYS	2.4
1	F	136	ILE	2.4
1	G	230	ALA	2.4
1	E	331	SER	2.4
1	E	234	ARG	2.4
1	F	266	LEU	2.4
1	E	187	ASP	2.4
1	G	300	THR	2.4
1	C	262	ASN	2.4
1	F	150	ASN	2.4
1	G	231	TYR	2.3
1	C	240	SER	2.3
1	F	302	LEU	2.3
1	D	102	PHE	2.3
1	E	124	GLU	2.3
1	E	306	THR	2.3
1	F	287	ASN	2.3
1	D	101	ILE	2.3
1	D	359	ILE	2.3
1	E	304	GLU	2.3
1	E	103	ALA	2.3
1	G	100	THR	2.3
1	C	264	VAL	2.3
1	F	123	GLU	2.3
1	E	193	GLY	2.3
1	G	271	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	136	ILE	2.3
1	G	194	VAL	2.3
1	F	83	ARG	2.3
1	A	245	MET	2.3
1	F	300	THR	2.3
1	G	135	ILE	2.3
1	A	261	LEU	2.3
1	D	310	PRO	2.3
1	A	330	THR	2.2
1	B	125	TYR	2.2
1	B	190	ASN	2.2
1	C	287	ASN	2.2
1	F	190	ASN	2.2
1	F	361	ASN	2.2
1	D	161	LEU	2.2
1	E	326	GLY	2.2
1	C	150	ASN	2.2
1	F	234	ARG	2.2
1	B	247	GLU	2.2
1	F	185	PHE	2.2
1	E	125	TYR	2.1
1	F	126	THR	2.1
1	C	154	PHE	2.1
1	G	124	GLU	2.1
1	A	121	PRO	2.1
1	F	31	ALA	2.1
1	A	309	VAL	2.1
1	D	305	ARG	2.1
1	F	94	ILE	2.1
1	G	312	ARG	2.1
1	F	188	PRO	2.1
1	E	325	GLY	2.1
1	E	189	ARG	2.1
1	D	186	ASP	2.1
1	B	246	LYS	2.1
1	G	297	ARG	2.1
1	G	148	THR	2.1
1	B	121	PRO	2.0
1	F	305	ARG	2.0
1	A	124	GLU	2.0
1	G	167	GLU	2.0
1	B	307	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	125	TYR	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, 95th 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
5	CL	G	1364	1/1	0.40	0.34	106,106,106,106	0
5	CL	A	1366	1/1	0.72	0.15	89,89,89,89	0
5	CL	B	1365	1/1	0.83	0.09	78,78,78,78	0
5	CL	D	1364	1/1	0.84	0.12	77,77,77,77	0
5	CL	E	1364	1/1	0.85	0.22	90,90,90,90	0
4	DQ8	F	801	26/26	0.87	0.25	60,75,84,110	0
4	DQ8	E	801	26/26	0.88	0.22	57,67,77,98	0
5	CL	A	1364	1/1	0.89	0.08	75,75,75,75	0
4	DQ8	A	801	26/26	0.89	0.23	43,54,63,85	0
5	CL	A	1365	1/1	0.90	0.07	95,95,95,95	0
5	CL	C	1369	1/1	0.92	0.11	97,97,97,97	0
4	DQ8	C	801	26/26	0.92	0.22	39,49,61,83	0
4	DQ8	B	801	26/26	0.93	0.22	44,53,67,82	0
4	DQ8	G	801	26/26	0.93	0.22	49,57,68,85	0
3	MG	F	701	1/1	0.93	0.15	50,50,50,50	0
4	DQ8	D	801	26/26	0.93	0.21	38,47,60,79	0
3	MG	C	701	1/1	0.93	0.23	40,40,40,40	0
5	CL	F	1364	1/1	0.95	0.15	89,89,89,89	0
5	CL	A	1367	1/1	0.95	0.19	73,73,73,73	0
3	MG	B	701	1/1	0.96	0.18	37,37,37,37	0
2	ADP	E	601	27/27	0.96	0.16	45,54,61,71	0
2	ADP	F	601	27/27	0.96	0.16	45,55,70,77	0

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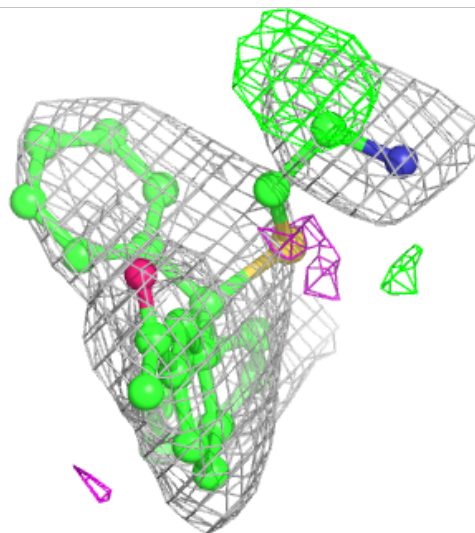
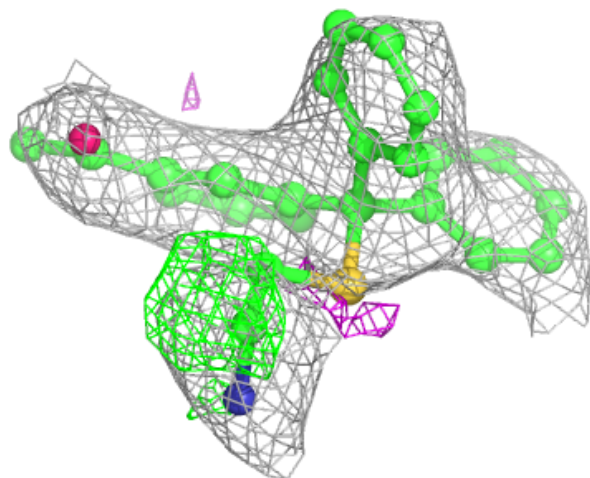
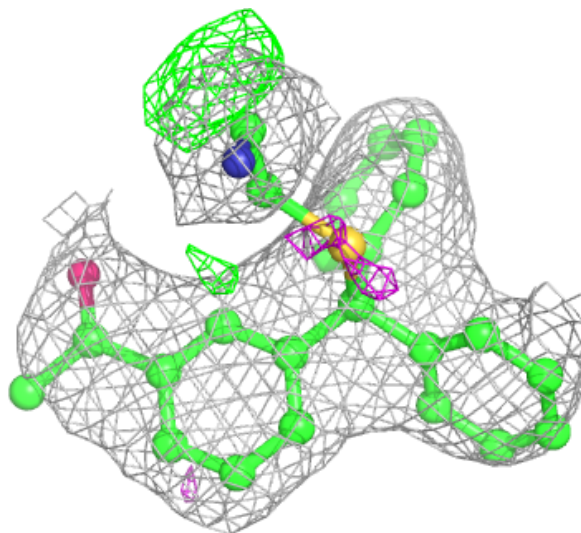
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	B	1364	1/1	0.96	0.32	80,80,80,80	0
3	MG	G	701	1/1	0.96	0.28	45,45,45,45	0
5	CL	D	1363	1/1	0.97	0.10	79,79,79,79	0
3	MG	D	701	1/1	0.97	0.18	35,35,35,35	0
5	CL	C	1367	1/1	0.97	0.29	62,62,62,62	0
5	CL	C	1368	1/1	0.97	0.09	56,56,56,56	0
3	MG	E	701	1/1	0.97	0.20	50,50,50,50	0
6	SO4	D	1362	5/5	0.97	0.12	54,54,63,68	0
2	ADP	B	601	27/27	0.98	0.16	35,42,48,58	0
2	ADP	G	601	27/27	0.98	0.14	46,54,59,64	0
2	ADP	C	601	27/27	0.98	0.16	28,38,42,48	0
2	ADP	D	601	27/27	0.98	0.14	28,40,45,51	0
2	ADP	A	601	27/27	0.98	0.13	34,41,47,50	0
3	MG	A	701	1/1	0.99	0.16	35,35,35,35	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.

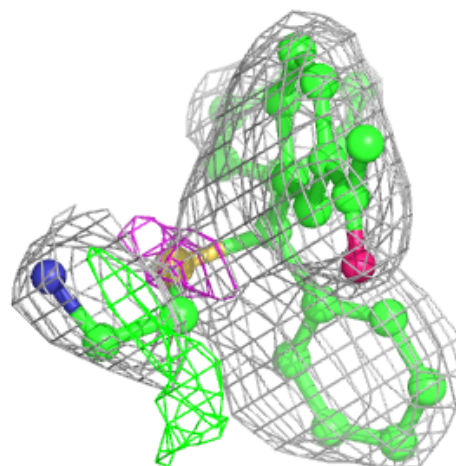
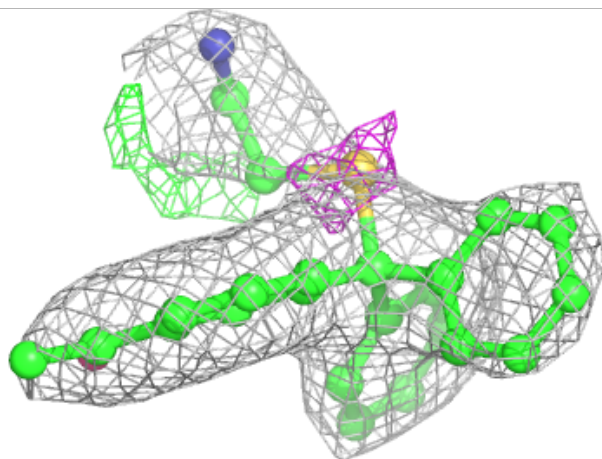
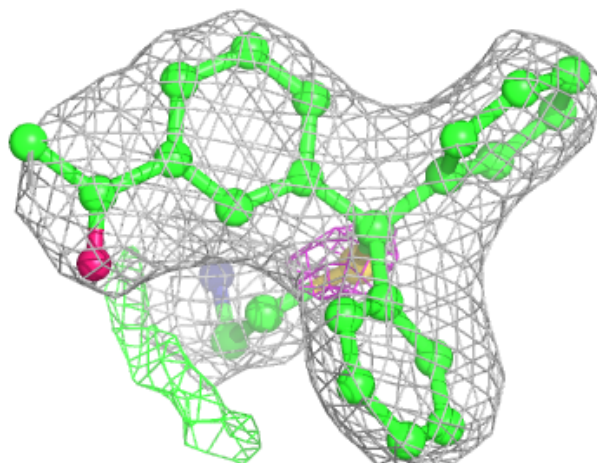
Electron density around DQ8 F 801:

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



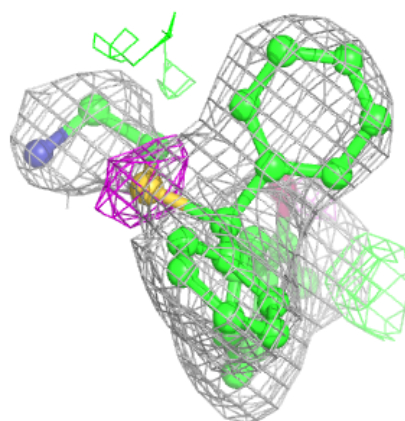
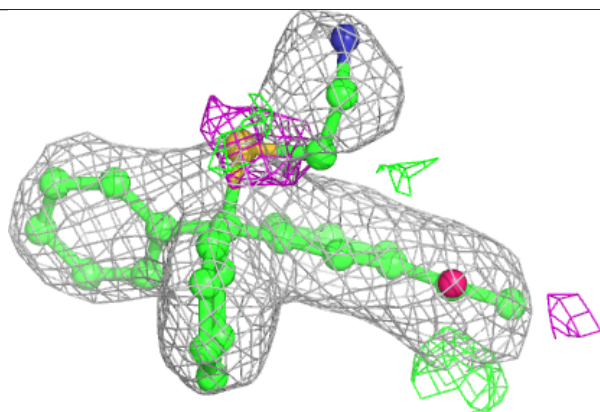
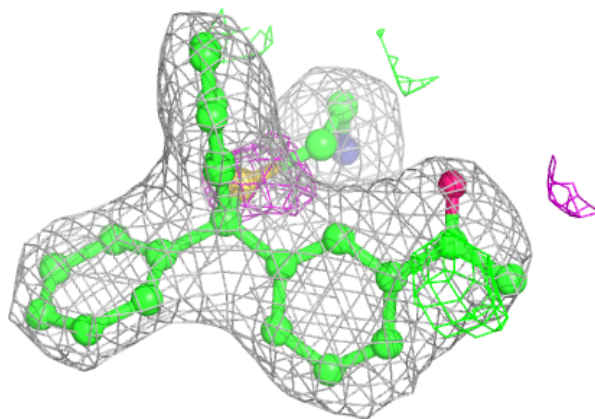
Electron density around DQ8 E 801:

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



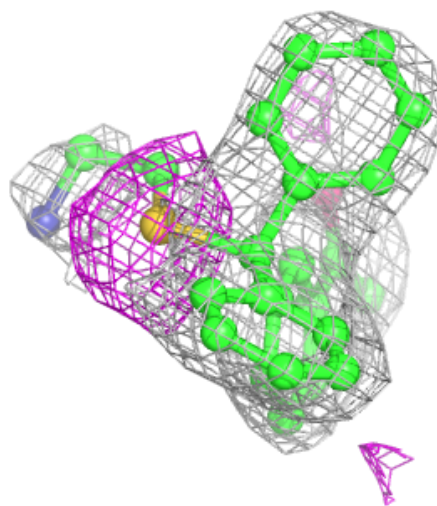
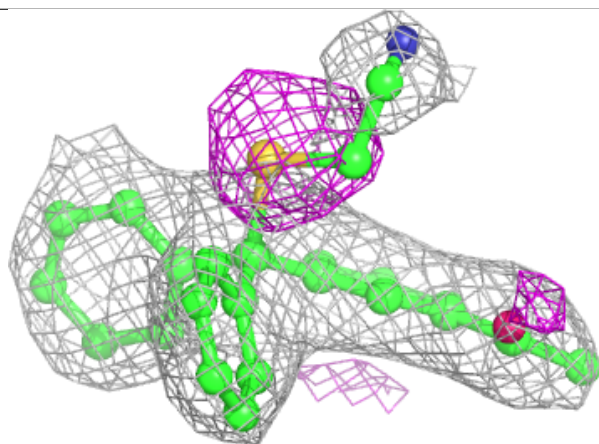
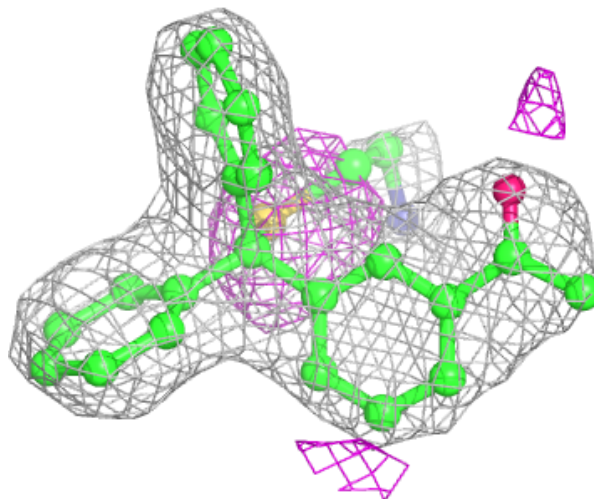
Electron density around DQ8 A 801:

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



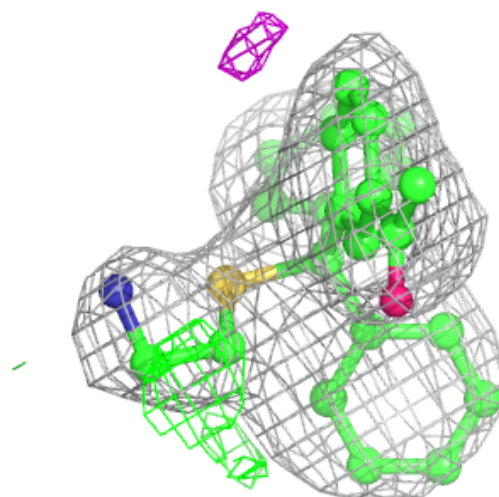
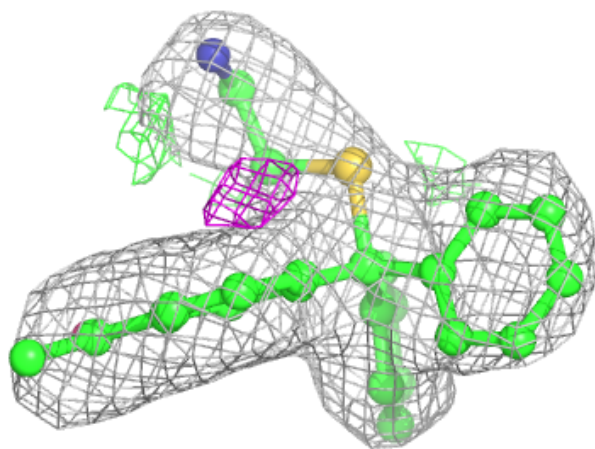
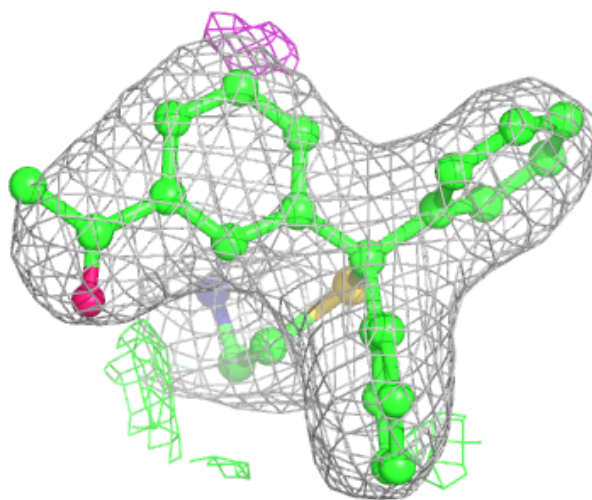
Electron density around DQ8 C 801:

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



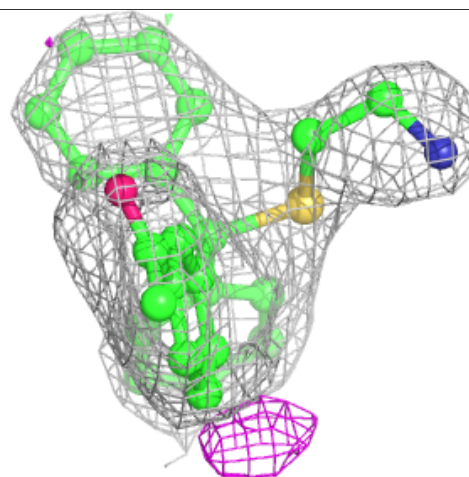
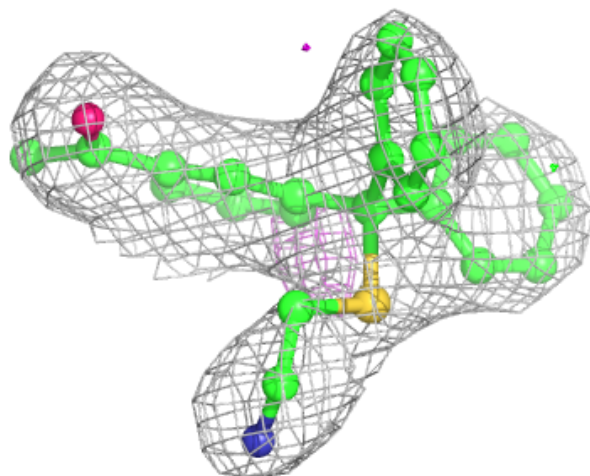
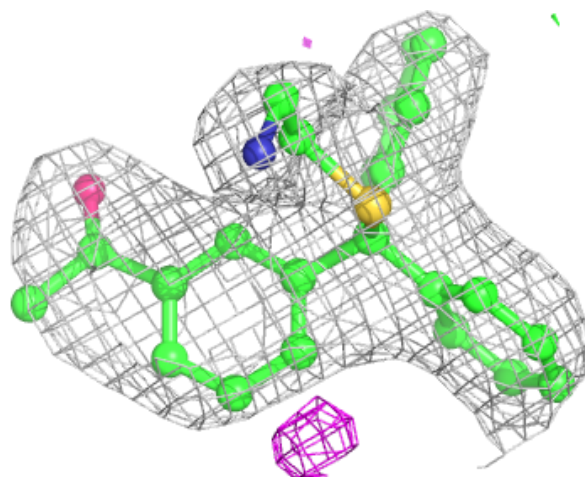
Electron density around DQ8 B 801:

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



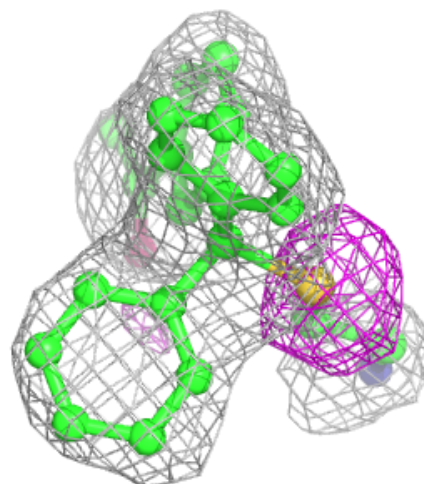
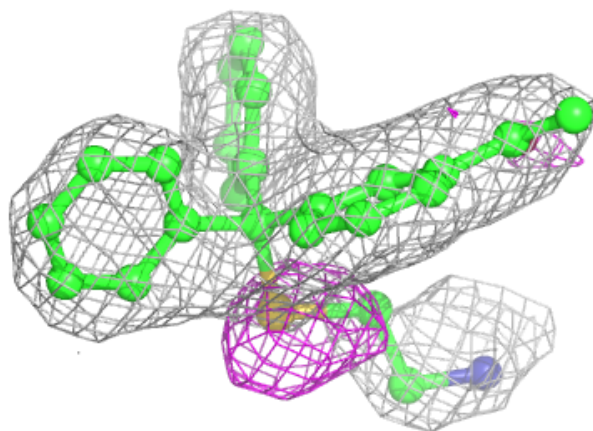
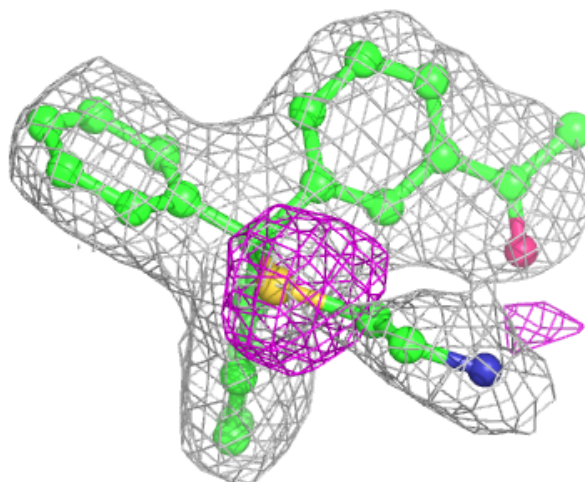
Electron density around DQ8 G 801:

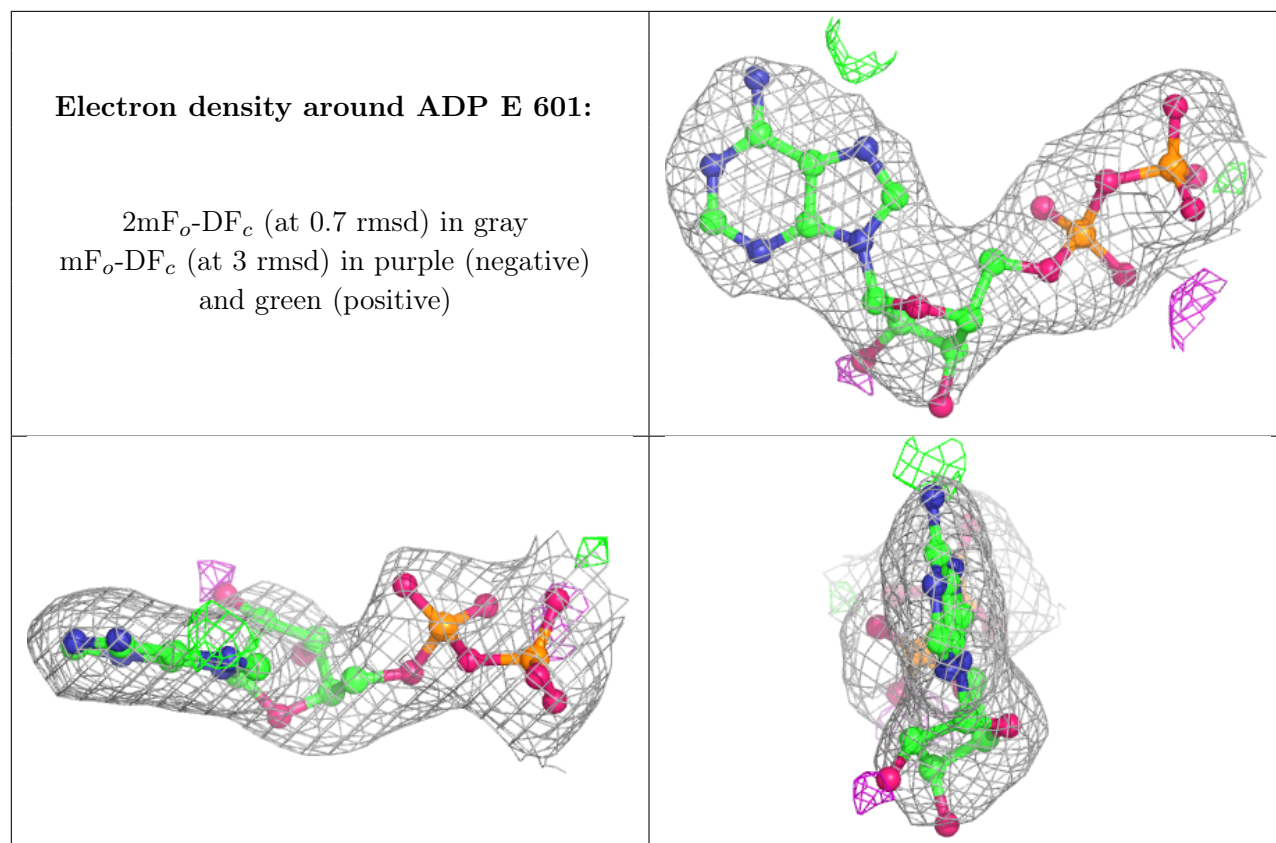
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DQ8 D 801:

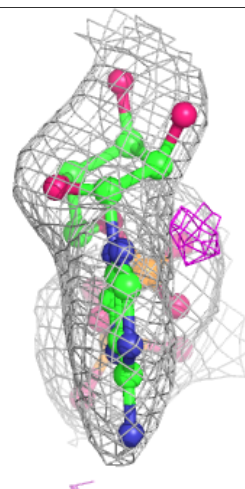
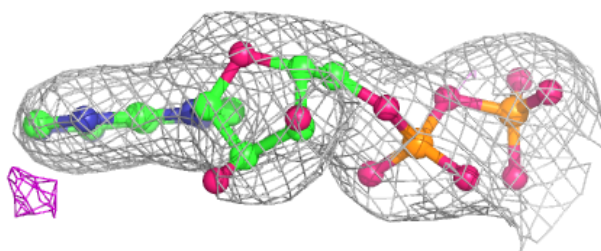
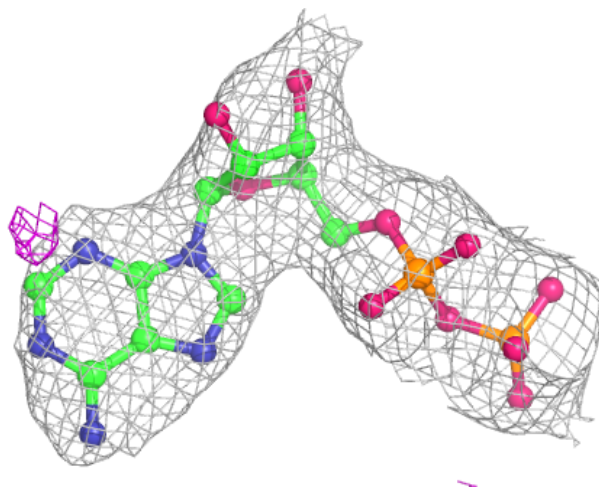
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

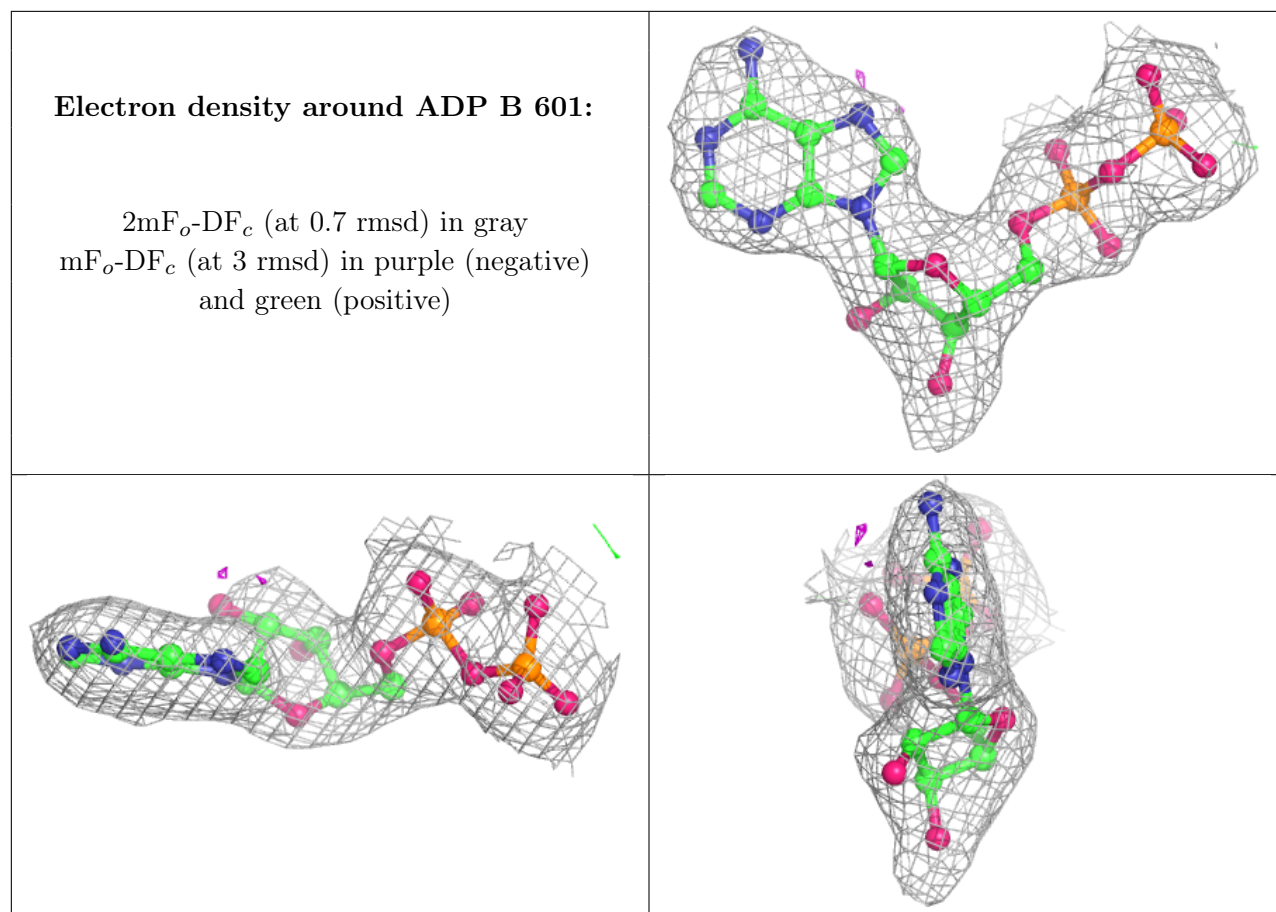


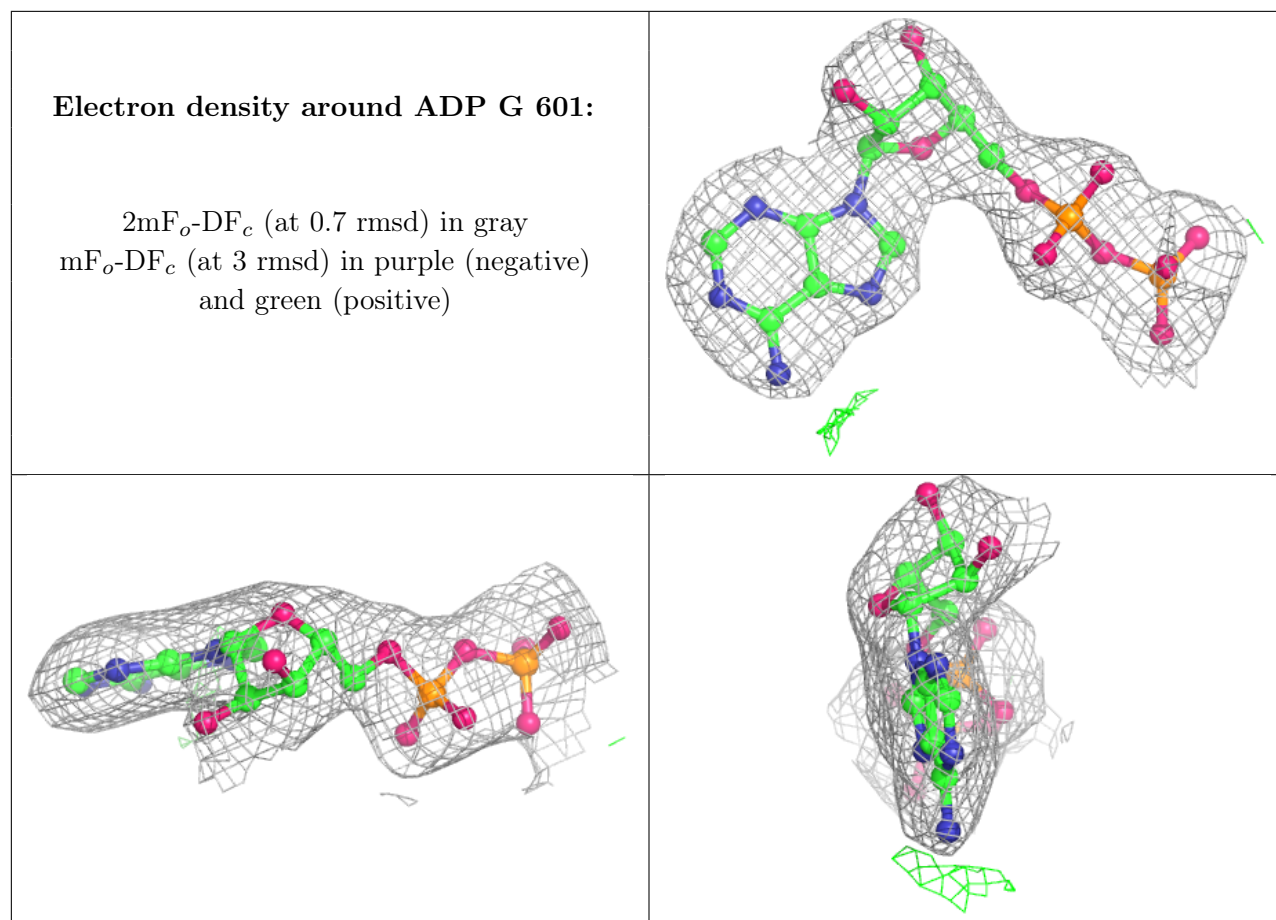


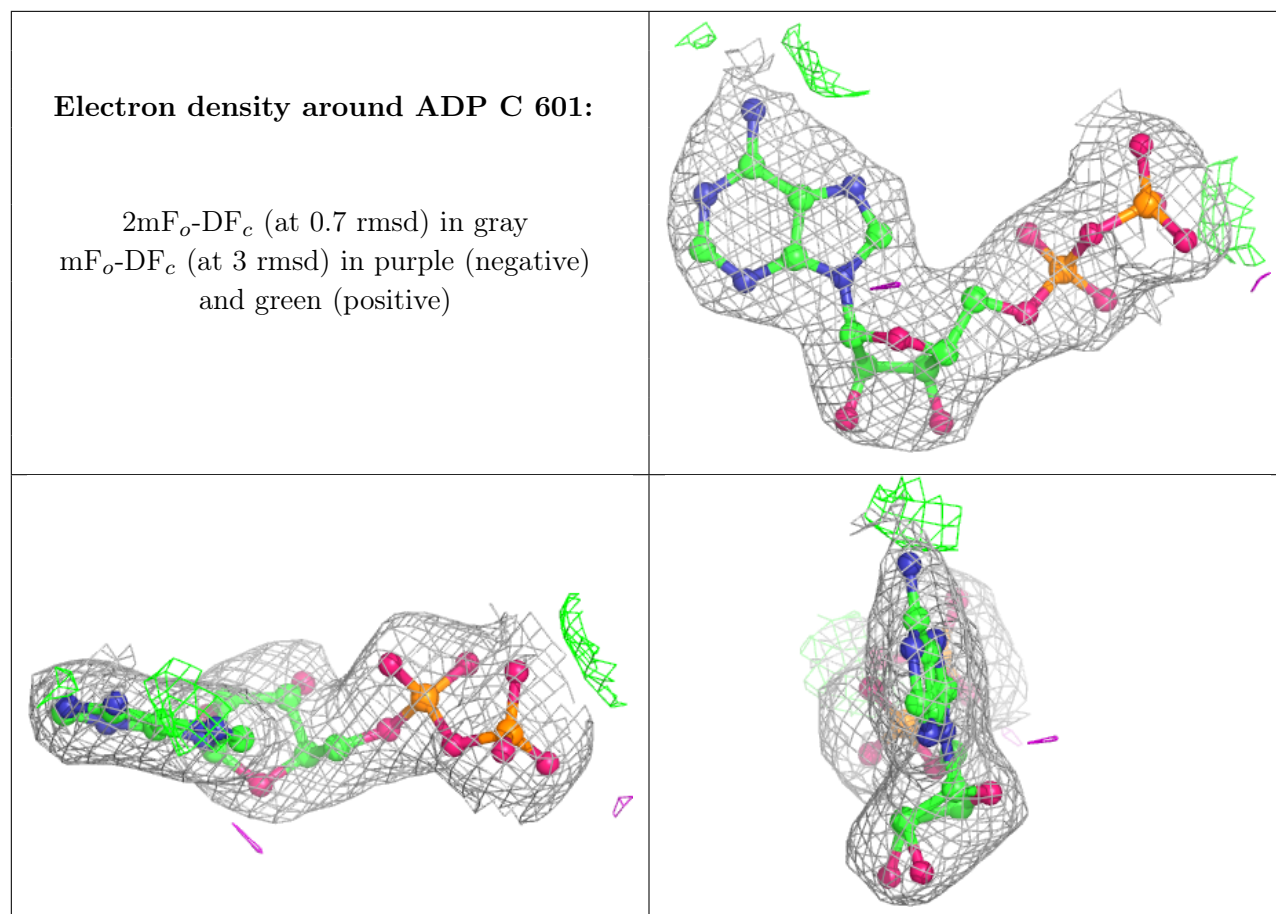
Electron density around ADP F 601:

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



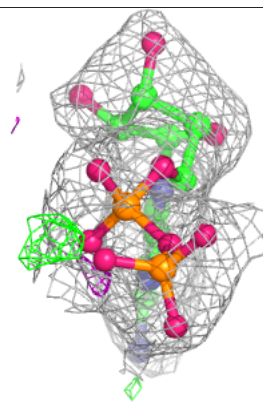
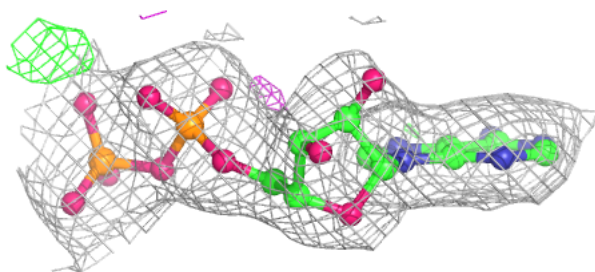
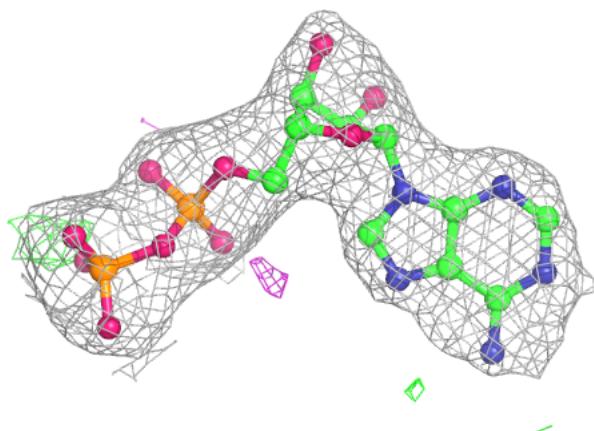


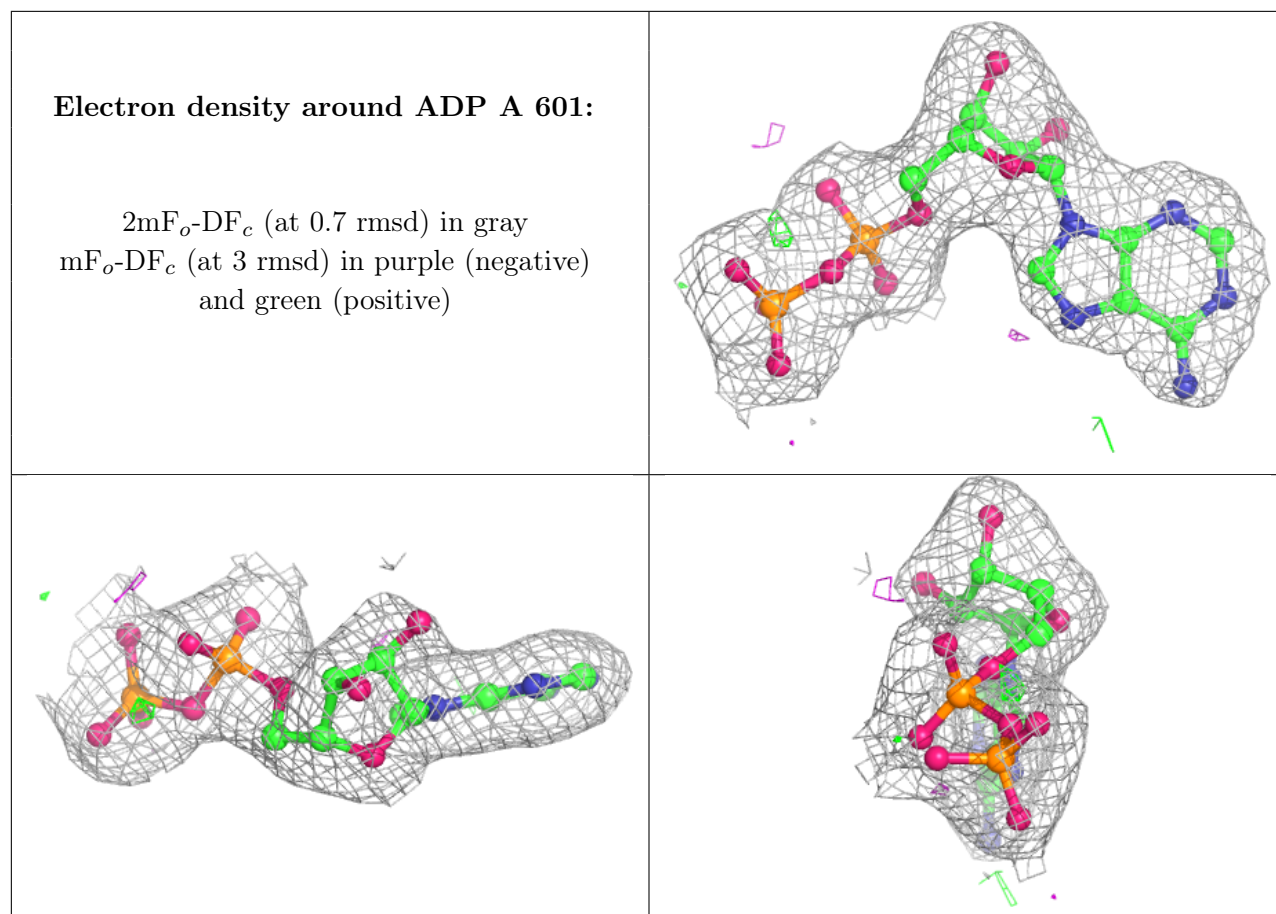




Electron density around ADP D 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.