



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2020 – 12:32 PM EDT

PDB ID : 6VVV
Title : Crystal structure of a Mycobacterium smegmatis transcription initiation complex with Rifampicin-resistant RNA polymerase
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

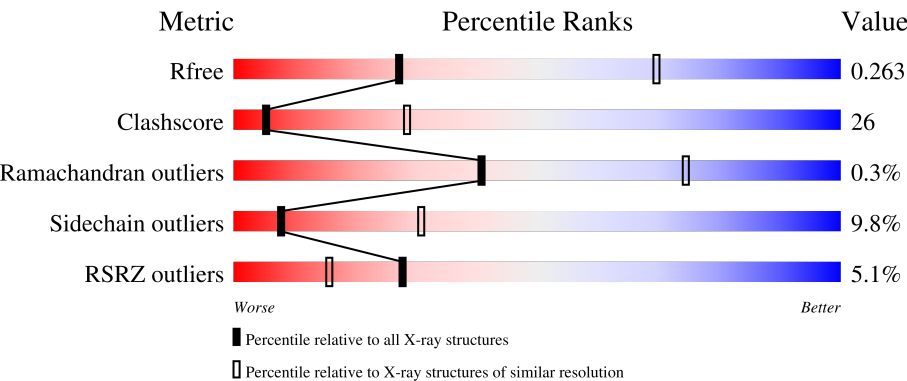
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	J	114	
2	A	350	
2	B	350	
2	T	350	
3	C	1169	

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Mol	Chain	Length	Quality of chain
4	D	1317	
5	E	107	
6	F	466	
7	O	31	
8	P	26	

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
9	SO4	D	1403	-	-	X	-
9	SO4	D	1405	-	-	X	-
9	SO4	D	1406	-	-	X	-
9	SO4	F	1201	-	-	X	-
9	SO4	F	1204	-	-	X	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22970 atoms, of which 16 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 RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	88	Total	C	N	O	S	0	0	0
			678	425	122	129	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	223	Total	C	N	O	S	0	0	0
			1645	1038	284	320	3			
2	B	235	Total	C	N	O	S	0	0	0
			1643	1037	293	312	1			
2	T	53	Total	C	N	O	S	0	0	0
			374	236	65	72	1			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	790	Total	C	N	O	S	0	0	0
			5774	3620	1008	1121	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	447	LEU	SER	conflict	UNP P60281

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1174	Total	C	N	O	S	0	0	0
			8679	5438	1548	1654	39			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	0	0	0
			586	372	100	114			

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	302	Total	C	N	O	S	0	0	0
			2349	1474	423	445	7			

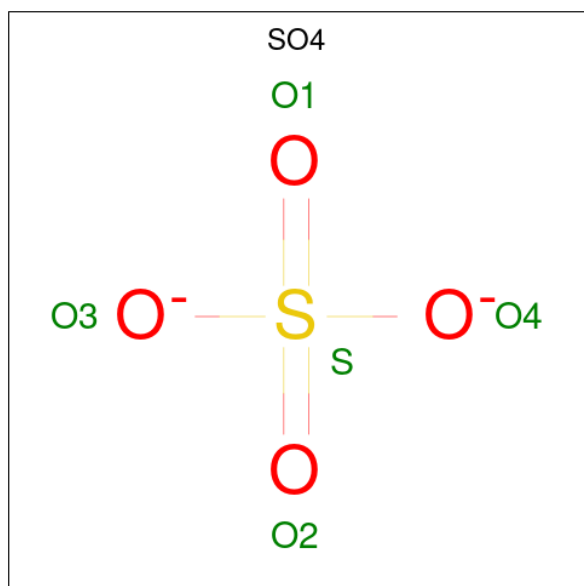
- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	31	Total	C	N	O	P	0	0	0
			635	306	114	185	30			

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			2	1	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		

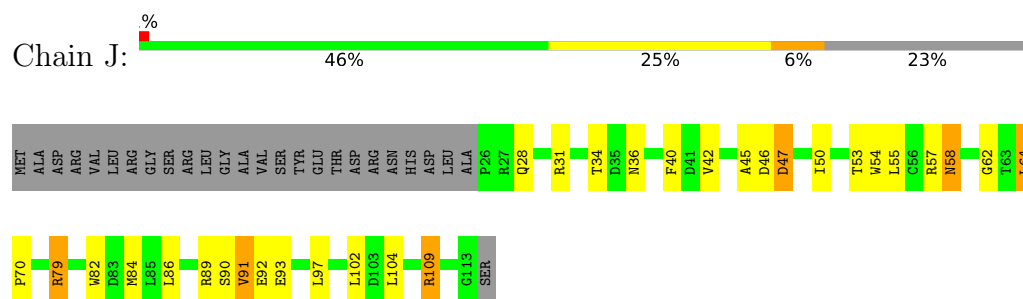
- Molecule 11 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	H	O	0	0
			3	2	1		
11	D	3	Total	H	O	0	0
			9	6	3		
11	F	3	Total	H	O	0	0
			9	6	3		
11	P	1	Total	H	O	0	0
			3	2	1		

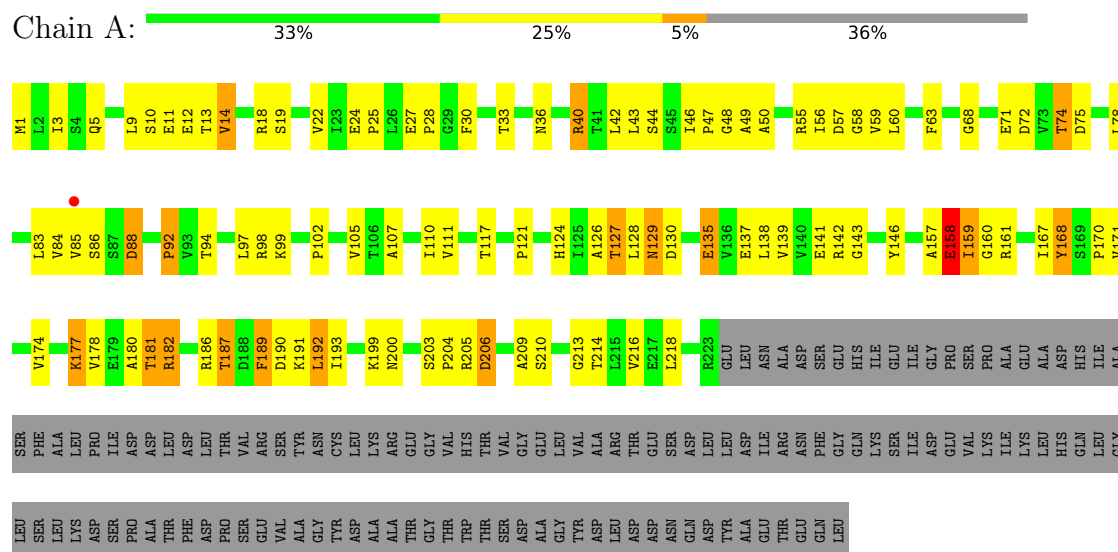
3 Residue-property plots

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

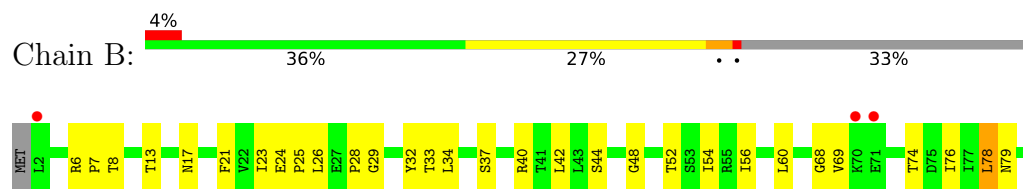
- Molecule 1: RNA polymerase-binding protein RbpA

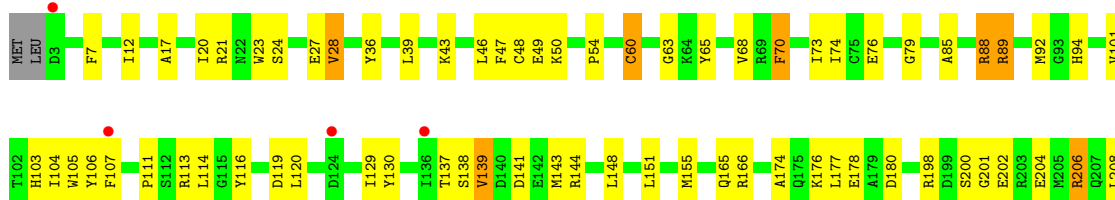


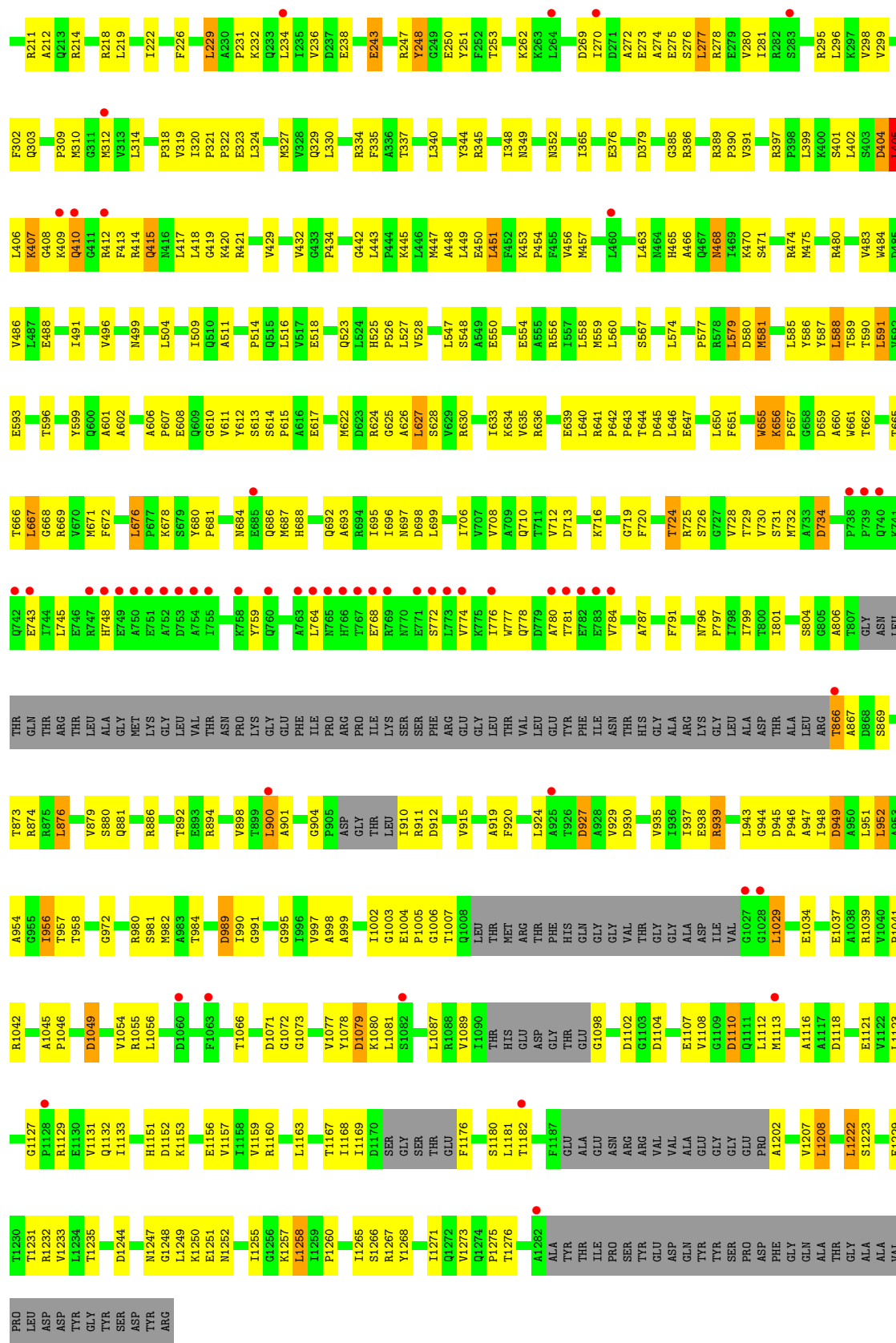
- Molecule 2: DNA-directed RNA polymerase subunit alpha



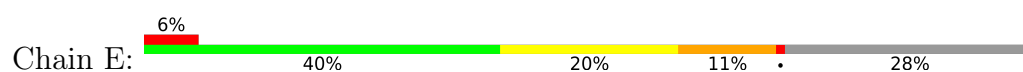
- Molecule 2: DNA-directed RNA polymerase subunit alpha



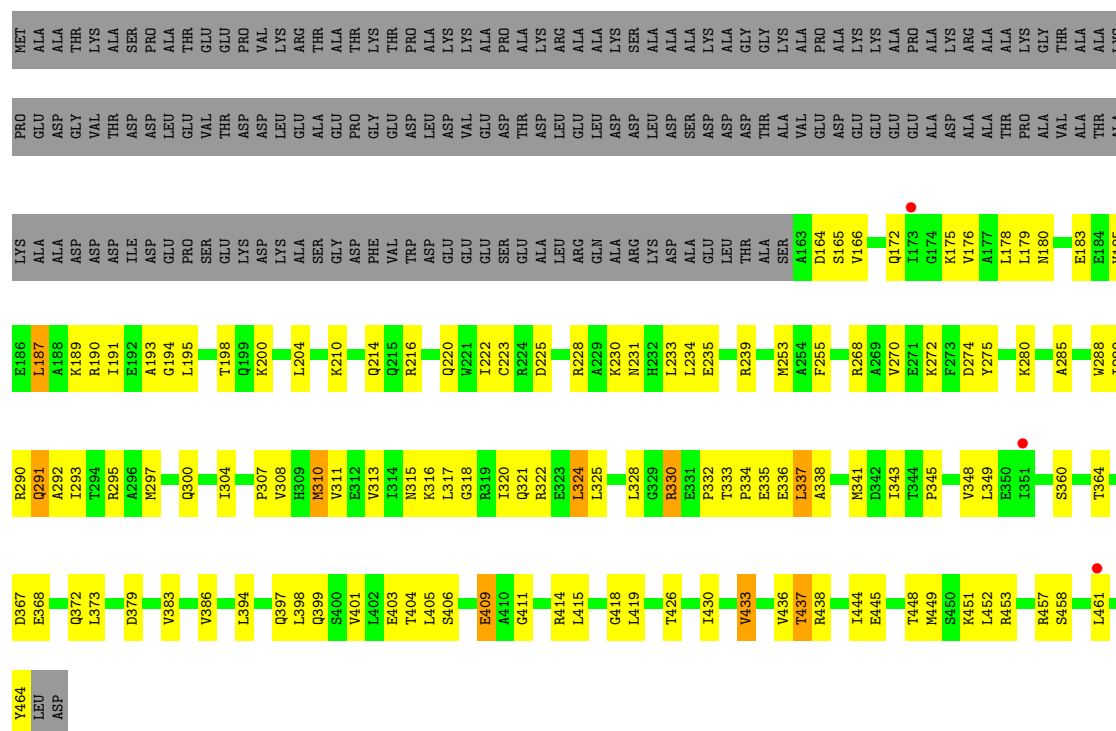




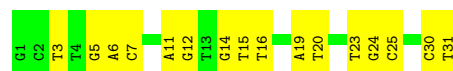
- Molecule 5: DNA-directed RNA polymerase subunit omega



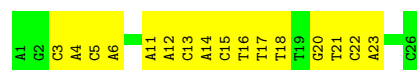
- Molecule 6: RNA polymerase sigma factor SigA



- Molecule 7: DNA (31-MER)



- Molecule 8: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.75Å 162.34Å 137.16Å 90.00° 111.27° 90.00°	Depositor
Resolution (Å)	49.83 – 3.20 49.83 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.83-3.20) 95.4 (49.83-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.19Å)	Xtriage
Refinement program	PHENIX v0	Depositor
R, R_{free}	0.234 , 0.262 0.236 , 0.263	Depositor DCC
R_{free} test set	1957 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	119.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22970	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

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	J	0.24	0/692	0.43	0/940
2	A	0.24	0/1671	0.46	0/2279
2	B	0.24	0/1670	0.47	1/2292 (0.0%)
2	T	0.22	0/376	0.35	0/511
3	C	0.25	0/5870	0.44	1/7988 (0.0%)
4	D	0.24	0/8815	0.42	2/11982 (0.0%)
5	E	0.24	0/597	0.40	0/814
6	F	0.22	0/2379	0.38	0/3218
7	O	0.51	0/712	0.94	0/1098
8	P	0.51	0/589	0.91	0/906
All	All	0.26	0/23371	0.48	4/32028 (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	J	0	1
2	B	0	2
3	C	0	5
4	D	0	1
5	E	0	1
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	984	LEU	CA-CB-CG	5.86	128.77	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	579	LEU	CA-CB-CG	5.78	128.59	115.30
2	B	206	ASP	CB-CG-OD2	5.21	122.99	118.30
4	D	405	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	156	GLY	Peptide
2	B	157	ALA	Peptide
3	C	1052	ALA	Peptide
3	C	171	VAL	Peptide
3	C	398	GLN	Peptide
3	C	916	ARG	Peptide
3	C	986	ASN	Peptide
4	D	407	LYS	Peptide
5	E	26	TYR	Peptide
1	J	109	ARG	Peptide

5.2 Too-close contacts

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	J	678	0	642	36	0
2	A	1645	0	1656	109	0
2	B	1643	0	1583	115	0
2	T	374	0	344	13	0
3	C	5774	0	5503	374	0
4	D	8679	0	8318	457	1
5	E	586	0	567	41	0
6	F	2349	0	2346	110	0
7	O	635	0	354	30	0
8	P	526	0	296	18	0
9	D	35	0	0	9	0
9	F	20	0	0	9	1
10	D	2	0	0	0	0
11	C	1	2	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	3	6	0	2	0
11	F	3	6	0	2	0
11	P	1	2	0	0	0
All	All	22954	16	21609	1170	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (1170) 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:J:68:ASP:HA	1:J:69:VAL:HG22	1.28	1.09
2:B:90:ASP:HA	2:B:142:ARG:HG3	1.35	1.09
3:C:758:GLU:HG2	3:C:798:THR:HG22	1.33	1.08
3:C:937:ILE:HD11	3:C:955:TYR:HB3	1.31	1.06
3:C:937:ILE:HD13	3:C:939:VAL:HG12	1.35	1.06
4:D:408:GLY:HA2	4:D:412:ARG:HB3	1.37	1.05
4:D:656:LYS:HA	4:D:659:ASP:HB2	1.44	0.98
3:C:1130:SER:HB2	3:C:1136:ILE:HD11	1.47	0.97
4:D:277:LEU:HD13	4:D:296:LEU:HD13	1.47	0.96
4:D:407:LYS:O	4:D:413:PHE:HB2	1.64	0.96
5:E:29:PRO:HG2	5:E:34:ASN:HB2	1.47	0.95
3:C:1058:ARG:HB3	3:C:1058:ARG:HH21	1.27	0.95
4:D:408:GLY:HA3	4:D:413:PHE:H	1.30	0.94
2:B:84:VAL:HB	2:B:199:LYS:HD3	1.49	0.94
4:D:647:GLU:HB2	4:D:655:TRP:HH2	1.33	0.93
3:C:798:THR:HG23	3:C:826:THR:HG21	1.49	0.93
2:B:102:PRO:HG3	2:B:130:ASP:HA	1.50	0.93
2:B:170:PRO:HB2	2:B:202:ILE:HD11	1.52	0.91
7:O:6:DA:H2''	7:O:7:DC:H5'	1.51	0.91
4:D:414:ARG:O	4:D:418:LEU:N	2.03	0.90
4:D:274:ALA:HA	4:D:277:LEU:HD11	1.52	0.90
3:C:1045:GLN:HG2	3:C:1087:THR:HG22	1.54	0.89
2:A:48:GLY:HA2	2:A:49:ALA:HB3	1.55	0.89
2:A:40:ARG:HD3	2:B:33:THR:HG22	1.53	0.88
4:D:579:LEU:HA	4:D:806:ALA:HB1	1.53	0.88
4:D:901:ALA:HB1	4:D:911:ARG:HA	1.54	0.88
6:F:444:ILE:O	6:F:448:THR:HG23	1.73	0.88
4:D:706:ILE:HD12	5:E:36:PRO:HB3	1.54	0.88
3:C:170:LEU:HD11	3:C:448:ALA:HB2	1.55	0.88
6:F:404:THR:OG1	6:F:457:ARG:NH2	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:THR:OG1	2:B:24:GLU:O	1.91	0.88
2:A:56:ILE:HB	2:A:59:VAL:HG22	1.55	0.88
3:C:760:ILE:HG22	3:C:796:LYS:HG3	1.53	0.88
3:C:1061:GLU:HB2	4:D:417:LEU:O	1.73	0.87
3:C:169:GLN:HB2	3:C:427:LEU:HD21	1.55	0.86
4:D:1004:GLU:HB3	4:D:1005:PRO:HD3	1.57	0.86
4:D:1276:THR:HG22	5:E:102:GLU:HG3	1.57	0.85
3:C:641:ILE:HD11	3:C:684:GLY:N	1.92	0.85
3:C:937:ILE:CD1	3:C:955:TYR:HB3	2.07	0.85
3:C:1058:ARG:NH1	4:D:418:LEU:HG	1.91	0.85
3:C:760:ILE:HA	3:C:796:LYS:HA	1.57	0.84
1:J:68:ASP:CA	1:J:69:VAL:HG22	2.07	0.84
4:D:408:GLY:HA3	4:D:413:PHE:N	1.93	0.84
4:D:499:ASN:HB2	4:D:509:ILE:HG12	1.60	0.84
4:D:647:GLU:HB2	4:D:655:TRP:CH2	2.13	0.84
6:F:438:ARG:NH1	8:P:20:DG:N7	2.26	0.84
1:J:68:ASP:HA	1:J:69:VAL:CG2	2.05	0.84
3:C:848:ASP:OD1	3:C:848:ASP:N	2.09	0.84
4:D:869:SER:HB3	4:D:1007:THR:HG22	1.60	0.84
2:B:21:PHE:HB2	2:B:194:ILE:HG22	1.59	0.84
1:J:28:GLN:HE21	1:J:46:ASP:HA	1.42	0.83
4:D:47:PHE:O	4:D:88:ARG:NH2	2.12	0.83
3:C:602:MET:HE3	3:C:883:LYS:HD3	1.60	0.82
2:A:55:ARG:HH21	2:A:160:GLY:HA3	1.44	0.82
2:A:40:ARG:HB3	2:A:40:ARG:HH11	1.42	0.82
5:E:84:LEU:HB2	5:E:85:GLN:HE21	1.44	0.82
3:C:1026:HIS:HB3	3:C:1031:LYS:HE2	1.62	0.82
2:B:102:PRO:HG3	2:B:131:LYS:H	1.45	0.81
4:D:1160:ARG:NH2	9:D:1405:SO4:O1	2.12	0.81
6:F:230:LYS:NZ	11:F:1301:HOH:O	2.10	0.81
5:E:40:LEU:HB3	5:E:50:LEU:HD11	1.62	0.81
4:D:222:ILE:HD13	4:D:243:GLU:HG2	1.63	0.81
4:D:991:GLY:HA2	4:D:1265:ILE:HD11	1.62	0.80
3:C:1043:ILE:H	3:C:1043:ILE:HD12	1.46	0.80
4:D:404:ASP:HA	4:D:409:LYS:HB3	1.62	0.80
3:C:1079:LEU:HD23	3:C:1083:LYS:HD2	1.61	0.80
6:F:280:LYS:HG2	7:O:30:DC:OP2	1.80	0.80
3:C:799:PRO:HA	3:C:823:VAL:HG12	1.62	0.79
6:F:290:ARG:NH1	9:F:1204:SO4:O1	2.13	0.79
4:D:218:ARG:NH2	9:D:1403:SO4:O4	2.15	0.79
4:D:944:GLY:HA2	4:D:980:ARG:HH22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:910:THR:HG23	4:D:730:VAL:HG23	1.64	0.79
7:O:19:DA:H2''	7:O:20:DT:O5'	1.81	0.79
3:C:1058:ARG:HH11	4:D:418:LEU:HG	1.44	0.79
1:J:69:VAL:HG23	1:J:69:VAL:O	1.81	0.79
3:C:1060:GLY:HA2	4:D:419:GLY:HA3	1.64	0.79
3:C:783:ILE:H	3:C:783:ILE:HD12	1.48	0.78
4:D:641:ARG:HA	4:D:656:LYS:HE3	1.66	0.78
1:J:92:GLU:OE1	1:J:92:GLU:N	2.16	0.78
6:F:324:LEU:HB3	6:F:332:PRO:HG3	1.64	0.78
4:D:656:LYS:HD3	4:D:656:LYS:H	1.49	0.78
3:C:763:ASP:OD2	3:C:821:ARG:NH1	2.17	0.77
3:C:602:MET:CE	3:C:883:LYS:HD3	2.14	0.77
5:E:84:LEU:H	5:E:84:LEU:HD12	1.46	0.77
4:D:1129:ARG:NH1	9:D:1408:SO4:O3	2.16	0.77
3:C:51:SER:OG	3:C:373:GLY:N	2.18	0.77
2:A:204:PRO:HD2	2:A:205:ARG:HH12	1.49	0.77
3:C:728:LEU:HD22	3:C:906:ILE:HG22	1.65	0.77
4:D:636:ARG:HD3	4:D:660:ALA:HB1	1.67	0.77
2:A:98:ARG:HG2	2:A:135:GLU:HG2	1.65	0.77
2:A:210:SER:HB2	2:B:229:SER:HB3	1.66	0.77
3:C:911:HIS:O	3:C:914:PRO:HD2	1.86	0.77
2:A:1:MET:N	2:B:142:ARG:O	2.18	0.76
8:P:11:DA:H2''	8:P:12:DA:O5'	1.85	0.76
3:C:1039:PRO:HG2	3:C:1048:LEU:O	1.85	0.76
2:B:143:GLY:HA3	2:B:168:TYR:CG	2.20	0.76
3:C:722:TYR:HB3	4:D:432:VAL:HG21	1.68	0.76
4:D:644:THR:O	4:D:647:GLU:HG2	1.85	0.76
2:A:187:THR:HG23	2:A:187:THR:O	1.85	0.76
3:C:849:ASP:O	3:C:850:ASP:HB2	1.86	0.76
3:C:1128:VAL:HG11	3:C:1136:ILE:HB	1.68	0.76
3:C:805:LEU:HD22	3:C:809:GLU:OE2	1.85	0.76
6:F:210:LYS:NZ	9:F:1201:SO4:O4	2.14	0.76
2:A:40:ARG:NH2	3:C:894:ASP:HB3	2.01	0.75
5:E:86:GLU:OE2	5:E:94:ARG:NH1	2.20	0.75
4:D:912:ASP:HB3	4:D:915:VAL:HG13	1.69	0.75
3:C:1058:ARG:NH2	3:C:1058:ARG:HB3	2.00	0.75
4:D:365:ILE:HD12	4:D:365:ILE:H	1.50	0.75
1:J:47:ASP:N	1:J:47:ASP:OD1	2.18	0.75
2:A:48:GLY:CA	2:A:49:ALA:HB3	2.16	0.74
3:C:492:SER:HB2	3:C:495:ALA:HB2	1.67	0.74
2:A:27:GLU:HB3	2:A:28:PRO:HD2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:TYR:CE2	2:B:178:VAL:HG21	2.22	0.74
4:D:734:ASP:N	4:D:734:ASP:OD1	2.20	0.74
3:C:984:LEU:HB3	3:C:985:PRO:HD2	1.70	0.74
3:C:754:LYS:HD2	4:D:39:LEU:HD12	1.69	0.74
3:C:773:ALA:O	3:C:782:ARG:NH2	2.21	0.74
3:C:641:ILE:CD1	3:C:685:GLN:H	2.01	0.74
4:D:49:GLU:HG2	4:D:88:ARG:HH21	1.52	0.74
3:C:641:ILE:HA	3:C:651:VAL:HA	1.68	0.73
3:C:654:ASP:OD2	3:C:686:ARG:NH2	2.20	0.73
3:C:796:LYS:HB3	3:C:826:THR:O	1.89	0.73
3:C:910:THR:CG2	4:D:730:VAL:HG23	2.19	0.73
2:A:157:ALA:O	2:A:158:GLU:HB2	1.88	0.73
3:C:850:ASP:O	3:C:852:LEU:HD23	1.88	0.73
4:D:655:TRP:CE3	4:D:655:TRP:HA	2.24	0.73
5:E:29:PRO:CG	5:E:34:ASN:HB2	2.18	0.73
6:F:308:VAL:HG21	7:O:23:DT:H73	1.69	0.73
2:B:6:ARG:O	2:B:25:PRO:HD2	1.87	0.73
3:C:721:ASN:H	3:C:721:ASN:HD22	1.36	0.73
4:D:611:VAL:HA	4:D:634:LYS:O	1.89	0.73
2:B:26:LEU:HB2	2:B:190:ASP:HB2	1.69	0.73
4:D:900:LEU:CD1	4:D:956:ILE:HD13	2.19	0.72
8:P:11:DA:H2''	8:P:12:DA:C5'	2.18	0.72
3:C:900:ASP:OD1	3:C:986:ASN:ND2	2.22	0.72
4:D:276:SER:O	4:D:280:VAL:HG23	1.90	0.72
4:D:415:GLN:HA	4:D:418:LEU:CB	2.19	0.72
4:D:614:SER:HB2	4:D:615:PRO:HD2	1.70	0.72
4:D:111:PRO:O	4:D:113:ARG:NH1	2.22	0.72
4:D:453:LYS:HB3	4:D:454:PRO:HD3	1.72	0.72
2:A:206:ASP:OD1	2:B:226:ASN:ND2	2.23	0.72
3:C:170:LEU:HD12	3:C:170:LEU:O	1.90	0.72
4:D:1229:GLU:O	4:D:1233:VAL:HG23	1.90	0.72
3:C:170:LEU:HG	3:C:447:LEU:O	1.90	0.71
4:D:269:ASP:HB3	4:D:272:ALA:HB3	1.71	0.71
1:J:84:MET:HE3	6:F:272:LYS:HE2	1.72	0.71
2:A:44:SER:HB3	3:C:893:GLU:OE1	1.90	0.71
4:D:1071:ASP:HB2	4:D:1073:GLY:N	2.05	0.71
3:C:1081:THR:HG22	3:C:1109:PRO:HG3	1.72	0.71
4:D:900:LEU:HD11	4:D:956:ILE:HD13	1.73	0.71
6:F:405:LEU:HD21	6:F:452:LEU:HD11	1.72	0.71
4:D:1041:PRO:HB3	4:D:1116:ALA:HB3	1.72	0.71
4:D:787:ALA:O	4:D:791:PHE:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:949:ASP:HA	4:D:952:LEU:HD22	1.73	0.71
4:D:901:ALA:HA	4:D:912:ASP:H	1.56	0.71
7:O:11:DA:H2"	7:O:12:DG:H5"	1.72	0.71
4:D:874:ARG:NH1	9:D:1406:SO4:O4	2.22	0.70
3:C:950:LEU:HD22	3:C:951:PRO:HD2	1.72	0.70
4:D:504:LEU:HD23	4:D:1004:GLU:HG2	1.72	0.70
6:F:330:ARG:NH2	6:F:336:GLU:OE2	2.22	0.70
4:D:344:TYR:O	4:D:348:ILE:HG22	1.92	0.70
4:D:376:GLU:OE2	6:F:165:SER:OG	2.07	0.70
3:C:400:VAL:O	3:C:401:GLU:HB2	1.90	0.70
6:F:405:LEU:HD21	6:F:452:LEU:CD1	2.22	0.70
2:A:210:SER:O	2:B:231:HIS:HB3	1.91	0.70
2:A:214:THR:OG1	2:B:231:HIS:HB2	1.92	0.70
3:C:598:MET:O	3:C:602:MET:HG3	1.91	0.70
4:D:389:ARG:NH1	6:F:164:ASP:OD2	2.23	0.70
6:F:210:LYS:NZ	9:F:1201:SO4:S	2.65	0.69
2:B:34:LEU:HD11	2:B:192:LEU:HD22	1.74	0.69
3:C:1086:ASP:O	3:C:1090:ARG:HG2	1.93	0.69
2:A:12:GLU:O	2:A:19:SER:HB2	1.92	0.69
3:C:60:ARG:HA	3:C:60:ARG:HH21	1.57	0.69
2:B:23:ILE:HD12	2:B:192:LEU:HD23	1.73	0.69
4:D:1248:GLY:O	4:D:1252:ASN:ND2	2.26	0.69
3:C:1078:GLU:HG3	3:C:1082:ILE:HD11	1.74	0.69
3:C:169:GLN:OE1	3:C:370:ARG:NH2	2.26	0.68
5:E:36:PRO:HG2	5:E:39:GLU:HG3	1.75	0.68
3:C:807:PRO:HB2	6:F:419:LEU:HD23	1.75	0.68
3:C:873:GLY:HA3	3:C:1028:VAL:HG11	1.75	0.68
3:C:937:ILE:HD13	3:C:939:VAL:CG1	2.19	0.68
3:C:1060:GLY:HA2	4:D:419:GLY:CA	2.23	0.68
4:D:920:PHE:O	4:D:1151:HIS:NE2	2.23	0.68
3:C:939:VAL:HG11	3:C:955:TYR:HD2	1.59	0.68
4:D:748:HIS:CD2	4:D:780:ALA:HB2	2.28	0.68
6:F:318:GLY:O	6:F:322:ARG:HG3	1.94	0.68
3:C:728:LEU:HD22	3:C:906:ILE:CG2	2.23	0.68
2:B:101:GLY:N	2:B:132:GLY:O	2.25	0.68
4:D:900:LEU:O	4:D:900:LEU:HD13	1.94	0.68
3:C:798:THR:HG23	3:C:826:THR:CG2	2.23	0.68
4:D:1071:ASP:N	4:D:1072:GLY:HA2	2.08	0.68
6:F:335:GLU:OE1	6:F:335:GLU:N	2.24	0.68
2:A:50:ALA:HB3	2:A:168:TYR:CE1	2.28	0.68
4:D:273:GLU:O	4:D:277:LEU:HG	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:GLN:OE1	1:J:50:ILE:HD11	1.94	0.68
3:C:649:ILE:HD11	3:C:679:PRO:HB3	1.77	0.67
3:C:640:VAL:O	3:C:652:MET:N	2.25	0.67
1:J:36:ASN:HD21	1:J:58:ASN:HD21	1.41	0.67
3:C:835:SER:O	3:C:866:GLN:HG2	1.94	0.67
7:O:6:DA:C2'	7:O:7:DC:H5'	2.23	0.67
8:P:20:DG:H2''	8:P:21:DT:H5'	1.76	0.67
6:F:409:GLU:CD	6:F:448:THR:HG21	2.15	0.67
3:C:989:GLY:O	3:C:990:GLU:HG3	1.94	0.67
4:D:277:LEU:CD1	4:D:296:LEU:HD13	2.23	0.67
3:C:369:LEU:HD23	3:C:501:GLY:O	1.94	0.67
4:D:589:THR:HG21	4:D:687:MET:HG2	1.75	0.67
4:D:143:MET:HG2	4:D:251:TYR:CE1	2.29	0.67
3:C:711:LEU:HD23	3:C:904:VAL:HA	1.77	0.67
4:D:599:TYR:HA	4:D:610:GLY:HA3	1.77	0.67
3:C:1035:ARG:NH2	3:C:1047:PRO:HB3	2.10	0.66
3:C:33:ALA:HB2	3:C:966:PRO:CG	2.25	0.66
4:D:1223:SER:HB2	4:D:1251:GLU:OE2	1.96	0.66
2:B:231:HIS:HD1	2:B:232:ILE:H	1.42	0.66
4:D:1275:PRO:HB3	5:E:79:LEU:HD11	1.78	0.66
4:D:155:MET:HE3	4:D:219:LEU:HB3	1.75	0.66
3:C:433:GLN:NE2	3:C:670:ASN:OD1	2.29	0.66
4:D:643:PRO:O	4:D:647:GLU:HB3	1.95	0.66
4:D:759:TYR:HA	4:D:764:LEU:CB	2.26	0.66
4:D:1079:ASP:N	4:D:1079:ASP:OD1	2.28	0.66
4:D:588:LEU:HD22	4:D:668:GLY:HA3	1.77	0.66
3:C:727:ILE:HG22	3:C:888:LYS:HB3	1.77	0.66
2:B:102:PRO:HG3	2:B:131:LYS:N	2.11	0.66
4:D:415:GLN:HA	4:D:418:LEU:HB3	1.78	0.66
3:C:1015:THR:OG1	4:D:731:SER:OG	2.13	0.65
3:C:976:LEU:HD22	4:D:732:MET:HE3	1.78	0.65
6:F:311:VAL:O	6:F:315:ASN:ND2	2.28	0.65
2:B:7:PRO:O	2:B:8:THR:HG23	1.97	0.65
4:D:404:ASP:HA	4:D:409:LYS:CB	2.25	0.65
4:D:585:LEU:HD12	4:D:692:GLN:HE21	1.61	0.65
4:D:930:ASP:CB	4:D:954:ALA:HB1	2.26	0.65
3:C:780:ILE:HG22	3:C:794:VAL:HG13	1.77	0.65
3:C:641:ILE:HD12	3:C:685:GLN:H	1.61	0.65
4:D:453:LYS:O	4:D:457:MET:HG3	1.97	0.65
4:D:612:TYR:HB2	4:D:635:VAL:HG12	1.79	0.65
4:D:708:VAL:O	4:D:712:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:PRO:HB2	5:E:33:THR:HG23	1.79	0.65
2:B:74:THR:CG2	4:D:611:VAL:HG21	2.27	0.64
6:F:345:PRO:HA	6:F:348:VAL:HG13	1.78	0.64
2:B:32:TYR:CZ	2:B:178:VAL:HG21	2.31	0.64
3:C:760:ILE:HG22	3:C:796:LYS:CG	2.27	0.64
3:C:602:MET:CE	3:C:1024:LEU:HD21	2.27	0.64
4:D:270:ILE:O	4:D:274:ALA:N	2.23	0.64
7:O:14:DG:H2''	7:O:15:DT:OP2	1.96	0.64
2:A:210:SER:HB2	2:B:229:SER:CB	2.26	0.64
4:D:463:LEU:HD22	4:D:465:HIS:CD2	2.32	0.64
1:J:109:ARG:NH2	6:F:214:GLN:OE1	2.27	0.64
5:E:76:VAL:HG22	5:E:77:GLY:H	1.63	0.64
2:A:36:ASN:HD21	2:A:40:ARG:HD2	1.62	0.64
4:D:590:THR:HG21	4:D:630:ARG:HH21	1.63	0.64
4:D:70:PHE:HB3	4:D:73:ILE:CD1	2.28	0.64
4:D:748:HIS:NE2	4:D:776:ILE:O	2.30	0.64
3:C:170:LEU:HA	3:C:369:LEU:HA	1.79	0.64
4:D:1249:LEU:HD12	4:D:1250:LYS:N	2.12	0.64
4:D:1275:PRO:HG3	5:E:76:VAL:HG11	1.80	0.64
3:C:680:ILE:HG12	3:C:693:ILE:O	1.98	0.64
3:C:939:VAL:HG23	3:C:943:VAL:HA	1.78	0.64
3:C:650:THR:HG22	3:C:660:SER:OG	1.98	0.63
2:A:88:ASP:N	2:A:88:ASP:OD1	2.31	0.63
4:D:869:SER:HB2	4:D:1029:LEU:HD21	1.80	0.63
4:D:320:ILE:HG12	4:D:321:PRO:HD2	1.79	0.63
4:D:550:GLU:O	4:D:554:GLU:HG3	1.98	0.63
3:C:379:GLN:HG2	3:C:421:PHE:HB2	1.80	0.63
5:E:26:TYR:O	5:E:26:TYR:CD1	2.52	0.63
6:F:190:ARG:HD2	6:F:225:ASP:OD2	1.98	0.63
6:F:239:ARG:HB2	7:O:31:DT:H1'	1.81	0.63
4:D:405:LEU:C	4:D:405:LEU:HD12	2.18	0.63
4:D:989:ASP:CG	5:E:46:SER:HB2	2.19	0.63
4:D:414:ARG:O	4:D:418:LEU:HB2	1.98	0.63
3:C:729:SER:HA	3:C:895:MET:HE1	1.81	0.63
3:C:708:LYS:NZ	3:C:737:VAL:O	2.31	0.63
6:F:180:ASN:OD1	6:F:183:GLU:HG3	1.99	0.63
3:C:939:VAL:HG23	3:C:943:VAL:HG22	1.80	0.62
4:D:176:LYS:O	4:D:180:ASP:N	2.29	0.62
3:C:872:ASP:N	3:C:872:ASP:OD1	2.30	0.62
6:F:290:ARG:HB3	9:F:1204:SO4:O1	1.98	0.62
6:F:307:PRO:O	6:F:311:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:901:GLY:O	3:C:903:PRO:HD3	1.99	0.62
4:D:20:ILE:HD13	4:D:318:PRO:HD3	1.80	0.62
3:C:33:ALA:HB2	3:C:966:PRO:HG2	1.80	0.62
6:F:253:MET:CE	6:F:300:GLN:HB2	2.29	0.62
6:F:210:LYS:NZ	9:F:1201:SO4:O2	2.33	0.62
6:F:338:ALA:HB1	6:F:343:ILE:O	2.00	0.62
2:B:68:GLY:CA	2:B:129:ASN:HB2	2.29	0.62
4:D:274:ALA:O	4:D:278:ARG:HG3	2.00	0.62
2:B:120:ASN:ND2	2:B:123:MET:SD	2.73	0.62
4:D:748:HIS:CE1	4:D:777:TRP:HA	2.34	0.62
1:J:42:VAL:HG13	4:D:74:ILE:HD12	1.81	0.62
4:D:327:MET:CE	6:F:304:ILE:HD11	2.30	0.62
1:J:90:SER:N	1:J:93:GLU:OE1	2.30	0.62
2:A:187:THR:CG2	2:A:187:THR:O	2.47	0.62
3:C:868:ARG:HH11	3:C:1027:LEU:HD12	1.65	0.62
4:D:585:LEU:HD12	4:D:692:GLN:NE2	2.15	0.62
3:C:1112:PHE:CE2	4:D:1255:ILE:HG22	2.34	0.62
3:C:798:THR:CG2	3:C:826:THR:HG21	2.28	0.62
4:D:590:THR:CG2	4:D:630:ARG:HE	2.12	0.62
7:O:19:DA:H4'	7:O:20:DT:OP1	2.00	0.62
4:D:408:GLY:CA	4:D:412:ARG:HB3	2.22	0.61
4:D:527:LEU:HD21	4:D:581:MET:CE	2.30	0.61
2:A:14:VAL:HG13	2:A:18:ARG:HG3	1.82	0.61
2:A:199:LYS:O	2:A:200:ASN:HB2	1.98	0.61
2:B:74:THR:HG23	4:D:611:VAL:HG21	1.81	0.61
4:D:1107:GLU:HB2	4:D:1110:ASP:OD1	2.01	0.61
6:F:448:THR:O	6:F:452:LEU:HD13	2.00	0.61
4:D:1129:ARG:O	4:D:1133:ILE:HG12	1.98	0.61
3:C:1070:TYR:CD1	4:D:559:MET:HG2	2.36	0.61
5:E:26:TYR:O	5:E:27:ASP:O	2.17	0.61
3:C:613:GLU:O	3:C:705:ALA:HB1	2.01	0.61
6:F:332:PRO:HG2	6:F:337:LEU:HD13	1.82	0.61
3:C:1058:ARG:HG2	4:D:421:ARG:HG2	1.83	0.61
4:D:527:LEU:HD21	4:D:581:MET:HE1	1.81	0.61
4:D:468:ASN:ND2	4:D:471:SER:OG	2.33	0.61
4:D:636:ARG:HB2	4:D:662:THR:HG22	1.82	0.61
1:J:89:ARG:NH2	6:F:274:ASP:OD1	2.33	0.61
3:C:635:ALA:HB2	3:C:693:ILE:HD11	1.83	0.61
3:C:1058:ARG:HA	4:D:421:ARG:HA	1.81	0.61
4:D:669:ARG:HH11	4:D:684:ASN:ND2	1.99	0.61
6:F:449:MET:HB3	6:F:453:ARG:HH12	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:924:LEU:HD21	4:D:943:LEU:HD11	1.83	0.60
2:T:272:VAL:HG13	2:T:275:LEU:HD23	1.82	0.60
3:C:159:ILE:HB	3:C:164:ARG:HD2	1.84	0.60
4:D:415:GLN:HA	4:D:418:LEU:HB2	1.81	0.60
2:B:32:TYR:CD1	3:C:1005:ARG:HB2	2.35	0.60
3:C:914:PRO:HG2	4:D:801:ILE:HG21	1.83	0.60
2:B:21:PHE:HB2	2:B:194:ILE:CG2	2.32	0.60
3:C:807:PRO:CB	6:F:419:LEU:HD23	2.30	0.60
4:D:1273:VAL:HG11	5:E:57:ARG:HB2	1.83	0.60
4:D:622:MET:HE2	4:D:667:LEU:HD13	1.83	0.60
3:C:710:LEU:HD13	3:C:1021:ILE:HG12	1.84	0.60
3:C:795:GLY:HA2	3:C:827:SER:OG	2.00	0.60
4:D:483:VAL:O	4:D:486:VAL:HG22	2.02	0.60
6:F:409:GLU:OE1	6:F:448:THR:HG21	2.01	0.60
3:C:172:ARG:O	3:C:173:SER:CB	2.49	0.59
3:C:613:GLU:HB3	3:C:708:LYS:HD3	1.82	0.59
4:D:1167:THR:HG23	4:D:1180:SER:CB	2.32	0.59
2:A:158:GLU:OE2	2:A:158:GLU:HA	2.01	0.59
2:A:48:GLY:HA2	2:A:49:ALA:CB	2.28	0.59
2:B:102:PRO:CG	2:B:131:LYS:H	2.16	0.59
3:C:589:GLU:N	3:C:589:GLU:OE1	2.25	0.59
4:D:442:GLY:HA3	4:D:523:GLN:HB2	1.82	0.59
2:B:68:GLY:HA2	2:B:129:ASN:HB2	1.84	0.59
4:D:636:ARG:CD	4:D:660:ALA:HB1	2.32	0.59
2:A:83:LEU:HD21	2:A:107:ALA:HB2	1.84	0.59
4:D:70:PHE:HB3	4:D:73:ILE:HD13	1.85	0.59
6:F:179:LEU:HD13	6:F:187:LEU:HD13	1.83	0.59
2:A:55:ARG:NH2	2:A:160:GLY:HA3	2.16	0.59
2:B:102:PRO:CG	2:B:130:ASP:HA	2.26	0.59
3:C:852:LEU:HD12	3:C:856:VAL:HG12	1.83	0.59
3:C:727:ILE:HG13	3:C:907:ILE:HB	1.85	0.59
4:D:665:THR:HG22	4:D:684:ASN:ND2	2.18	0.59
3:C:444:ARG:HH21	3:C:491:LEU:HD23	1.67	0.59
7:O:31:DT:H5'	7:O:31:DT:H6	1.68	0.59
2:B:84:VAL:HB	2:B:199:LYS:CD	2.29	0.59
3:C:732:LEU:HA	3:C:737:VAL:CG1	2.33	0.59
4:D:581:MET:O	4:D:585:LEU:HG	2.03	0.59
4:D:901:ALA:CB	4:D:912:ASP:H	2.16	0.59
4:D:404:ASP:CA	4:D:409:LYS:HB3	2.32	0.58
6:F:430:ILE:O	6:F:433:VAL:HG13	2.02	0.58
3:C:156:THR:HG22	3:C:165:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:781:THR:O	4:D:784:VAL:HG22	2.04	0.58
4:D:113:ARG:HH22	4:D:1232:ARG:HD2	1.67	0.58
4:D:1006:GLY:HA2	4:D:1029:LEU:HD11	1.85	0.58
4:D:656:LYS:CA	4:D:659:ASP:HB2	2.28	0.58
4:D:901:ALA:HA	4:D:912:ASP:HB2	1.85	0.58
4:D:23:TRP:HB3	4:D:92:MET:HE3	1.86	0.58
3:C:30:VAL:HG11	3:C:954:LEU:HG	1.84	0.58
3:C:780:ILE:HD12	3:C:781:VAL:O	2.04	0.58
6:F:320:ILE:O	6:F:324:LEU:HB2	2.04	0.58
3:C:874:ASP:OD1	3:C:1028:VAL:HG22	2.04	0.58
3:C:955:TYR:H	3:C:955:TYR:HD1	1.52	0.58
4:D:222:ILE:CD1	4:D:243:GLU:HG2	2.31	0.58
8:P:11:DA:H4'	8:P:12:DA:OP1	2.02	0.58
2:A:46:ILE:HB	2:A:170:PRO:HD2	1.86	0.58
4:D:901:ALA:HA	4:D:912:ASP:CB	2.33	0.58
6:F:414:ARG:O	6:F:418:GLY:N	2.37	0.58
3:C:1034:ALA:HB2	4:D:447:MET:HG3	1.85	0.58
4:D:397:ARG:NH2	6:F:360:SER:OG	2.37	0.58
5:E:57:ARG:HD3	5:E:57:ARG:O	2.04	0.58
3:C:742:HIS:CD2	3:C:868:ARG:HG3	2.39	0.58
3:C:1014:VAL:HG13	4:D:729:THR:HG21	1.86	0.58
4:D:796:ASN:OD1	4:D:797:PRO:HD2	2.03	0.58
6:F:397:GLN:O	6:F:401:VAL:HG23	2.03	0.58
2:A:203:SER:HB2	2:A:205:ARG:NH1	2.18	0.57
3:C:1085:ASP:OD2	4:D:420:LYS:HE2	2.04	0.57
4:D:1168:ILE:H	4:D:1180:SER:HA	1.69	0.57
4:D:443:LEU:HD22	4:D:514:PRO:HB3	1.86	0.57
4:D:901:ALA:CA	4:D:912:ASP:H	2.16	0.57
1:J:69:VAL:O	1:J:69:VAL:CG2	2.53	0.57
2:A:85:VAL:HG22	2:A:86:SER:H	1.69	0.57
3:C:771:VAL:HG23	3:C:772:LEU:HD12	1.86	0.57
4:D:938:GLU:OE1	4:D:938:GLU:N	2.31	0.57
2:B:88:ASP:N	2:B:88:ASP:OD1	2.36	0.57
3:C:935:TRP:HB2	3:C:982:SER:O	2.05	0.57
4:D:1247:ASN:O	4:D:1260:PRO:HG3	2.05	0.57
4:D:874:ARG:HD3	9:D:1406:SO4:O4	2.04	0.57
6:F:295:ARG:NH2	7:O:24:DG:O6	2.36	0.57
2:T:279:THR:HG23	2:T:282:ASP:HB2	1.86	0.57
3:C:641:ILE:HD11	3:C:684:GLY:H	1.69	0.57
3:C:648:TYR:CD2	3:C:650:THR:HG23	2.39	0.57
4:D:1041:PRO:HB3	4:D:1116:ALA:CB	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:636:ARG:HG3	4:D:662:THR:HG22	1.87	0.57
4:D:768:GLU:O	4:D:772:SER:N	2.32	0.57
2:A:30:PHE:CE1	2:B:40:ARG:HG3	2.39	0.57
3:C:909:ASN:OD1	3:C:910:THR:N	2.38	0.57
3:C:939:VAL:HG11	3:C:955:TYR:CD2	2.38	0.57
4:D:466:ALA:HB2	4:D:475:MET:CE	2.35	0.57
4:D:656:LYS:HE2	4:D:656:LYS:O	2.04	0.57
4:D:725:ARG:NH1	11:D:1501:HOH:O	2.19	0.57
4:D:1132:GLN:NE2	4:D:1163:LEU:HD12	2.19	0.57
2:B:56:ILE:HG12	2:B:136:VAL:HG23	1.86	0.57
4:D:587:TYR:O	4:D:590:THR:HG22	2.05	0.57
2:A:124:HIS:NE2	2:A:127:THR:HG22	2.19	0.56
3:C:1058:ARG:HD3	4:D:419:GLY:C	2.25	0.56
4:D:636:ARG:HG3	4:D:662:THR:CG2	2.35	0.56
2:A:10:SER:HB2	2:A:22:VAL:HG13	1.87	0.56
4:D:990:ILE:HD12	4:D:990:ILE:H	1.69	0.56
2:B:68:GLY:C	2:B:129:ASN:HB2	2.24	0.56
2:B:156:GLY:O	2:B:157:ALA:HB2	2.04	0.56
2:B:24:GLU:OE2	2:B:191:LYS:HD3	2.04	0.56
3:C:1042:MET:HA	6:F:379:ASP:HB2	1.87	0.56
3:C:939:VAL:O	3:C:939:VAL:HG13	2.05	0.56
4:D:417:LEU:HD12	4:D:874:ARG:HH21	1.69	0.56
4:D:1268:TYR:O	5:E:52:ILE:HG13	2.05	0.56
6:F:272:LYS:HE3	7:O:25:DC:OP1	2.05	0.56
2:B:68:GLY:O	2:B:129:ASN:HB2	2.05	0.56
3:C:55:LEU:HD22	3:C:373:GLY:O	2.06	0.56
3:C:602:MET:HE2	3:C:1024:LEU:HD21	1.87	0.56
3:C:758:GLU:HG2	3:C:798:THR:CG2	2.20	0.56
4:D:1252:ASN:HB3	4:D:1257:LYS:HB3	1.87	0.56
4:D:155:MET:CE	4:D:219:LEU:HB3	2.35	0.56
3:C:51:SER:HB2	3:C:371:THR:OG1	2.06	0.56
3:C:764:ILE:HB	3:C:767:VAL:HG21	1.87	0.56
4:D:432:VAL:HG22	4:D:434:PRO:HD3	1.88	0.56
2:T:279:THR:HG23	2:T:282:ASP:CB	2.36	0.56
3:C:973:GLU:H	3:C:973:GLU:CD	2.08	0.56
2:B:48:GLY:O	2:B:143:GLY:N	2.36	0.56
3:C:1041:SER:N	3:C:1048:LEU:HD22	2.20	0.56
3:C:984:LEU:HD13	3:C:984:LEU:H	1.70	0.56
4:D:28:VAL:HG21	4:D:46:LEU:HD23	1.87	0.56
6:F:290:ARG:NH1	9:F:1204:SO4:S	2.79	0.56
6:F:308:VAL:HG21	7:O:23:DT:C7	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:LEU:O	2:A:171:VAL:HG11	2.06	0.56
4:D:949:ASP:OD1	4:D:949:ASP:N	2.38	0.56
4:D:706:ILE:CD1	5:E:36:PRO:HB3	2.32	0.56
1:J:28:GLN:HE21	1:J:46:ASP:CA	2.15	0.56
4:D:1118:ASP:HB3	4:D:1121:GLU:HB2	1.88	0.55
4:D:1252:ASN:OD1	4:D:1257:LYS:HD3	2.06	0.55
3:C:587:PHE:CD2	3:C:923:LEU:HB2	2.41	0.55
8:P:5:DC:H2''	8:P:6:DA:C8	2.40	0.55
4:D:881:GLN:HB2	4:D:1249:LEU:HD11	1.88	0.55
4:D:129:ILE:HD11	4:D:130:TYR:CE2	2.40	0.55
2:T:256:LEU:HD22	2:T:297:VAL:HG22	1.89	0.55
3:C:622:GLU:HB3	3:C:703:GLU:HB2	1.89	0.55
4:D:706:ILE:O	4:D:710:GLN:HG3	2.05	0.55
5:E:76:VAL:HG22	5:E:77:GLY:N	2.21	0.55
2:B:54:ILE:HG13	2:B:162:ILE:HD11	1.88	0.55
4:D:468:ASN:OD1	4:D:470:LYS:HB2	2.06	0.55
4:D:642:PRO:HD3	4:D:656:LYS:HG2	1.88	0.55
4:D:1276:THR:CG2	5:E:102:GLU:HG3	2.34	0.55
6:F:234:LEU:HD23	6:F:270:VAL:HG21	1.88	0.55
3:C:1103:ILE:HG13	4:D:548:SER:HA	1.88	0.55
5:E:30:LEU:O	5:E:33:THR:HG22	2.06	0.55
3:C:167:VAL:HG23	3:C:427:LEU:O	2.06	0.55
4:D:636:ARG:CB	4:D:662:THR:HG22	2.37	0.55
4:D:73:ILE:O	4:D:73:ILE:HG13	2.06	0.55
2:A:48:GLY:O	2:A:142:ARG:HG3	2.06	0.55
2:A:40:ARG:CD	2:B:33:THR:HG22	2.30	0.55
3:C:935:TRP:HA	3:C:984:LEU:HD13	1.88	0.55
4:D:404:ASP:OD1	4:D:409:LYS:HD3	2.07	0.55
4:D:1276:THR:HG22	5:E:102:GLU:CG	2.31	0.55
4:D:1153:LYS:O	4:D:1157:VAL:HG23	2.07	0.55
4:D:676:LEU:HD23	4:D:676:LEU:N	2.22	0.55
3:C:1003:ASP:HB2	3:C:1010:PHE:CZ	2.42	0.55
3:C:754:LYS:HD3	4:D:329:GLN:OE1	2.07	0.55
3:C:899:PRO:HD2	3:C:992:MET:SD	2.47	0.55
4:D:1049:ASP:HB2	4:D:1078:TYR:OH	2.06	0.55
6:F:228:ARG:HB3	9:F:1202:SO4:O4	2.07	0.54
3:C:718:GLU:H	4:D:724:THR:HG22	1.73	0.54
3:C:898:LEU:HD23	3:C:1001:LEU:CD2	2.38	0.54
4:D:1087:LEU:HA	4:D:1113:MET:HG2	1.88	0.54
4:D:1123:LEU:HD22	4:D:1208:LEU:HB2	1.88	0.54
8:P:17:DT:H2''	8:P:18:DT:C5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:811:LEU:O	3:C:815:ILE:HG13	2.08	0.54
3:C:937:ILE:HG13	3:C:955:TYR:O	2.07	0.54
2:B:94:THR:HA	2:B:138:LEU:O	2.07	0.54
3:C:984:LEU:CD1	3:C:984:LEU:H	2.19	0.54
4:D:43:LYS:HE2	4:D:50:LYS:CD	2.37	0.54
3:C:911:HIS:CE1	4:D:580:ASP:HA	2.43	0.54
6:F:178:LEU:HD21	6:F:239:ARG:HH11	1.72	0.54
6:F:333:THR:N	6:F:336:GLU:OE1	2.36	0.54
2:T:254:LEU:HB2	2:T:256:LEU:HG	1.88	0.54
2:B:180:ALA:HA	2:B:189:PHE:O	2.08	0.54
3:C:590:HIS:HD2	3:C:923:LEU:CD1	2.21	0.54
4:D:927:ASP:N	4:D:927:ASP:OD2	2.32	0.54
3:C:939:VAL:HG23	3:C:943:VAL:CA	2.37	0.54
6:F:185:VAL:HG13	6:F:275:TYR:CD1	2.42	0.54
6:F:239:ARG:CB	7:O:31:DT:H1'	2.38	0.54
2:A:14:VAL:HG12	2:A:19:SER:HA	1.90	0.54
2:B:102:PRO:HG3	2:B:130:ASP:CA	2.30	0.54
2:B:44:SER:HA	2:B:145:GLY:HA2	1.89	0.54
2:B:174:VAL:HA	2:B:195:ASP:O	2.08	0.54
2:A:40:ARG:NH1	2:B:33:THR:HG22	2.23	0.54
3:C:32:PHE:HE1	3:C:963:VAL:HG13	1.74	0.54
4:D:567:SER:HB2	4:D:574:LEU:HD13	1.89	0.54
4:D:642:PRO:HG3	4:D:661:TRP:CE2	2.42	0.54
2:B:76:ILE:HA	2:B:79:ASN:HB2	1.89	0.53
3:C:868:ARG:NH1	3:C:1027:LEU:HD12	2.23	0.53
7:O:31:DT:C6	7:O:31:DT:H5'	2.43	0.53
3:C:400:VAL:HG22	3:C:401:GLU:H	1.73	0.53
4:D:1071:ASP:HB2	4:D:1073:GLY:H	1.73	0.53
4:D:586:TYR:CD1	4:D:804:SER:HA	2.44	0.53
3:C:60:ARG:N	3:C:60:ARG:HD2	2.23	0.53
4:D:901:ALA:HB2	4:D:915:VAL:HG11	1.90	0.53
6:F:293:ILE:O	6:F:297:MET:HG3	2.09	0.53
7:O:5:DG:H2''	7:O:6:DA:OP2	2.08	0.53
2:A:129:ASN:H	2:A:129:ASN:HD22	1.54	0.53
2:A:178:VAL:HG12	2:A:192:LEU:HB3	1.91	0.53
3:C:729:SER:HA	3:C:895:MET:CE	2.38	0.53
6:F:426:THR:O	6:F:430:ILE:HG13	2.08	0.53
4:D:138:SER:HB3	4:D:253:THR:OG1	2.08	0.53
4:D:567:SER:HB2	4:D:574:LEU:CD1	2.38	0.53
5:E:30:LEU:N	5:E:30:LEU:HD12	2.23	0.53
3:C:39:LEU:O	3:C:41:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1066:THR:HG23	4:D:1077:VAL:HG22	1.90	0.53
4:D:139:VAL:CG1	4:D:231:PRO:HD3	2.39	0.53
4:D:295:ARG:O	4:D:299:VAL:HG23	2.08	0.53
1:J:109:ARG:HH22	6:F:214:GLN:CD	2.11	0.53
4:D:1176:PHE:CB	4:D:1202:ALA:HA	2.39	0.53
4:D:748:HIS:CG	4:D:780:ALA:HB2	2.44	0.53
3:C:106:VAL:HG11	3:C:120:TYR:CE1	2.44	0.53
4:D:646:LEU:O	4:D:650:LEU:HG	2.08	0.53
3:C:718:GLU:H	4:D:724:THR:CG2	2.20	0.53
3:C:748:ILE:O	3:C:859:LEU:HD23	2.09	0.53
3:C:805:LEU:HD12	3:C:810:ARG:NH1	2.24	0.53
4:D:200:SER:O	4:D:204:GLU:HG3	2.09	0.53
4:D:262:LYS:HG3	4:D:310:MET:CE	2.39	0.53
4:D:929:VAL:HA	4:D:935:VAL:HA	1.91	0.53
8:P:14:DA:H2''	8:P:15:DC:H5'	1.91	0.53
4:D:27:GLU:HB2	4:D:94:HIS:CE1	2.43	0.53
2:A:28:PRO:HG3	4:D:624:ARG:NH2	2.24	0.52
3:C:498:ASN:HB2	3:C:502:PHE:O	2.09	0.52
2:A:186:ARG:O	2:A:187:THR:HG22	2.09	0.52
3:C:171:VAL:O	3:C:172:ARG:O	2.27	0.52
4:D:139:VAL:HG11	4:D:231:PRO:HD3	1.91	0.52
4:D:463:LEU:O	4:D:465:HIS:N	2.41	0.52
4:D:666:THR:OG1	4:D:669:ARG:HG3	2.09	0.52
4:D:745:LEU:HA	4:D:748:HIS:HB3	1.91	0.52
7:O:15:DT:H2''	7:O:16:DT:OP2	2.10	0.52
3:C:712:VAL:HG12	3:C:1017:GLY:O	2.10	0.52
4:D:28:VAL:HG11	4:D:319:VAL:HG21	1.90	0.52
7:O:15:DT:H1'	7:O:16:DT:H5''	1.91	0.52
3:C:1114:VAL:O	3:C:1118:GLU:HG3	2.09	0.52
6:F:316:LYS:HG2	6:F:341:MET:HE3	1.90	0.52
2:A:48:GLY:O	2:A:143:GLY:N	2.40	0.52
2:B:54:ILE:O	2:B:162:ILE:HG12	2.09	0.52
3:C:865:ALA:C	3:C:866:GLN:HG3	2.29	0.52
1:J:53:THR:HA	1:J:62:GLY:O	2.09	0.52
4:D:103:HIS:CE1	4:D:105:TRP:HB2	2.44	0.52
4:D:401:SER:OG	4:D:404:ASP:OD1	2.26	0.52
4:D:655:TRP:HE3	4:D:655:TRP:HA	1.72	0.52
8:P:17:DT:H2''	8:P:18:DT:H5'	1.90	0.52
4:D:1123:LEU:HA	4:D:1131:VAL:CG2	2.40	0.52
4:D:92:MET:HG2	4:D:321:PRO:HD3	1.92	0.52
3:C:51:SER:OG	3:C:371:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:591:ASP:OD2	3:C:880:HIS:ND1	2.39	0.52
4:D:627:LEU:HD13	4:D:667:LEU:HD12	1.91	0.52
6:F:175:LYS:HD3	6:F:175:LYS:O	2.10	0.52
6:F:185:VAL:HG13	6:F:275:TYR:HD1	1.75	0.52
8:P:14:DA:H2''	8:P:15:DC:C5'	2.40	0.52
4:D:404:ASP:CG	4:D:409:LYS:HD3	2.30	0.52
4:D:695:ILE:O	4:D:699:LEU:HG	2.10	0.52
6:F:185:VAL:O	6:F:189:LYS:HG3	2.10	0.52
2:A:57:ASP:OD1	2:A:58:GLY:N	2.44	0.51
4:D:904:GLY:HA2	4:D:910:ILE:CB	2.40	0.51
6:F:411:GLY:O	6:F:415:LEU:HG	2.09	0.51
3:C:1074:TYR:CE1	4:D:1258:LEU:HD21	2.45	0.51
4:D:1034:GLU:OE2	4:D:1042:ARG:N	2.40	0.51
2:T:284:LEU:HD12	2:T:294:ILE:HD12	1.91	0.51
4:D:1055:ARG:HA	4:D:1102:ASP:OD1	2.09	0.51
4:D:23:TRP:HB3	4:D:92:MET:CE	2.41	0.51
4:D:466:ALA:HB2	4:D:475:MET:HE1	1.92	0.51
6:F:324:LEU:HD23	6:F:328:LEU:HD13	1.90	0.51
3:C:1058:ARG:HD2	3:C:1058:ARG:C	2.31	0.51
4:D:60:CYS:SG	4:D:63:GLY:N	2.72	0.51
4:D:748:HIS:NE2	4:D:777:TRP:HA	2.25	0.51
2:A:40:ARG:HH21	3:C:894:ASP:HB3	1.71	0.51
3:C:776:ASP:HB2	3:C:777:GLU:OE1	2.10	0.51
3:C:985:PRO:HB2	3:C:989:GLY:HA2	1.91	0.51
4:D:499:ASN:CB	4:D:509:ILE:HG12	2.37	0.51
2:A:30:PHE:CD1	2:B:40:ARG:HG3	2.45	0.51
2:A:56:ILE:HB	2:A:59:VAL:CG2	2.35	0.51
2:A:50:ALA:HB3	2:A:168:TYR:CD1	2.45	0.51
3:C:616:LEU:HB2	3:C:709:ASN:ND2	2.26	0.51
3:C:753:THR:HG22	3:C:758:GLU:HG3	1.93	0.51
4:D:669:ARG:HH11	4:D:684:ASN:HD21	1.59	0.51
3:C:753:THR:CG2	3:C:758:GLU:HG3	2.40	0.51
2:B:78:LEU:CD1	4:D:636:ARG:HH21	2.24	0.51
4:D:647:GLU:CB	4:D:655:TRP:HH2	2.16	0.51
2:B:183:VAL:HG11	2:B:189:PHE:CE1	2.46	0.51
4:D:886:ARG:NH1	11:D:1502:HOH:O	2.34	0.51
2:B:33:THR:OG1	2:B:34:LEU:N	2.43	0.51
2:B:69:VAL:HG12	2:B:128:LEU:HA	1.92	0.51
6:F:285:ALA:O	6:F:289:ILE:HG13	2.10	0.51
4:D:998:ALA:O	4:D:1002:ILE:HG13	2.11	0.50
4:D:177:LEU:HD12	4:D:201:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:588:LEU:HD22	4:D:668:GLY:CA	2.40	0.50
4:D:948:ILE:O	4:D:952:LEU:HD13	2.11	0.50
3:C:650:THR:HG22	3:C:660:SER:CB	2.41	0.50
3:C:754:LYS:CD	4:D:39:LEU:HD12	2.41	0.50
4:D:957:THR:O	4:D:958:THR:HG23	2.11	0.50
3:C:896:PRO:HB3	3:C:1010:PHE:HE2	1.75	0.50
6:F:449:MET:HB3	6:F:453:ARG:NH1	2.25	0.50
3:C:932:LYS:HG2	3:C:1018:TYR:CE2	2.46	0.50
4:D:1222:LEU:HD23	4:D:1244:ASP:OD2	2.11	0.50
7:O:6:DA:OP2	7:O:6:DA:H8	1.94	0.50
3:C:939:VAL:CG2	3:C:943:VAL:HG22	2.41	0.50
4:D:1271:ILE:HG23	5:E:103:HIS:HB2	1.93	0.50
4:D:151:LEU:HD13	4:D:226:PHE:HE2	1.76	0.50
4:D:780:ALA:O	4:D:784:VAL:HG13	2.11	0.50
4:D:892:THR:OG1	4:D:894:ARG:NH1	2.40	0.50
1:J:36:ASN:HD21	1:J:58:ASN:ND2	2.08	0.50
8:P:13:DC:H2"	8:P:14:DA:C8	2.47	0.50
2:B:182:ARG:HD2	2:B:184:GLU:HA	1.94	0.50
3:C:1110:GLU:OE2	4:D:89:ARG:HD3	2.12	0.50
4:D:391:VAL:HG12	4:D:399:LEU:HD22	1.93	0.50
2:A:204:PRO:HD2	2:A:205:ARG:NH1	2.21	0.50
2:A:74:THR:O	2:A:78:LEU:HG	2.10	0.50
3:C:852:LEU:H	3:C:852:LEU:HD23	1.76	0.50
6:F:373:LEU:HD23	6:F:373:LEU:O	2.12	0.50
1:J:79:ARG:NH2	7:O:25:DC:OP1	2.45	0.50
2:A:146:TYR:HD2	2:A:167:ILE:HG12	1.77	0.50
3:C:935:TRP:HA	3:C:984:LEU:CD1	2.42	0.50
4:D:211:ARG:HG3	4:D:214:ARG:NH2	2.27	0.50
4:D:672:PHE:CE1	4:D:687:MET:HG3	2.47	0.50
2:B:143:GLY:HA3	2:B:168:TYR:CD1	2.46	0.50
3:C:640:VAL:HG23	3:C:685:GLN:O	2.12	0.50
3:C:704:MET:HE3	3:C:706:LEU:HD21	1.94	0.50
3:C:796:LYS:HE3	3:C:826:THR:CG2	2.42	0.50
3:C:1084:SER:HB2	4:D:421:ARG:O	2.11	0.50
3:C:789:ASP:HA	3:C:830:VAL:HG22	1.94	0.49
3:C:712:VAL:HG21	3:C:908:LEU:HD12	1.94	0.49
4:D:54:PRO:O	4:D:88:ARG:HG3	2.12	0.49
4:D:601:ALA:HA	4:D:608:GLU:HG2	1.94	0.49
4:D:796:ASN:HB3	4:D:799:ILE:HG12	1.93	0.49
4:D:912:ASP:HB3	4:D:915:VAL:CG1	2.40	0.49
5:E:28:THR:HG23	5:E:28:THR:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LEU:N	2:B:138:LEU:HD12	2.27	0.49
4:D:866:THR:HG23	4:D:867:ALA:H	1.77	0.49
6:F:233:LEU:HD23	6:F:270:VAL:HG13	1.94	0.49
1:J:82:TRP:CZ2	1:J:86:LEU:HD13	2.47	0.49
2:A:146:TYR:CG	3:C:734:GLU:HG2	2.47	0.49
3:C:52:PHE:HZ	3:C:150:MET:HE2	1.76	0.49
3:C:801:GLY:HA2	3:C:802:GLU:C	2.32	0.49
4:D:1152:ASP:O	4:D:1156:GLU:HG3	2.13	0.49
4:D:407:LYS:NZ	4:D:409:LYS:HD2	2.27	0.49
4:D:869:SER:HB3	4:D:1007:THR:CG2	2.37	0.49
4:D:413:PHE:HZ	4:D:874:ARG:NH2	2.10	0.49
3:C:33:ALA:HB2	3:C:966:PRO:HG3	1.93	0.49
3:C:1124:LEU:HD13	4:D:12:ILE:HD11	1.94	0.49
4:D:972:GLY:N	9:D:1405:SO4:O4	2.34	0.49
4:D:174:ALA:O	4:D:178:GLU:HG3	2.13	0.49
4:D:876:LEU:HB3	4:D:999:ALA:HB1	1.94	0.49
6:F:310:MET:HA	6:F:313:VAL:HG12	1.94	0.49
2:B:87:SER:OG	2:B:116:VAL:HG12	2.13	0.49
4:D:113:ARG:NH2	4:D:1232:ARG:HD2	2.28	0.49
3:C:1061:GLU:OE2	4:D:417:LEU:HD22	2.12	0.49
2:T:292:LYS:HG2	8:P:16:DT:OP1	2.12	0.49
2:A:12:GLU:HG2	2:A:13:THR:H	1.77	0.49
2:A:48:GLY:CA	2:A:49:ALA:CB	2.85	0.49
5:E:35:PRO:HG2	5:E:40:LEU:HD11	1.93	0.49
4:D:511:ALA:HB3	4:D:560:LEU:HA	1.93	0.49
3:C:123:PRO:HA	3:C:147:ASP:HA	1.95	0.49
3:C:610:VAL:HG22	3:C:739:THR:O	2.12	0.49
4:D:720:PHE:O	4:D:724:THR:HG23	2.13	0.49
2:T:257:THR:O	2:T:260:SER:N	2.43	0.49
2:A:177:LYS:HB3	2:A:177:LYS:NZ	2.27	0.49
3:C:602:MET:HE1	3:C:1024:LEU:HD21	1.94	0.49
4:D:327:MET:HE1	6:F:304:ILE:HD11	1.95	0.49
1:J:28:GLN:NE2	1:J:46:ASP:O	2.45	0.49
2:A:159:ILE:C	2:A:159:ILE:HD13	2.34	0.49
2:B:170:PRO:CB	2:B:202:ILE:HD11	2.35	0.49
3:C:840:GLY:C	3:C:841:ILE:HD12	2.32	0.49
2:A:181:THR:OG1	2:A:189:PHE:HE2	1.96	0.48
2:B:143:GLY:HA3	2:B:168:TYR:CD2	2.48	0.48
2:B:183:VAL:O	2:B:184:GLU:CB	2.61	0.48
3:C:1058:ARG:CB	3:C:1058:ARG:HH21	2.13	0.48
3:C:792:ILE:HD12	3:C:792:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:937:ILE:CG1	3:C:955:TYR:HB3	2.43	0.48
4:D:990:ILE:HD12	4:D:990:ILE:N	2.26	0.48
2:A:11:GLU:CD	2:A:205:ARG:HG2	2.34	0.48
3:C:414:VAL:O	3:C:418:ILE:HG12	2.14	0.48
3:C:976:LEU:HD13	4:D:732:MET:CE	2.42	0.48
4:D:743:GLU:OE1	4:D:743:GLU:HA	2.14	0.48
4:D:1071:ASP:HB2	4:D:1072:GLY:CA	2.42	0.48
6:F:187:LEU:O	6:F:191:ILE:HG13	2.13	0.48
4:D:1078:TYR:CE2	4:D:1112:LEU:HD11	2.49	0.48
4:D:320:ILE:CG1	4:D:321:PRO:HD2	2.43	0.48
3:C:812:LEU:HD21	6:F:398:LEU:HD21	1.94	0.48
2:B:179:GLU:O	2:B:191:LYS:N	2.46	0.48
3:C:648:TYR:HD2	3:C:650:THR:HG23	1.78	0.48
4:D:385:GLY:HA3	4:D:390:PRO:HG3	1.95	0.48
6:F:255:PHE:N	9:F:1203:SO4:O3	2.39	0.48
7:O:19:DA:H2'	7:O:20:DT:C6	2.48	0.48
2:A:43:LEU:HD11	2:A:174:VAL:HB	1.95	0.48
2:A:94:THR:HG22	2:A:139:VAL:HG22	1.96	0.48
3:C:641:ILE:HD11	3:C:685:GLN:H	1.79	0.48
3:C:952:GLU:HA	3:C:955:TYR:CE1	2.48	0.48
4:D:85:ALA:O	4:D:88:ARG:HB2	2.14	0.48
5:E:49:ALA:O	5:E:53:TYR:HB2	2.14	0.48
2:B:156:GLY:O	2:B:157:ALA:CB	2.61	0.48
2:B:202:ILE:O	2:B:202:ILE:HD12	2.13	0.48
3:C:1043:ILE:HD12	3:C:1043:ILE:N	2.23	0.48
3:C:635:ALA:CA	3:C:693:ILE:HD11	2.43	0.48
3:C:766:ASN:O	3:C:767:VAL:HG13	2.12	0.48
4:D:656:LYS:N	4:D:656:LYS:HD3	2.22	0.48
2:A:216:VAL:HG13	2:B:216:VAL:HG23	1.96	0.48
2:A:42:LEU:O	2:A:46:ILE:HG12	2.14	0.48
2:A:9:LEU:CD2	2:B:225:LEU:HD11	2.44	0.48
2:B:124:HIS:HE1	2:B:127:THR:HG23	1.79	0.48
3:C:1108:ILE:N	3:C:1108:ILE:HD12	2.29	0.48
4:D:596:THR:HG21	4:D:625:GLY:O	2.13	0.48
1:J:64:LEU:HD23	1:J:65:ILE:H	1.78	0.48
3:C:372:VAL:HA	3:C:375:LEU:HD12	1.96	0.48
4:D:48:CYS:SG	4:D:50:LYS:HB2	2.54	0.48
1:J:67:GLY:O	1:J:69:VAL:HG22	2.14	0.48
2:A:92:PRO:HG3	2:A:141:GLU:HG3	1.96	0.48
2:A:159:ILE:HG23	2:A:160:GLY:N	2.29	0.48
2:B:110:ILE:HD12	2:B:138:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:973:GLU:OE1	3:C:973:GLU:N	2.42	0.48
4:D:599:TYR:HA	4:D:610:GLY:CA	2.43	0.47
6:F:290:ARG:HD2	9:F:1204:SO4:O1	2.14	0.47
1:J:97:LEU:HD22	6:F:193:ALA:HB2	1.96	0.47
3:C:602:MET:HE1	3:C:883:LYS:HD3	1.95	0.47
5:E:40:LEU:CB	5:E:50:LEU:HD11	2.41	0.47
3:C:1053:GLN:HG2	3:C:1055:GLY:H	1.79	0.47
3:C:638:THR:HG23	3:C:688:GLU:HA	1.95	0.47
4:D:1006:GLY:CA	4:D:1029:LEU:HD11	2.43	0.47
2:A:40:ARG:HH11	2:A:40:ARG:CB	2.21	0.47
3:C:641:ILE:HD13	3:C:641:ILE:O	2.14	0.47
3:C:826:THR:O	3:C:826:THR:HG23	2.14	0.47
4:D:250:GLU:N	4:D:250:GLU:OE1	2.47	0.47
4:D:602:ALA:HB3	4:D:607:PRO:C	2.34	0.47
3:C:1041:SER:HB3	3:C:1044:THR:O	2.15	0.47
3:C:635:ALA:CB	3:C:693:ILE:HD11	2.44	0.47
3:C:708:LYS:HG3	3:C:737:VAL:HG23	1.97	0.47
3:C:717:TRP:HB2	3:C:907:ILE:HG21	1.96	0.47
4:D:405:LEU:O	4:D:412:ARG:HD2	2.14	0.47
4:D:596:THR:HG22	4:D:626:ALA:O	2.14	0.47
6:F:190:ARG:NH2	6:F:225:ASP:OD2	2.43	0.47
1:J:28:GLN:HG2	1:J:46:ASP:HA	1.96	0.47
2:A:40:ARG:HH11	2:B:33:THR:HG22	1.79	0.47
3:C:370:ARG:HH11	3:C:378:ASN:ND2	2.13	0.47
3:C:755:LEU:HD23	3:C:799:PRO:HB2	1.95	0.47
4:D:693:ALA:O	4:D:697:ASN:ND2	2.45	0.47
4:D:468:ASN:HD22	4:D:468:ASN:H	1.63	0.47
2:A:107:ALA:HB3	2:A:121:PRO:HA	1.97	0.47
2:B:52:THR:HG21	2:B:141:GLU:OE2	2.15	0.47
3:C:110:VAL:HG23	3:C:111:ASP:OD2	2.15	0.47
3:C:641:ILE:HG13	3:C:682:ASP:O	2.15	0.47
3:C:632:VAL:HG22	3:C:694:ALA:O	2.15	0.47
4:D:491:ILE:CD1	4:D:516:LEU:HD21	2.45	0.47
7:O:16:DT:C6	7:O:16:DT:H5'	2.50	0.47
2:B:222:ALA:HA	2:B:225:LEU:HD13	1.96	0.47
3:C:911:HIS:HE1	4:D:580:ASP:OD1	1.98	0.47
3:C:718:GLU:HG2	4:D:724:THR:HG21	1.96	0.47
4:D:898:VAL:HG11	4:D:919:ALA:HB2	1.95	0.47
4:D:951:LEU:O	4:D:956:ILE:HD11	2.14	0.47
5:E:84:LEU:HB2	5:E:85:GLN:NE2	2.20	0.47
3:C:1114:VAL:HG13	4:D:324:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1128:VAL:HG11	3:C:1136:ILE:CB	2.41	0.47
3:C:783:ILE:HG13	3:C:841:ILE:HD13	1.96	0.47
8:P:11:DA:H2''	8:P:12:DA:H5'	1.95	0.47
4:D:1258:LEU:HD12	4:D:1258:LEU:HA	1.71	0.47
2:A:33:THR:CG2	2:B:37:SER:HA	2.45	0.46
3:C:929:TRP:NE1	3:C:993:VAL:HB	2.29	0.46
3:C:984:LEU:HB3	3:C:985:PRO:CD	2.44	0.46
3:C:30:VAL:HG11	3:C:954:LEU:CD2	2.45	0.46
3:C:967:VAL:HG23	3:C:968:PHE:H	1.79	0.46
2:B:230:GLU:OE1	2:B:230:GLU:HA	2.12	0.46
4:D:143:MET:HG2	4:D:251:TYR:HE1	1.77	0.46
4:D:177:LEU:O	4:D:177:LEU:HD23	2.14	0.46
4:D:774:VAL:O	4:D:778:GLN:N	2.35	0.46
8:P:22:DC:H2''	8:P:23:DA:H5'	1.97	0.46
2:B:183:VAL:HG12	2:B:186:ARG:H	1.81	0.46
3:C:400:VAL:HG22	3:C:401:GLU:N	2.30	0.46
3:C:727:ILE:HA	3:C:888:LYS:O	2.16	0.46
4:D:1167:THR:HA	4:D:1181:LEU:H	1.80	0.46
4:D:106:TYR:HB3	4:D:312:MET:CE	2.46	0.46
4:D:1268:TYR:CE1	5:E:49:ALA:HB2	2.51	0.46
6:F:253:MET:HE2	6:F:300:GLN:HB2	1.97	0.46
1:J:65:ILE:HG22	1:J:65:ILE:O	2.15	0.46
2:A:137:GLU:C	2:A:138:LEU:HD12	2.36	0.46
2:B:113:PRO:O	2:B:116:VAL:HG22	2.16	0.46
2:B:231:HIS:O	2:B:232:ILE:HG13	2.15	0.46
3:C:1112:PHE:O	3:C:1115:LEU:HB3	2.16	0.46
3:C:976:LEU:HD13	4:D:732:MET:HE3	1.97	0.46
4:D:39:LEU:HD13	4:D:335:PHE:HZ	1.81	0.46
4:D:692:GLN:O	4:D:696:ILE:HG13	2.15	0.46
2:A:85:VAL:HG22	2:A:86:SER:N	2.31	0.46
3:C:723:GLU:O	3:C:724:ASP:OD1	2.34	0.46
4:D:991:GLY:CA	4:D:1265:ILE:HD11	2.38	0.46
4:D:65:TYR:OH	4:D:76:GLU:OE2	2.30	0.46
6:F:458:SER:O	6:F:461:LEU:N	2.48	0.46
2:T:264:LEU:HB3	2:T:269:VAL:CG2	2.46	0.46
4:D:1046:PRO:HG2	4:D:1081:LEU:CD2	2.45	0.46
4:D:43:LYS:HG3	4:D:50:LYS:HD3	1.98	0.46
6:F:216:ARG:O	6:F:220:GLN:HG3	2.15	0.46
6:F:321:GLN:HA	6:F:337:LEU:HD11	1.97	0.46
6:F:272:LYS:HE3	7:O:25:DC:P	2.55	0.46
3:C:711:LEU:N	3:C:905:ASP:OD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:445:LYS:HB2	4:D:484:TRP:CZ3	2.51	0.46
2:A:27:GLU:HB3	2:A:28:PRO:CD	2.43	0.46
3:C:1048:LEU:HD23	3:C:1048:LEU:O	2.16	0.46
3:C:410:ASN:O	3:C:413:PRO:HD2	2.16	0.46
4:D:24:SER:HB2	4:D:94:HIS:HB3	1.98	0.46
4:D:385:GLY:CA	4:D:390:PRO:HG3	2.46	0.46
3:C:1078:GLU:OE2	4:D:547:LEU:HB2	2.16	0.46
4:D:876:LEU:O	4:D:879:VAL:HG12	2.16	0.46
4:D:982:MET:HE2	4:D:1153:LYS:HD2	1.97	0.46
2:A:24:GLU:OE1	2:A:191:LYS:HD3	2.16	0.46
3:C:1119:LEU:HD23	4:D:406:LEU:HD22	1.97	0.46
3:C:726:ILE:O	3:C:887:GLY:N	2.48	0.46
3:C:768:SER:O	3:C:771:VAL:HG22	2.16	0.46
4:D:404:ASP:CB	4:D:409:LYS:HB3	2.46	0.46
5:E:53:TYR:CE1	5:E:103:HIS:HB3	2.51	0.46
5:E:98:GLY:O	5:E:100:LEU:HD12	2.16	0.46
6:F:321:GLN:O	6:F:325:LEU:HB2	2.15	0.46
3:C:1116:LEU:HG	3:C:1126:VAL:HG21	1.98	0.45
3:C:844:PHE:O	3:C:859:LEU:N	2.40	0.45
3:C:896:PRO:O	3:C:904:VAL:HG13	2.16	0.45
7:O:5:DG:H2"	7:O:6:DA:C8	2.51	0.45
2:B:188:ASP:N	2:B:188:ASP:OD1	2.37	0.45
4:D:68:VAL:HG12	4:D:68:VAL:O	2.16	0.45
6:F:367:ASP:O	6:F:368:GLU:CB	2.64	0.45
2:A:33:THR:HG21	2:B:37:SER:HA	1.98	0.45
2:A:63:PHE:HE1	3:C:741:ILE:HD13	1.81	0.45
4:D:345:ARG:O	4:D:349:ASN:HB2	2.17	0.45
4:D:602:ALA:H	4:D:608:GLU:HA	1.82	0.45
1:J:31:ARG:O	1:J:64:LEU:HD23	2.17	0.45
1:J:79:ARG:NH2	1:J:84:MET:HG2	2.31	0.45
2:A:5:GLN:HG3	2:A:25:PRO:HG3	1.99	0.45
2:A:3:ILE:O	2:A:3:ILE:HG13	2.16	0.45
3:C:712:VAL:O	3:C:1016:VAL:HA	2.16	0.45
3:C:810:ARG:O	3:C:813:ARG:HB2	2.16	0.45
3:C:873:GLY:HA3	3:C:1028:VAL:CG1	2.46	0.45
3:C:917:MET:O	3:C:918:ASN:C	2.55	0.45
4:D:248:TYR:HA	4:D:251:TYR:CE2	2.50	0.45
4:D:295:ARG:O	4:D:298:VAL:HG22	2.16	0.45
4:D:480:ARG:O	4:D:483:VAL:HG22	2.16	0.45
4:D:88:ARG:O	4:D:323:GLU:HG2	2.16	0.45
2:A:78:LEU:HD13	3:C:611:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:GLY:O	2:B:216:VAL:HG12	2.17	0.45
2:B:91:GLU:HB3	2:B:92:PRO:HD2	1.98	0.45
3:C:812:LEU:N	3:C:812:LEU:HD23	2.32	0.45
4:D:1046:PRO:HG2	4:D:1081:LEU:HD21	1.98	0.45
4:D:410:GLN:HA	4:D:410:GLN:HE21	1.82	0.45
4:D:76:GLU:H	4:D:76:GLU:CD	2.19	0.45
2:B:155:SER:O	2:B:156:GLY:C	2.55	0.45
2:B:28:PRO:HA	2:B:29:GLY:HA2	1.59	0.45
3:C:1002:PHE:HA	3:C:1009:PRO:HA	1.98	0.45
4:D:17:ALA:O	4:D:21:ARG:HG3	2.16	0.45
2:A:71:GLU:OE2	2:A:126:ALA:HA	2.17	0.45
3:C:370:ARG:HH11	3:C:378:ASN:HD22	1.65	0.45
3:C:446:LEU:HD21	3:C:491:LEU:HB2	1.99	0.45
3:C:764:ILE:HG23	3:C:765:PRO:HD2	1.99	0.45
4:D:103:HIS:HB3	4:D:106:TYR:HD2	1.82	0.45
6:F:445:GLU:O	6:F:449:MET:HG2	2.17	0.45
2:T:264:LEU:HD22	2:T:269:VAL:HG21	1.98	0.45
2:A:138:LEU:HD12	2:A:138:LEU:N	2.31	0.45
3:C:169:GLN:HB2	3:C:427:LEU:CD2	2.37	0.45
3:C:945:ASP:N	3:C:945:ASP:OD1	2.50	0.45
4:D:1132:GLN:HG2	4:D:1159:VAL:HG12	1.98	0.45
2:B:147:VAL:O	2:B:147:VAL:HG13	2.17	0.45
3:C:805:LEU:HD12	3:C:810:ARG:CZ	2.47	0.45
3:C:980:LEU:HB3	3:C:995:ALA:HA	1.99	0.45
2:A:68:GLY:CA	2:A:129:ASN:HD21	2.30	0.45
4:D:1265:ILE:HG22	4:D:1266:SER:N	2.32	0.45
3:C:34:LYS:C	3:C:35:LEU:HD12	2.36	0.44
3:C:506:PRO:HA	3:C:521:TYR:HA	1.99	0.44
3:C:727:ILE:CG2	3:C:888:LYS:HB3	2.46	0.44
4:D:599:TYR:HB2	4:D:633:ILE:HA	1.99	0.44
4:D:981:SER:HB3	4:D:984:THR:OG1	2.17	0.44
7:O:11:DA:C2'	7:O:12:DG:H5''	2.43	0.44
8:P:20:DG:H2''	8:P:21:DT:C5'	2.45	0.44
2:A:105:VAL:HG23	2:A:128:LEU:HD13	1.99	0.44
2:B:13:THR:HG23	2:B:13:THR:O	2.17	0.44
2:B:32:TYR:CE1	3:C:1005:ARG:HD3	2.52	0.44
3:C:1072:ALA:HB1	4:D:554:GLU:OE2	2.17	0.44
3:C:506:PRO:HG2	3:C:576:GLN:OE1	2.17	0.44
3:C:626:ALA:HB3	3:C:702:GLY:O	2.17	0.44
3:C:783:ILE:N	3:C:783:ILE:HD12	2.26	0.44
4:D:613:SER:N	4:D:617:GLU:OE1	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:876:LEU:CD1	3:C:886:ILE:HD11	2.48	0.44
4:D:198:ARG:O	4:D:202:GLU:HG3	2.16	0.44
4:D:386:ARG:HH12	4:D:1231:THR:HG21	1.83	0.44
2:A:182:ARG:HH22	4:D:624:ARG:HG3	1.81	0.44
2:B:231:HIS:H	2:B:231:HIS:CD2	2.35	0.44
3:C:1044:THR:OG1	3:C:1046:GLN:HG3	2.17	0.44
2:A:97:LEU:HD22	2:A:110:ILE:HG12	2.00	0.44
3:C:727:ILE:C	3:C:728:LEU:HD23	2.37	0.44
2:A:174:VAL:O	3:C:901:GLY:HA3	2.17	0.44
4:D:581:MET:HB3	4:D:719:GLY:HA3	1.99	0.44
4:D:639:GLU:O	4:D:678:LYS:NZ	2.51	0.44
5:E:26:TYR:O	5:E:26:TYR:HD1	1.98	0.44
1:J:45:ALA:HB2	4:D:73:ILE:HD12	1.98	0.44
3:C:760:ILE:HB	3:C:795:GLY:O	2.18	0.44
4:D:386:ARG:NH1	4:D:1231:THR:HG21	2.32	0.44
4:D:636:ARG:HD3	4:D:660:ALA:CB	2.42	0.44
2:A:102:PRO:HD3	2:A:130:ASP:HA	1.99	0.44
2:B:199:LYS:HB2	2:B:199:LYS:HE3	1.78	0.44
2:B:24:GLU:HA	2:B:25:PRO:HA	1.73	0.44
3:C:391:VAL:O	3:C:395:MET:HG2	2.18	0.44
3:C:498:ASN:CG	3:C:499:PRO:HD2	2.38	0.44
3:C:649:ILE:HD11	3:C:679:PRO:CB	2.47	0.44
4:D:924:LEU:CD2	4:D:943:LEU:HD11	2.48	0.44
6:F:175:LYS:HD3	6:F:175:LYS:C	2.38	0.44
3:C:1122:LEU:HD23	4:D:105:TRP:CH2	2.53	0.44
4:D:1127:GLY:O	4:D:1131:VAL:HG23	2.17	0.44
2:A:214:THR:HG23	2:B:232:ILE:HB	1.99	0.44
3:C:896:PRO:HB3	3:C:1010:PHE:CE2	2.52	0.44
3:C:1026:HIS:CB	3:C:1031:LYS:HE2	2.41	0.44
3:C:1094:TYR:O	3:C:1098:VAL:HG23	2.18	0.44
3:C:937:ILE:HD12	3:C:937:ILE:N	2.33	0.44
4:D:1041:PRO:HD3	4:D:1118:ASP:HA	2.00	0.44
4:D:1231:THR:HB	9:D:1407:SO4:O3	2.18	0.44
4:D:139:VAL:HG12	4:D:231:PRO:HG3	1.99	0.44
4:D:270:ILE:HG13	4:D:270:ILE:H	1.62	0.44
4:D:443:LEU:HD23	4:D:448:ALA:HB2	1.99	0.44
4:D:327:MET:HE2	6:F:304:ILE:HD11	2.00	0.44
7:O:16:DT:H6	7:O:16:DT:H5'	1.82	0.44
2:B:112:PRO:HB2	2:B:116:VAL:HG23	2.00	0.43
2:B:68:GLY:HA2	2:B:129:ASN:CB	2.47	0.43
3:C:852:LEU:HD11	3:C:857:ASN:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:114:LEU:HD23	4:D:114:LEU:HA	1.83	0.43
4:D:119:ASP:C	4:D:120:LEU:HD12	2.39	0.43
4:D:397:ARG:O	4:D:397:ARG:HG3	2.18	0.43
4:D:668:GLY:HA2	4:D:671:MET:CE	2.47	0.43
4:D:876:LEU:HA	4:D:876:LEU:HD12	1.83	0.43
6:F:394:LEU:HB2	6:F:464:TYR:CD1	2.53	0.43
2:B:211:ALA:O	2:B:215:LEU:HB2	2.18	0.43
2:A:214:THR:CG2	2:B:232:ILE:HD12	2.48	0.43
3:C:379:GLN:HG2	3:C:421:PHE:CB	2.47	0.43
3:C:638:THR:HG23	3:C:687:VAL:O	2.18	0.43
3:C:728:LEU:HD11	3:C:886:ILE:HD13	2.01	0.43
2:A:72:ASP:OD1	2:A:75:ASP:N	2.47	0.43
3:C:1061:GLU:HA	3:C:1061:GLU:OE1	2.18	0.43
3:C:165:VAL:HG23	3:C:431:MET:HB2	2.00	0.43
4:D:676:LEU:HD23	4:D:676:LEU:H	1.81	0.43
4:D:726:SER:OG	4:D:728:VAL:HG23	2.19	0.43
4:D:943:LEU:HA	4:D:943:LEU:HD23	1.84	0.43
2:A:130:ASP:OD1	2:A:130:ASP:N	2.51	0.43
3:C:822:GLU:H	3:C:822:GLU:CD	2.21	0.43
3:C:742:HIS:HD2	3:C:868:ARG:HG3	1.82	0.43
4:D:129:ILE:HD11	4:D:130:TYR:CZ	2.53	0.43
4:D:525:HIS:O	4:D:528:VAL:HG22	2.18	0.43
4:D:748:HIS:HE2	4:D:777:TRP:HA	1.83	0.43
4:D:1276:THR:HG23	5:E:101:LEU:HA	2.00	0.43
4:D:236:VAL:HG12	4:D:236:VAL:O	2.18	0.43
4:D:340:LEU:HG	4:D:402:LEU:HD21	2.00	0.43
4:D:880:SER:O	4:D:995:GLY:HA3	2.17	0.43
3:C:1102:ASN:ND2	5:E:59:ARG:HB3	2.33	0.43
3:C:729:SER:N	3:C:905:ASP:O	2.51	0.43
4:D:218:ARG:NH2	9:D:1403:SO4:S	2.92	0.43
4:D:636:ARG:CG	4:D:662:THR:HG22	2.47	0.43
4:D:640:LEU:O	4:D:656:LYS:HE3	2.19	0.43
6:F:437:THR:HG1	7:O:3:DT:P	2.42	0.43
2:A:180:ALA:HA	2:A:190:ASP:HA	2.00	0.43
3:C:85:SER:HA	3:C:86:PRO:HA	1.84	0.43
4:D:104:ILE:HD12	4:D:379:ASP:HB3	2.01	0.43
4:D:1108:VAL:O	4:D:1108:VAL:HG12	2.19	0.43
4:D:226:PHE:O	4:D:229:LEU:HB2	2.18	0.43
4:D:606:ALA:HB1	4:D:607:PRO:HD2	1.99	0.43
5:E:95:GLU:HB3	5:E:101:LEU:HD21	2.01	0.43
2:B:42:LEU:O	2:B:171:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:VAL:HG23	3:C:111:ASP:N	2.34	0.43
3:C:1130:SER:CB	3:C:1136:ILE:HD11	2.32	0.43
3:C:30:VAL:CG1	3:C:954:LEU:HG	2.48	0.43
4:D:1089:VAL:HG13	4:D:1098:GLY:C	2.39	0.43
4:D:1231:THR:O	4:D:1235:THR:HG23	2.19	0.43
4:D:556:ARG:HG2	5:E:32:ILE:CD1	2.49	0.43
3:C:1138:MET:HA	3:C:1138:MET:HE2	2.00	0.43
3:C:444:ARG:NH2	3:C:492:SER:O	2.52	0.43
3:C:493:VAL:HG23	3:C:578:VAL:O	2.19	0.43
3:C:648:TYR:CE2	3:C:650:THR:HG23	2.54	0.43
4:D:327:MET:SD	4:D:337:THR:HB	2.59	0.43
4:D:447:MET:O	4:D:451:LEU:HB2	2.19	0.43
4:D:686:GLN:O	4:D:688:HIS:N	2.49	0.43
1:J:97:LEU:HD12	11:F:1302:HOH:O	2.18	0.43
2:A:36:ASN:ND2	2:A:40:ARG:HD2	2.30	0.43
2:B:145:GLY:O	2:B:168:TYR:HB2	2.19	0.43
2:A:209:ALA:CB	2:B:226:ASN:HB3	2.49	0.43
3:C:644:VAL:O	3:C:644:VAL:HG23	2.18	0.43
3:C:704:MET:CE	3:C:706:LEU:HD21	2.49	0.43
4:D:262:LYS:HG3	4:D:310:MET:HE3	2.01	0.43
3:C:877:ALA:O	3:C:1022:LEU:HG	2.19	0.42
4:D:1037:GLU:HG2	4:D:1039:ARG:CZ	2.49	0.42
4:D:348:ILE:HD11	4:D:352:ASN:ND2	2.34	0.42
7:O:5:DG:H2"	7:O:6:DA:H8	1.84	0.42
2:A:213:GLY:HA3	2:B:231:HIS:CD2	2.54	0.42
2:B:54:ILE:HG22	2:B:138:LEU:HA	2.01	0.42
2:B:176:TYR:HD1	2:B:176:TYR:H	1.67	0.42
3:C:412:ARG:N	3:C:413:PRO:HD2	2.34	0.42
3:C:986:ASN:OD1	3:C:986:ASN:N	2.40	0.42
4:D:1249:LEU:HB3	4:D:1260:PRO:HD2	2.00	0.42
4:D:641:ARG:HA	4:D:642:PRO:HD3	1.90	0.42
3:C:1069:ALA:HB1	4:D:997:VAL:HG22	2.00	0.42
6:F:291:GLN:HG3	6:F:292:ALA:N	2.33	0.42
6:F:436:VAL:HG23	6:F:437:THR:O	2.18	0.42
1:J:97:LEU:HD23	1:J:97:LEU:O	2.19	0.42
3:C:1008:GLU:H	3:C:1008:GLU:HG2	1.57	0.42
3:C:736:ASP:OD1	3:C:869:LYS:HE2	2.18	0.42
4:D:116:TYR:O	4:D:295:ARG:HG3	2.20	0.42
3:C:1036:SER:HB3	4:D:450:GLU:O	2.19	0.42
4:D:577:PRO:HA	4:D:581:MET:HE1	2.01	0.42
4:D:641:ARG:CA	4:D:656:LYS:HE3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:179:LEU:HD13	6:F:187:LEU:CD1	2.48	0.42
6:F:280:LYS:NZ	7:O:30:DC:OP1	2.52	0.42
6:F:451:LYS:O	6:F:457:ARG:HD2	2.19	0.42
2:T:256:LEU:HB3	2:T:260:SER:HB2	2.01	0.42
2:B:147:VAL:CG1	2:B:166:SER:HB2	2.49	0.42
3:C:44:LEU:HD22	3:C:444:ARG:HH12	1.85	0.42
3:C:491:LEU:HG	3:C:492:SER:N	2.35	0.42
3:C:643:GLU:HA	3:C:643:GLU:OE2	2.20	0.42
4:D:404:ASP:O	4:D:409:LYS:N	2.52	0.42
4:D:451:LEU:HD12	4:D:451:LEU:HA	1.86	0.42
6:F:198:THR:OG1	6:F:223:CYS:SG	2.69	0.42
2:A:99:LYS:HG2	2:A:105:VAL:HG22	2.01	0.42
2:B:107:ALA:HB3	2:B:120:ASN:O	2.19	0.42
3:C:965:THR:O	3:C:965:THR:OG1	2.27	0.42
2:A:60:LEU:HB3	2:A:159:ILE:HD11	2.01	0.42
2:B:113:PRO:HD2	2:B:116:VAL:HG21	2.00	0.42
2:B:17:ASN:HB3	2:B:198:THR:O	2.19	0.42
2:B:218:LEU:O	2:B:221:LEU:HG	2.20	0.42
3:C:430:PHE:O	3:C:442:HIS:HE1	2.02	0.42
4:D:525:HIS:CG	4:D:526:PRO:HD2	2.54	0.42
6:F:194:GLY:HA2	6:F:222:ILE:HG22	2.01	0.42
6:F:399:GLN:NE2	6:F:403:GLU:OE2	2.52	0.42
3:C:966:PRO:HG2	3:C:969:ASP:O	2.19	0.42
4:D:945:ASP:HB3	4:D:946:PRO:HD3	2.02	0.42
4:D:900:LEU:HD12	4:D:956:ILE:HD13	2.01	0.42
4:D:989:ASP:OD2	5:E:46:SER:HB2	2.20	0.42
6:F:200:LYS:O	6:F:204:LEU:HG	2.18	0.42
6:F:268:ARG:HD3	6:F:288:TRP:CH2	2.55	0.42
8:P:17:DT:H1'	8:P:18:DT:H5''	2.02	0.42
2:A:11:GLU:OE1	2:A:205:ARG:HG2	2.19	0.42
2:A:46:ILE:HA	2:A:47:PRO:HD3	1.89	0.42
2:B:183:VAL:HG13	2:B:185:GLN:HG3	2.02	0.42
3:C:619:THR:OG1	3:C:620:GLY:N	2.53	0.42
4:D:1054:VAL:HG12	4:D:1104:ASP:O	2.20	0.42
4:D:229:LEU:HA	4:D:229:LEU:HD23	1.90	0.42
2:A:40:ARG:HE	3:C:1005:ARG:HA	1.85	0.42
3:C:751:ARG:CB	3:C:856:VAL:HA	2.50	0.42
3:C:778:ARG:HG3	3:C:778:ARG:H	1.59	0.42
4:D:262:LYS:HG3	4:D:310:MET:HE1	2.01	0.42
4:D:405:LEU:C	4:D:405:LEU:CD1	2.87	0.42
4:D:680:TYR:CG	4:D:681:PRO:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:3:DC:H2"	8:P:4:DA:C8	2.55	0.42
2:A:78:LEU:HD13	3:C:611:ARG:NH1	2.34	0.42
3:C:1028:VAL:HG12	4:D:429:VAL:CG1	2.50	0.42
3:C:792:ILE:HD12	3:C:792:ILE:H	1.85	0.42
4:D:103:HIS:ND1	4:D:105:TRP:HB2	2.34	0.42
4:D:1151:HIS:ND1	4:D:1153:LYS:HG2	2.34	0.42
4:D:231:PRO:O	4:D:232:LYS:HB2	2.20	0.42
6:F:185:VAL:HG12	6:F:189:LYS:HE3	2.01	0.42
1:J:54:TRP:CH2	4:D:79:GLY:HA2	2.54	0.42
2:A:92:PRO:HG3	2:A:141:GLU:CG	2.50	0.41
3:C:771:VAL:HG23	3:C:772:LEU:CD1	2.50	0.41
3:C:587:PHE:CZ	3:C:927:LEU:HD12	2.55	0.41
4:D:1268:TYR:HE1	5:E:49:ALA:HB2	1.84	0.41
4:D:745:LEU:HD21	4:D:780:ALA:HB1	2.02	0.41
4:D:881:GLN:HE22	4:D:1250:LYS:HE2	1.84	0.41
3:C:811:LEU:HD23	6:F:398:LEU:HD13	2.02	0.41
3:C:1043:ILE:H	3:C:1043:ILE:CD1	2.21	0.41
3:C:663:LEU:O	3:C:665:LYS:HG2	2.20	0.41
3:C:1124:LEU:HD11	4:D:105:TRP:HZ3	1.86	0.41
6:F:164:ASP:OD1	6:F:166:VAL:N	2.53	0.41
6:F:253:MET:HE3	6:F:300:GLN:HB2	2.01	0.41
6:F:333:THR:HB	6:F:334:PRO:CD	2.50	0.41
6:F:333:THR:HB	6:F:334:PRO:HD2	2.02	0.41
2:B:174:VAL:HG22	2:B:196:VAL:HA	2.01	0.41
3:C:1062:MET:HE2	11:C:1201:HOH:O	2.19	0.41
3:C:54:TRP:HD1	3:C:61:TRP:CZ2	2.38	0.41
4:D:602:ALA:HB3	4:D:607:PRO:O	2.19	0.41
4:D:656:LYS:N	4:D:657:PRO:CD	2.83	0.41
2:B:54:ILE:HG13	2:B:162:ILE:CD1	2.50	0.41
3:C:1001:LEU:HD21	3:C:1016:VAL:HG11	2.01	0.41
4:D:348:ILE:HD11	4:D:352:ASN:HD21	1.86	0.41
1:J:91:VAL:HG22	1:J:92:GLU:OE1	2.19	0.41
2:A:193:ILE:C	2:A:193:ILE:HD12	2.41	0.41
2:B:124:HIS:CE1	2:B:127:THR:HG23	2.56	0.41
2:B:86:SER:O	2:B:117:THR:HG22	2.21	0.41
3:C:150:MET:HA	3:C:150:MET:HE2	2.02	0.41
4:D:206:ARG:HD3	4:D:206:ARG:C	2.41	0.41
4:D:340:LEU:HG	4:D:402:LEU:CD2	2.50	0.41
4:D:421:ARG:NH2	9:D:1404:SO4:O4	2.54	0.41
3:C:597:LEU:HD23	3:C:597:LEU:O	2.21	0.41
3:C:587:PHE:HZ	3:C:927:LEU:HD12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1004:GLU:HB3	4:D:1005:PRO:CD	2.39	0.41
4:D:1080:LYS:C	4:D:1081:LEU:HG	2.41	0.41
4:D:248:TYR:HA	4:D:251:TYR:HE2	1.85	0.41
4:D:937:ILE:CD1	4:D:947:ALA:HB1	2.50	0.41
4:D:944:GLY:CA	4:D:980:ARG:HH22	2.26	0.41
3:C:1003:ASP:HB2	3:C:1010:PHE:CE1	2.55	0.41
3:C:755:LEU:HD12	3:C:755:LEU:O	2.20	0.41
4:D:88:ARG:O	4:D:322:PRO:HD2	2.20	0.41
4:D:924:LEU:HB2	4:D:939:ARG:HA	2.03	0.41
6:F:291:GLN:OE1	7:O:25:DC:N4	2.53	0.41
3:C:1128:VAL:CG1	3:C:1136:ILE:H	2.33	0.41
3:C:169:GLN:O	3:C:370:ARG:N	2.43	0.41
3:C:636:ASP:N	3:C:636:ASP:OD1	2.54	0.41
4:D:248:TYR:HB3	4:D:251:TYR:CD2	2.56	0.41
4:D:272:ALA:O	4:D:275:GLU:HG2	2.21	0.41
4:D:273:GLU:OE1	4:D:295:ARG:NH2	2.54	0.41
4:D:365:ILE:CD1	4:D:365:ILE:H	2.21	0.41
4:D:496:VAL:HG13	4:D:514:PRO:HG3	2.03	0.41
4:D:496:VAL:HG22	4:D:514:PRO:HG3	2.02	0.41
4:D:581:MET:HE2	4:D:716:LYS:HA	2.01	0.41
4:D:947:ALA:O	4:D:951:LEU:HG	2.21	0.41
8:P:3:DC:H2"	8:P:4:DA:H8	1.85	0.41
2:A:1:MET:O	2:A:1:MET:HG2	2.21	0.41
3:C:44:LEU:HD22	3:C:444:ARG:NH1	2.36	0.41
3:C:447:LEU:HD23	3:C:447:LEU:HA	1.65	0.41
3:C:787:VAL:HG22	3:C:836:GLY:O	2.21	0.41
3:C:807:PRO:HB2	6:F:419:LEU:CD2	2.47	0.41
4:D:1045:ALA:HA	4:D:1046:PRO:HD3	1.92	0.41
2:B:182:ARG:HD2	2:B:184:GLU:H	1.86	0.41
3:C:897:PHE:HE2	3:C:1004:GLY:HA2	1.86	0.41
3:C:1102:ASN:OD1	3:C:1102:ASN:N	2.53	0.41
3:C:120:TYR:CE2	3:C:150:MET:HB2	2.56	0.41
3:C:986:ASN:O	3:C:987:ARG:C	2.59	0.41
4:D:1208:LEU:HA	4:D:1208:LEU:HD23	1.87	0.41
6:F:183:GLU:O	6:F:187:LEU:HD12	2.21	0.41
6:F:364:THR:HG23	6:F:364:THR:O	2.20	0.41
1:J:69:VAL:N	1:J:70:PRO:CD	2.84	0.41
2:T:284:LEU:O	2:T:284:LEU:HD23	2.21	0.41
3:C:24:PRO:HG2	3:C:688:GLU:HB2	2.03	0.40
3:C:436:PRO:HG2	3:C:704:MET:CE	2.51	0.40
3:C:678:ARG:O	3:C:695:ASP:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:760:ILE:CA	3:C:796:LYS:HA	2.41	0.40
3:C:915:ARG:HA	3:C:915:ARG:HD2	1.70	0.40
4:D:1167:THR:OG1	4:D:1207:VAL:HG21	2.22	0.40
4:D:166:ARG:HD3	4:D:212:ALA:HB3	2.01	0.40
4:D:250:GLU:CD	4:D:250:GLU:H	2.23	0.40
4:D:633:ILE:HD12	4:D:633:ILE:C	2.41	0.40
1:J:34:THR:CG2	1:J:40:PHE:HE1	2.33	0.40
2:A:157:ALA:HB1	2:A:161:ARG:HE	1.86	0.40
3:C:1059:PHE:CE1	3:C:1063:GLU:HB3	2.56	0.40
4:D:302:PHE:CE2	4:D:309:PRO:HA	2.56	0.40
4:D:407:LYS:HZ2	4:D:409:LYS:HD2	1.85	0.40
3:C:1047:PRO:O	4:D:421:ARG:HD3	2.22	0.40
2:A:182:ARG:HH12	4:D:624:ARG:NH1	2.18	0.40
6:F:364:THR:HA	6:F:372:GLN:HA	2.04	0.40
2:B:231:HIS:CG	2:B:232:ILE:H	2.38	0.40
3:C:1035:ARG:CZ	3:C:1047:PRO:HB3	2.51	0.40
3:C:446:LEU:N	3:C:446:LEU:HD23	2.36	0.40
3:C:950:LEU:HA	3:C:950:LEU:HD23	1.79	0.40
3:C:952:GLU:HA	3:C:955:TYR:HE1	1.86	0.40
4:D:28:VAL:CG1	4:D:319:VAL:HG21	2.51	0.40
4:D:591:LEU:HD23	4:D:591:LEU:HA	1.90	0.40
4:D:676:LEU:CD2	4:D:676:LEU:N	2.84	0.40
6:F:231:ASN:O	6:F:235:GLU:HG3	2.22	0.40
2:A:214:THR:O	2:A:218:LEU:HB2	2.22	0.40
3:C:764:ILE:HB	3:C:767:VAL:CG2	2.49	0.40
3:C:875:LYS:HB3	3:C:875:LYS:HE2	1.76	0.40
4:D:404:ASP:OD1	4:D:404:ASP:N	2.53	0.40
4:D:580:ASP:HB3	4:D:720:PHE:CE2	2.57	0.40
4:D:651:PHE:CD2	4:D:651:PHE:N	2.89	0.40
4:D:873:THR:OG1	4:D:1003:GLY:HA3	2.22	0.40
3:C:1003:ASP:OD1	3:C:1006:SER:N	2.37	0.40
4:D:668:GLY:HA2	4:D:671:MET:HE2	2.03	0.40
2:T:286:ILE:HG22	2:T:289:PHE:CB	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:628:SER:OG	9:F:1201:SO4:O4[1_554]	1.88	0.32

5.3 Torsion angles

5.3.1 Protein backbone

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	J	86/114 (75%)	80 (93%)	6 (7%)	0	100	100
2	A	221/350 (63%)	208 (94%)	11 (5%)	2 (1%)	17	56
2	B	233/350 (67%)	213 (91%)	16 (7%)	4 (2%)	9	42
2	T	51/350 (15%)	50 (98%)	1 (2%)	0	100	100
3	C	774/1169 (66%)	720 (93%)	52 (7%)	2 (0%)	41	74
4	D	1160/1317 (88%)	1118 (96%)	41 (4%)	1 (0%)	51	83
5	E	73/107 (68%)	69 (94%)	3 (4%)	1 (1%)	11	46
6	F	300/466 (64%)	296 (99%)	4 (1%)	0	100	100
All	All	2898/4223 (69%)	2754 (95%)	134 (5%)	10 (0%)	41	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1169	ILE
5	E	27	ASP
2	A	158	GLU
3	C	172	ARG
2	B	157	ALA
2	B	231	HIS
2	B	234	ILE
3	C	850	ASP
2	A	92	PRO
2	B	156	GLY

5.3.2 Protein sidechains

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	J	68/98 (69%)	57 (84%)	11 (16%)	2	11
2	A	178/297 (60%)	158 (89%)	20 (11%)	6	25
2	B	162/297 (54%)	148 (91%)	14 (9%)	10	38
2	T	35/297 (12%)	31 (89%)	4 (11%)	5	24
3	C	579/984 (59%)	520 (90%)	59 (10%)	7	29
4	D	853/1095 (78%)	779 (91%)	74 (9%)	10	37
5	E	60/86 (70%)	46 (77%)	14 (23%)	1	3
6	F	241/379 (64%)	224 (93%)	17 (7%)	14	47
All	All	2176/3533 (62%)	1963 (90%)	213 (10%)	8	31

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	ASP
1	J	55	LEU
1	J	57	ARG
1	J	58	ASN
1	J	64	LEU
1	J	66	GLU
1	J	69	VAL
1	J	79	ARG
1	J	91	VAL
1	J	102	LEU
1	J	104	LEU
2	A	14	VAL
2	A	40	ARG
2	A	74	THR
2	A	84	VAL
2	A	88	ASP
2	A	111	VAL
2	A	117	THR
2	A	127	THR
2	A	129	ASN
2	A	135	GLU
2	A	158	GLU
2	A	159	ILE
2	A	168	TYR

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Mol	Chain	Res	Type
2	A	177	LYS
2	A	181	THR
2	A	182	ARG
2	A	187	THR
2	A	189	PHE
2	A	192	LEU
2	A	206	ASP
2	B	60	LEU
2	B	78	LEU
2	B	84	VAL
2	B	88	ASP
2	B	98	ARG
2	B	138	LEU
2	B	151	GLN
2	B	176	TYR
2	B	185	GLN
2	B	188	ASP
2	B	198	THR
2	B	200	ASN
2	B	218	LEU
2	B	230	GLU
3	C	60	ARG
3	C	84	LEU
3	C	111	ASP
3	C	119	THR
3	C	124	LEU
3	C	153	GLU
3	C	377	GLN
3	C	427	LEU
3	C	434	ASN
3	C	437	LEU
3	C	446	LEU
3	C	447	LEU
3	C	505	THR
3	C	579	SER
3	C	607	VAL
3	C	611	ARG
3	C	619	THR
3	C	623	LEU
3	C	627	ILE
3	C	632	VAL
3	C	636	ASP

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Mol	Chain	Res	Type
3	C	641	ILE
3	C	669	SER
3	C	721	ASN
3	C	724	ASP
3	C	727	ILE
3	C	737	VAL
3	C	753	THR
3	C	754	LYS
3	C	775	LEU
3	C	777	GLU
3	C	778	ARG
3	C	804	GLU
3	C	830	VAL
3	C	848	ASP
3	C	850	ASP
3	C	851	GLU
3	C	852	LEU
3	C	859	LEU
3	C	866	GLN
3	C	872	ASP
3	C	915	ARG
3	C	927	LEU
3	C	936	ASN
3	C	937	ILE
3	C	945	ASP
3	C	954	LEU
3	C	972	GLN
3	C	983	THR
3	C	984	LEU
3	C	988	ASP
3	C	1008	GLU
3	C	1022	LEU
3	C	1024	LEU
3	C	1045	GLN
3	C	1053	GLN
3	C	1058	ARG
3	C	1091	VAL
3	C	1137	GLU
4	D	7	PHE
4	D	28	VAL
4	D	36	TYR
4	D	60	CYS

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Mol	Chain	Res	Type
4	D	70	PHE
4	D	88	ARG
4	D	89	ARG
4	D	101	VAL
4	D	107	PHE
4	D	137	THR
4	D	139	VAL
4	D	141	ASP
4	D	144	ARG
4	D	148	LEU
4	D	165	GLN
4	D	206	ARG
4	D	208	LEU
4	D	229	LEU
4	D	234	LEU
4	D	238	GLU
4	D	243	GLU
4	D	247	ARG
4	D	248	TYR
4	D	277	LEU
4	D	281	ILE
4	D	303	GLN
4	D	314	LEU
4	D	330	LEU
4	D	334	ARG
4	D	404	ASP
4	D	405	LEU
4	D	410	GLN
4	D	415	GLN
4	D	449	LEU
4	D	451	LEU
4	D	456	VAL
4	D	468	ASN
4	D	474	ARG
4	D	488	GLU
4	D	518	GLU
4	D	558	LEU
4	D	581	MET
4	D	588	LEU
4	D	591	LEU
4	D	593	GLU
4	D	627	LEU

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Mol	Chain	Res	Type
4	D	645	ASP
4	D	655	TRP
4	D	656	LYS
4	D	667	LEU
4	D	676	LEU
4	D	698	ASP
4	D	713	ASP
4	D	724	THR
4	D	734	ASP
4	D	866	THR
4	D	876	LEU
4	D	900	LEU
4	D	927	ASP
4	D	939	ARG
4	D	949	ASP
4	D	952	LEU
4	D	956	ILE
4	D	989	ASP
4	D	1029	LEU
4	D	1049	ASP
4	D	1056	LEU
4	D	1079	ASP
4	D	1110	ASP
4	D	1182	THR
4	D	1208	LEU
4	D	1222	LEU
4	D	1258	LEU
4	D	1267	ARG
5	E	27	ASP
5	E	32	ILE
5	E	34	ASN
5	E	37	ILE
5	E	50	LEU
5	E	53	TYR
5	E	57	ARG
5	E	59	ARG
5	E	80	VAL
5	E	84	LEU
5	E	85	GLN
5	E	101	LEU
5	E	102	GLU
5	E	103	HIS

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Mol	Chain	Res	Type
6	F	172	GLN
6	F	176	VAL
6	F	187	LEU
6	F	195	LEU
6	F	291	GLN
6	F	310	MET
6	F	317	LEU
6	F	324	LEU
6	F	330	ARG
6	F	337	LEU
6	F	349	LEU
6	F	383	VAL
6	F	386	VAL
6	F	406	SER
6	F	409	GLU
6	F	433	VAL
6	F	437	THR
2	T	252	ASP
2	T	255	ASP
2	T	279	THR
2	T	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	28	GLN
1	J	58	ASN
2	A	36	ASN
2	A	129	ASN
2	B	124	HIS
2	B	226	ASN
3	C	48	GLN
3	C	377	GLN
3	C	378	ASN
3	C	433	GLN
3	C	590	HIS
3	C	700	GLN
3	C	721	ASN
3	C	911	HIS
3	C	936	ASN
3	C	1046	GLN
3	C	1057	GLN

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Mol	Chain	Res	Type
4	D	165	GLN
4	D	245	GLN
4	D	267	ASN
4	D	368	ASN
4	D	410	GLN
4	D	468	ASN
4	D	515	GLN
4	D	564	ASN
4	D	600	GLN
4	D	684	ASN
4	D	686	GLN
4	D	692	GLN
4	D	765	ASN
4	D	881	GLN
4	D	897	ASN
4	D	1140	GLN
4	D	1146	GLN
4	D	1228	GLN
5	E	85	GLN
6	F	326	GLN
6	F	395	GLN
6	F	397	GLN

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
9	SO4	F	1201	-	4,4,4	0.15	0	6,6,6	0.06	0
9	SO4	D	1403	-	4,4,4	0.15	0	6,6,6	0.07	0
9	SO4	D	1404	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	D	1406	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	F	1204	-	4,4,4	0.13	0	6,6,6	0.09	0
9	SO4	D	1402	-	0,1,4	0.00	-	-	-	-
9	SO4	D	1405	-	4,4,4	0.14	0	6,6,6	0.06	0
9	SO4	F	1203	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	F	1202	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	D	1407	-	4,4,4	0.15	0	6,6,6	0.05	0
9	SO4	D	1408	-	4,4,4	0.14	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

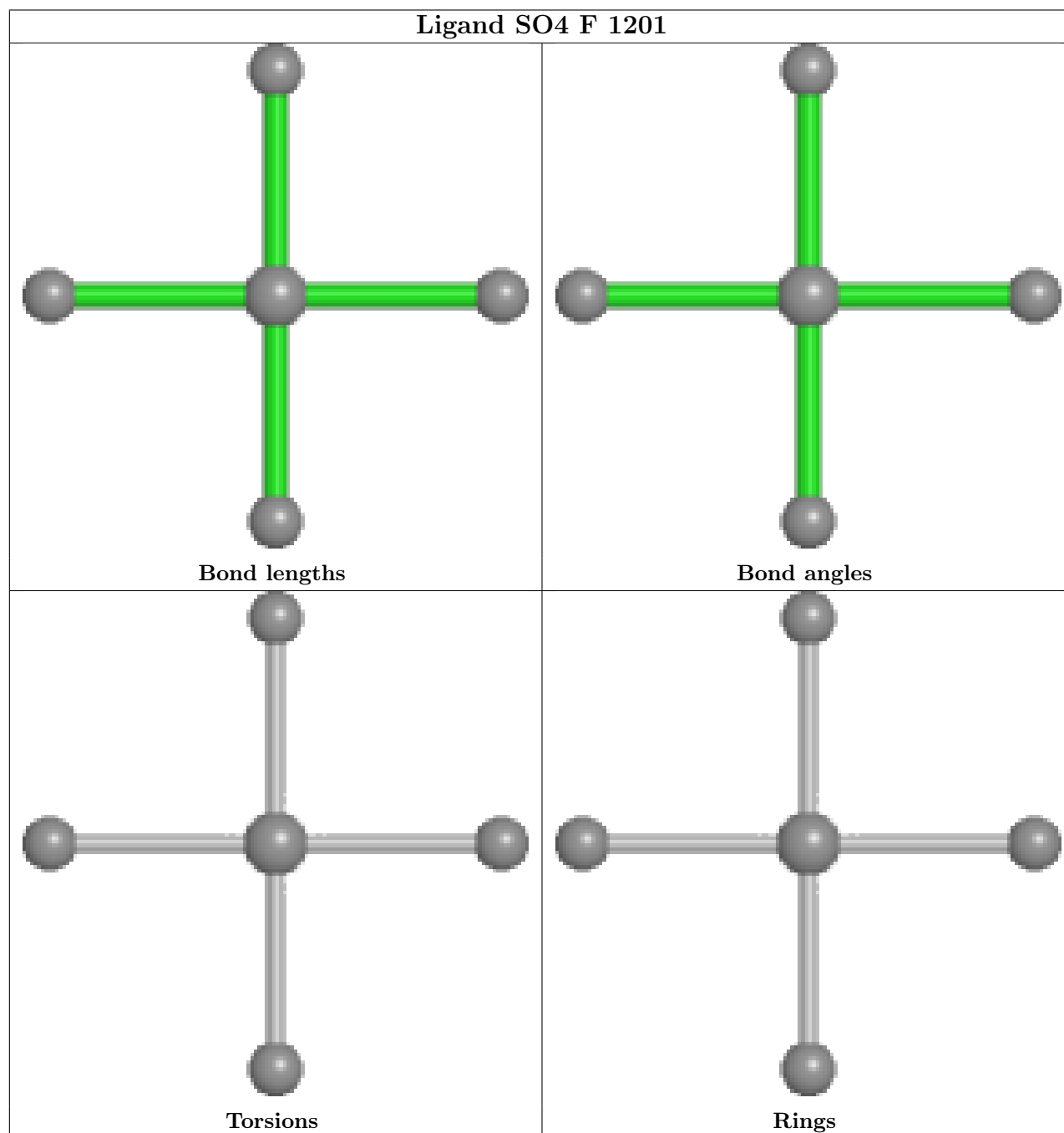
There are no ring outliers.

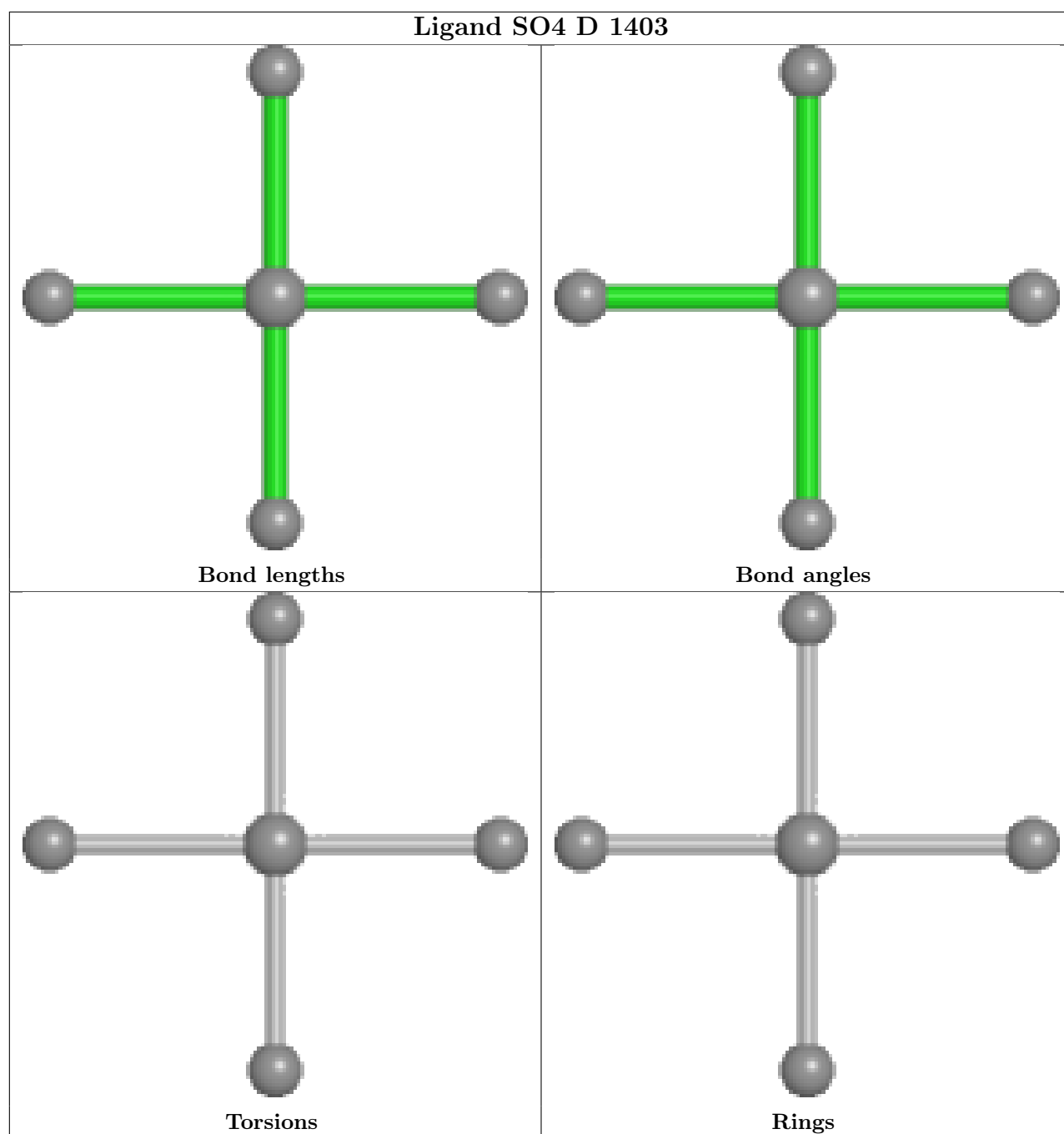
10 monomers are involved in 19 short contacts:

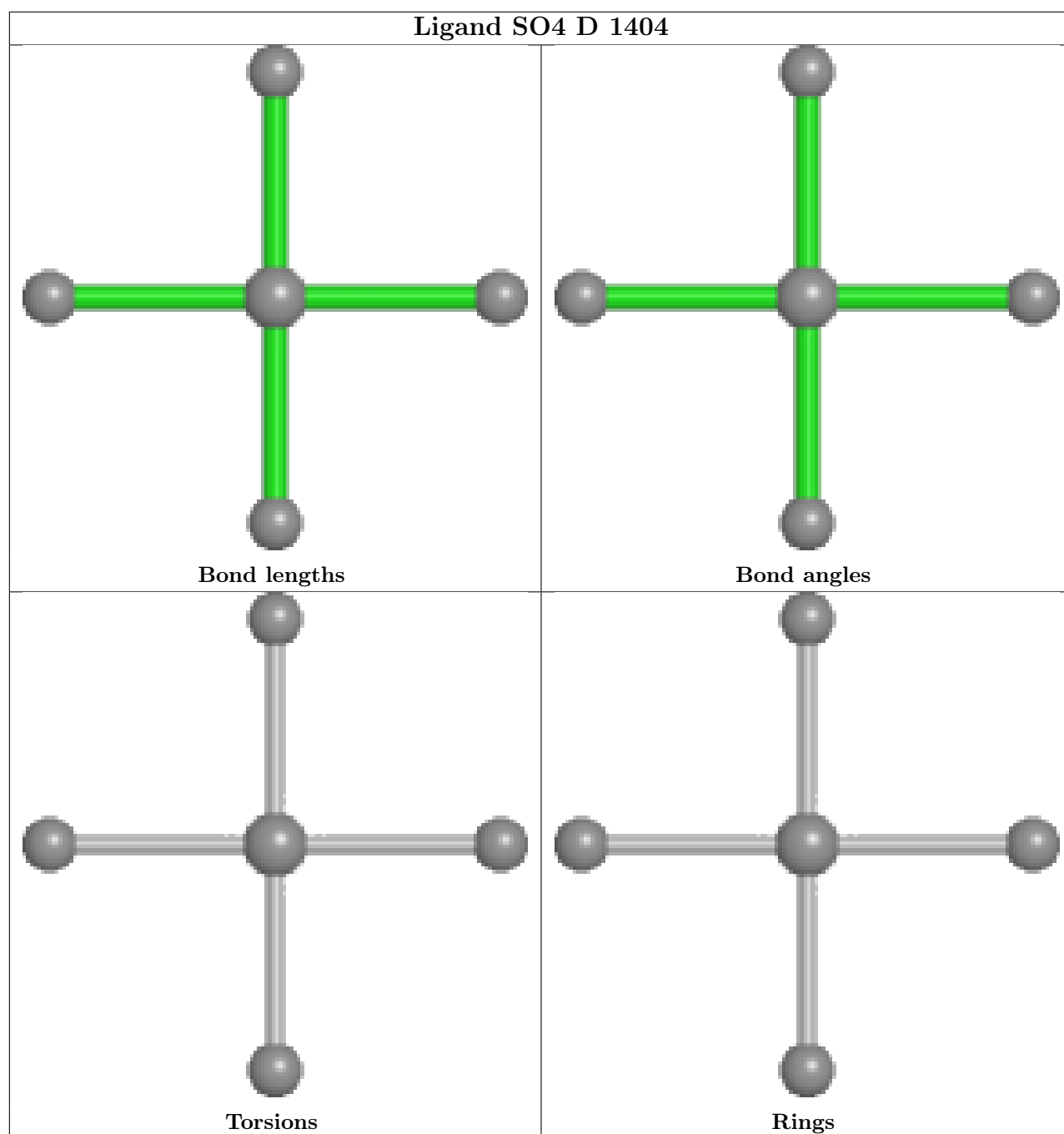
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1201	SO4	3	1
9	D	1403	SO4	2	0
9	D	1404	SO4	1	0
9	D	1406	SO4	2	0
9	F	1204	SO4	4	0
9	D	1405	SO4	2	0
9	F	1203	SO4	1	0
9	F	1202	SO4	1	0
9	D	1407	SO4	1	0
9	D	1408	SO4	1	0

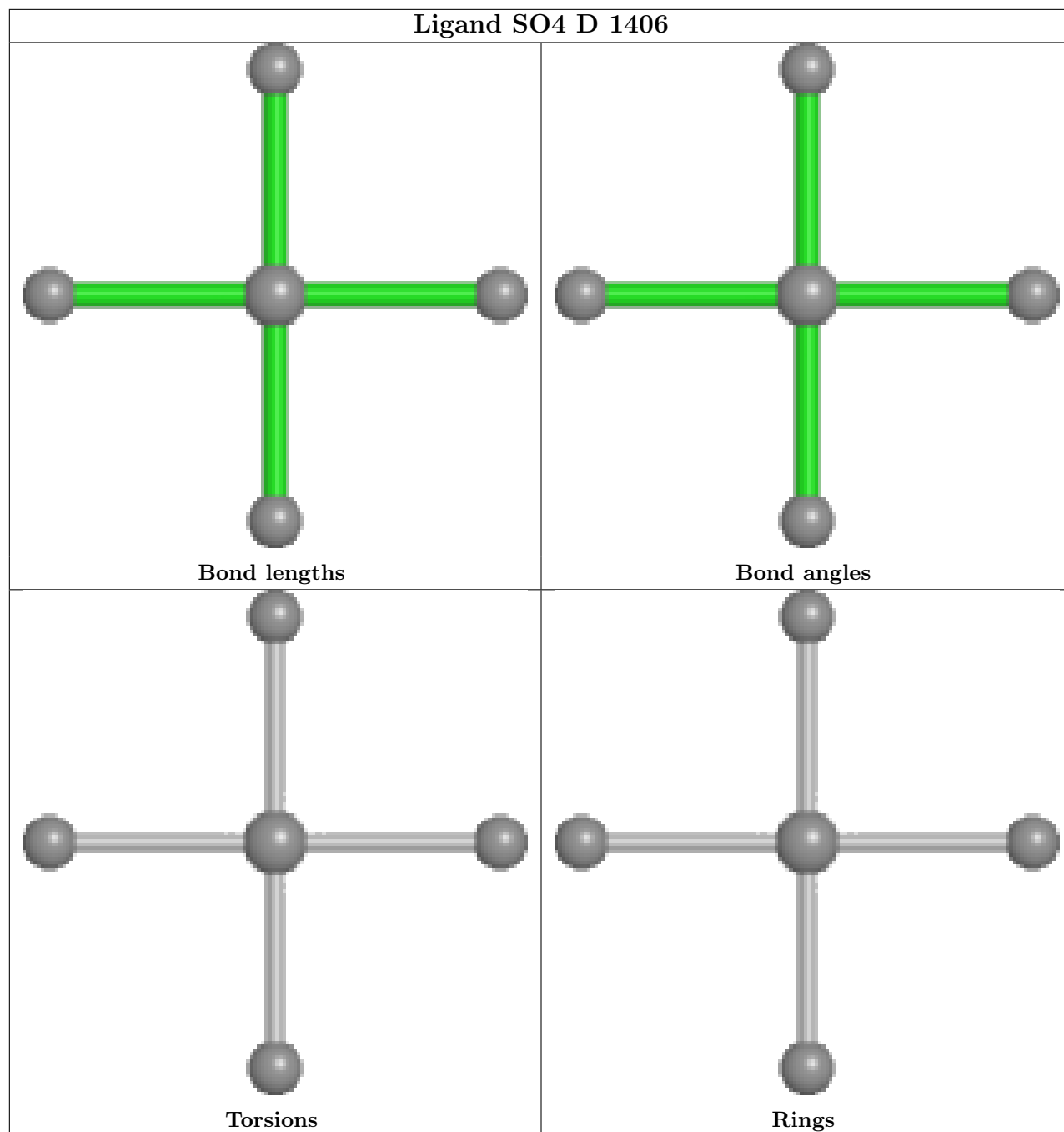
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

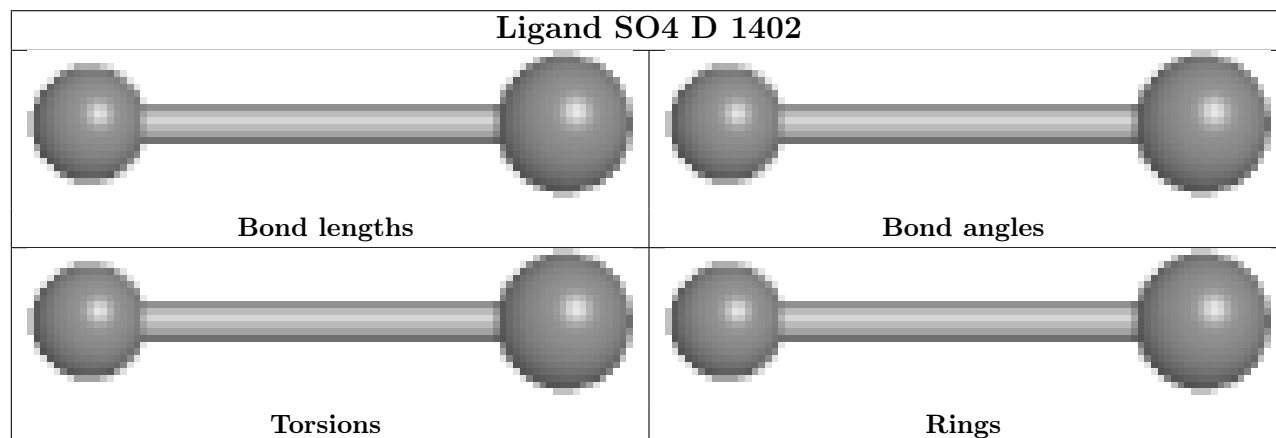
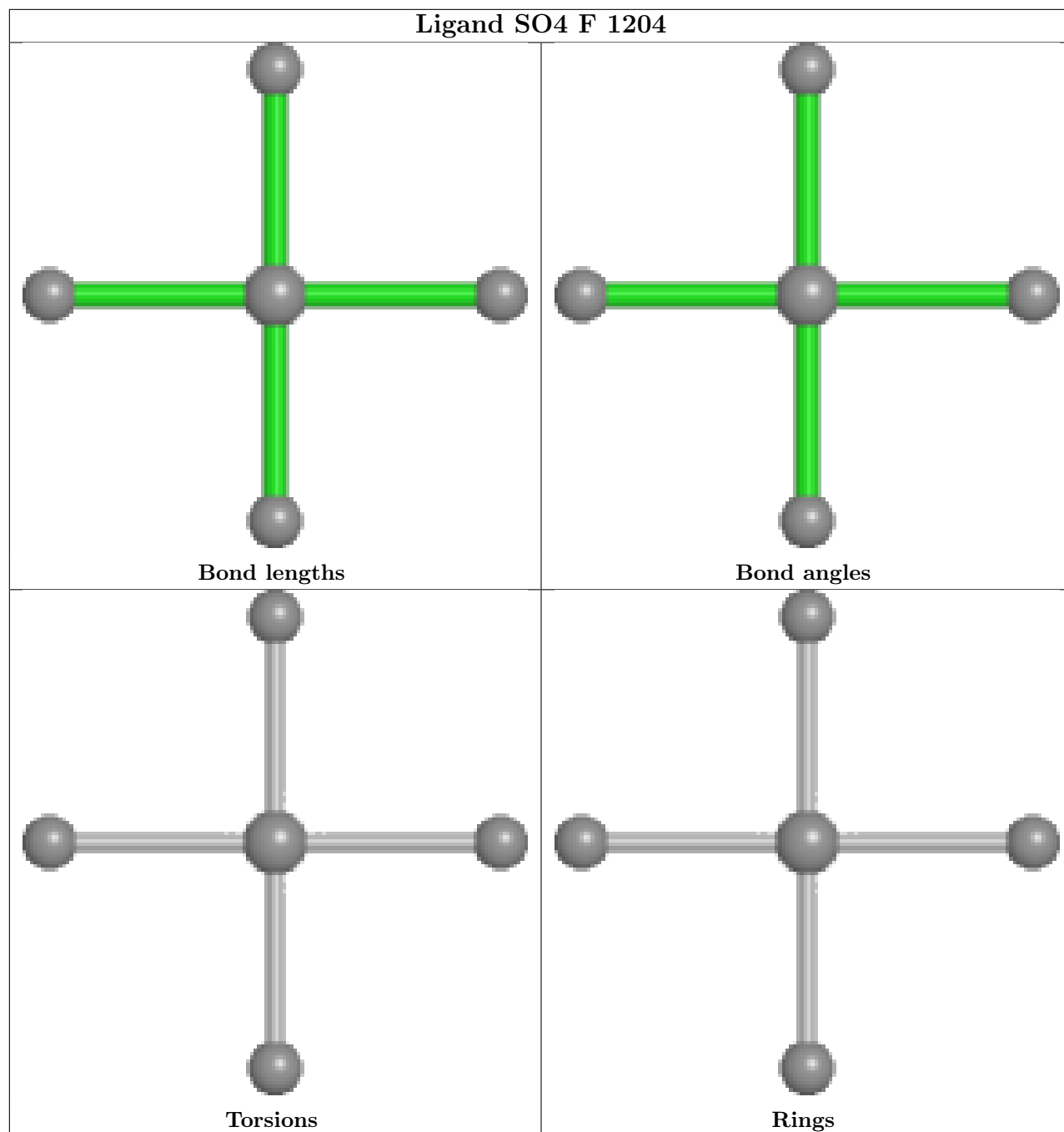
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

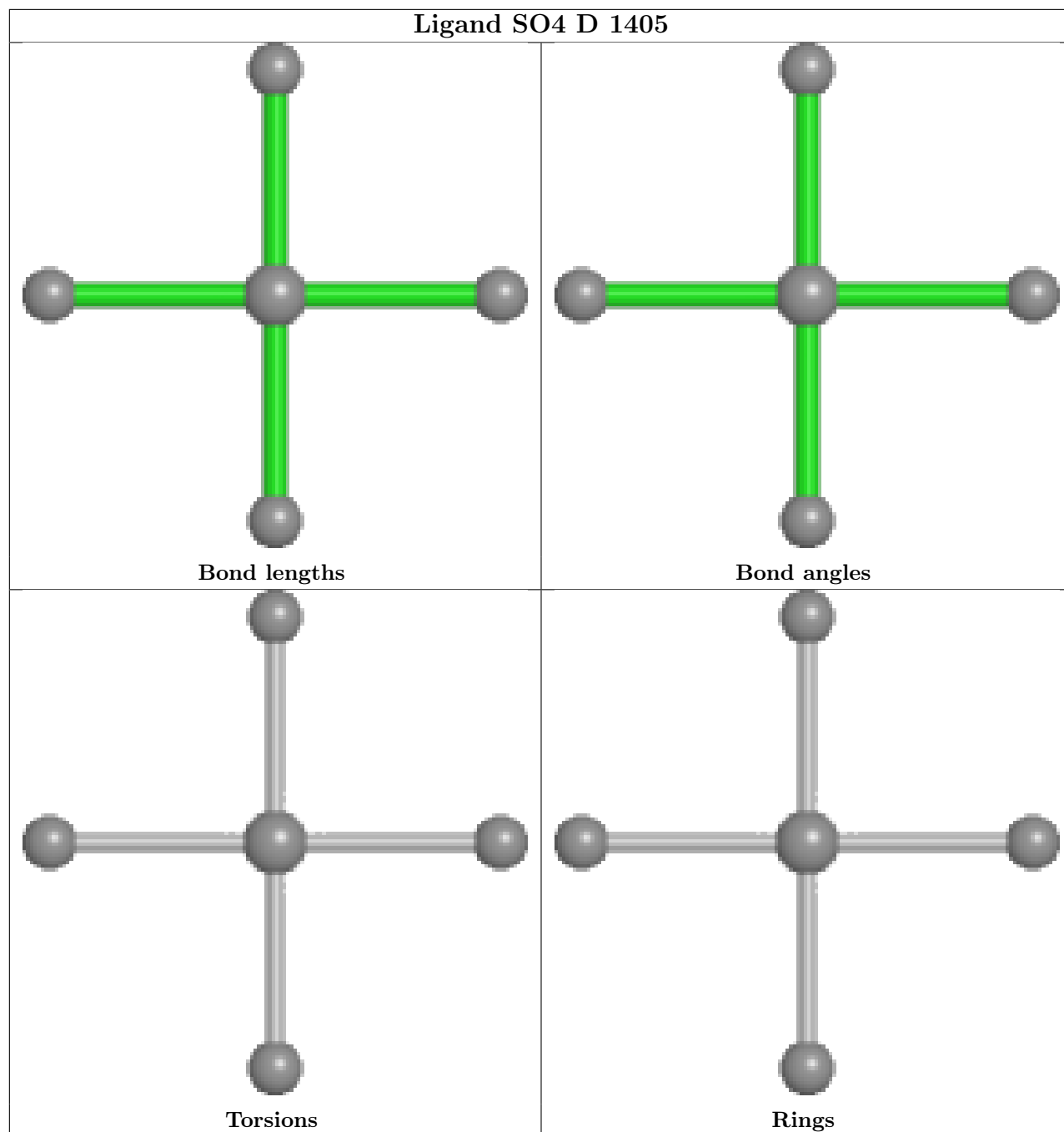


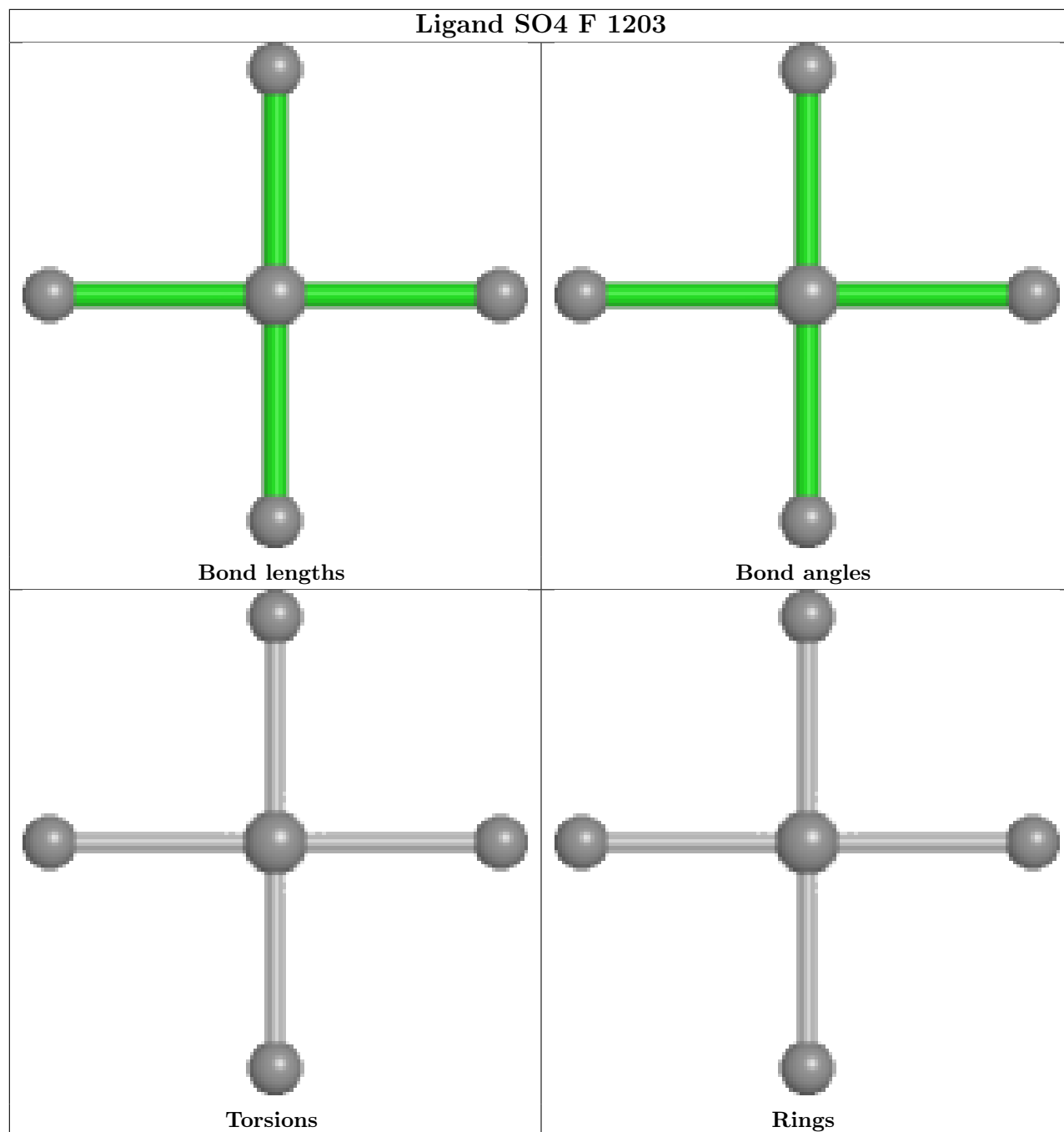


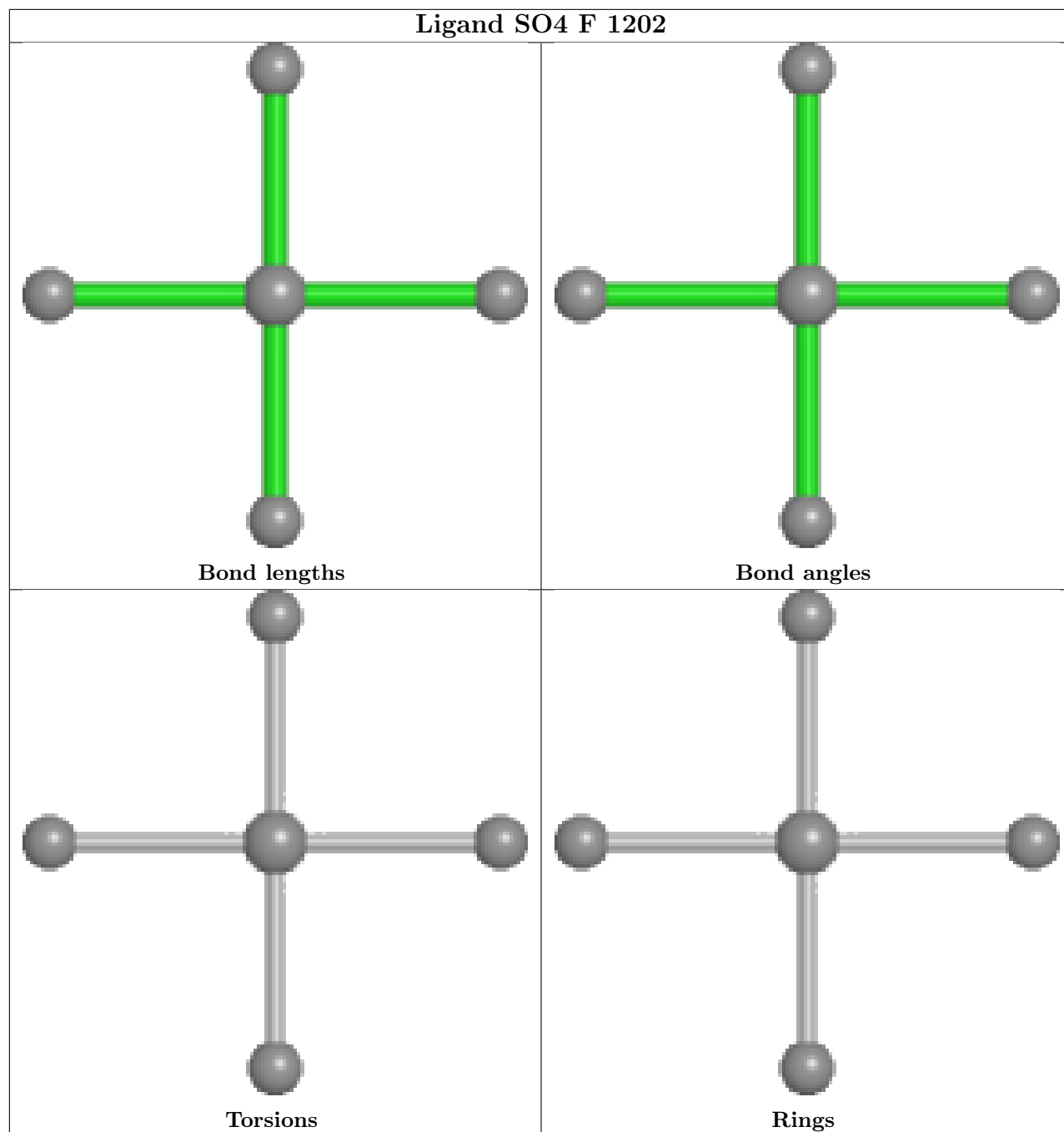


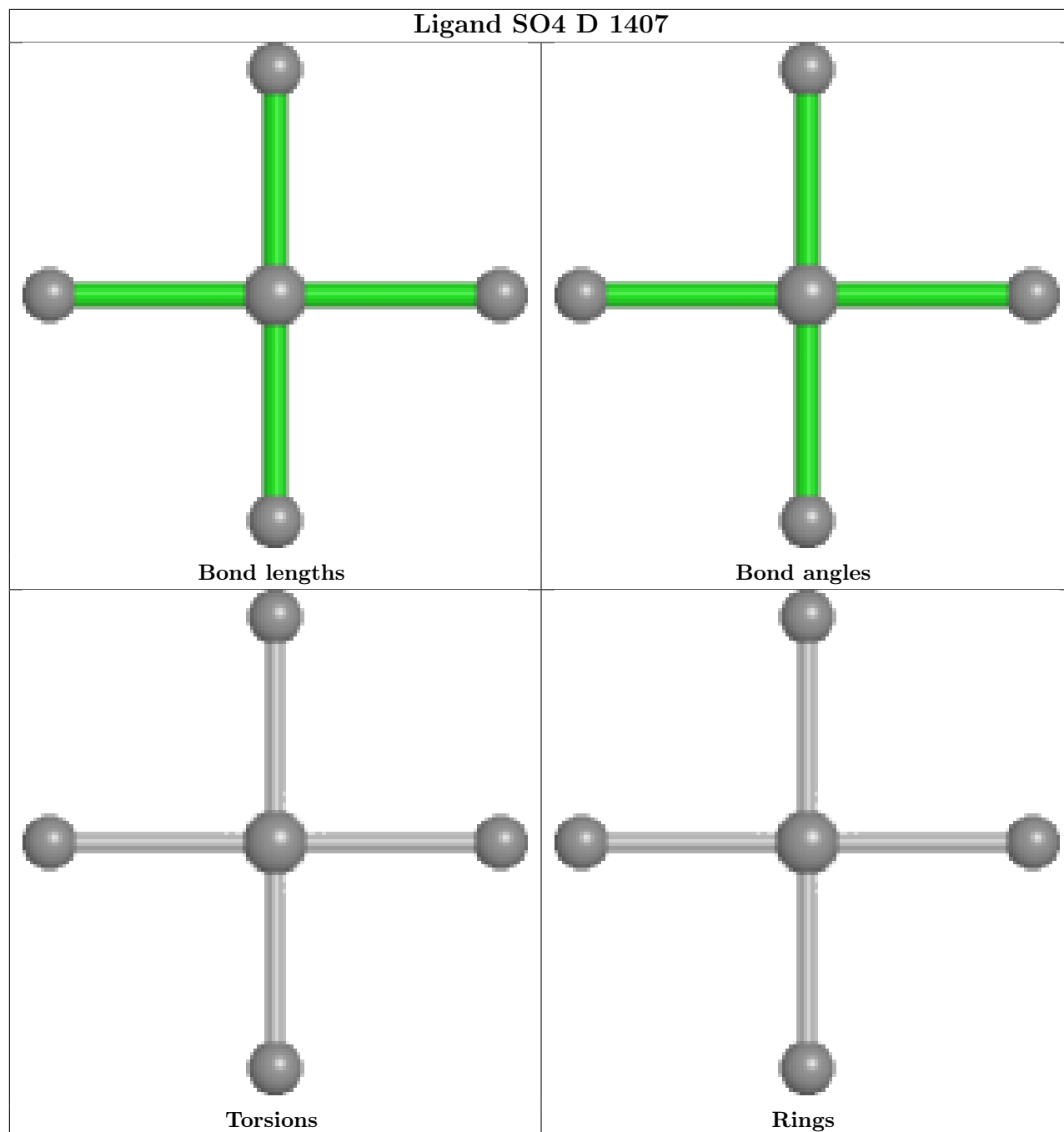


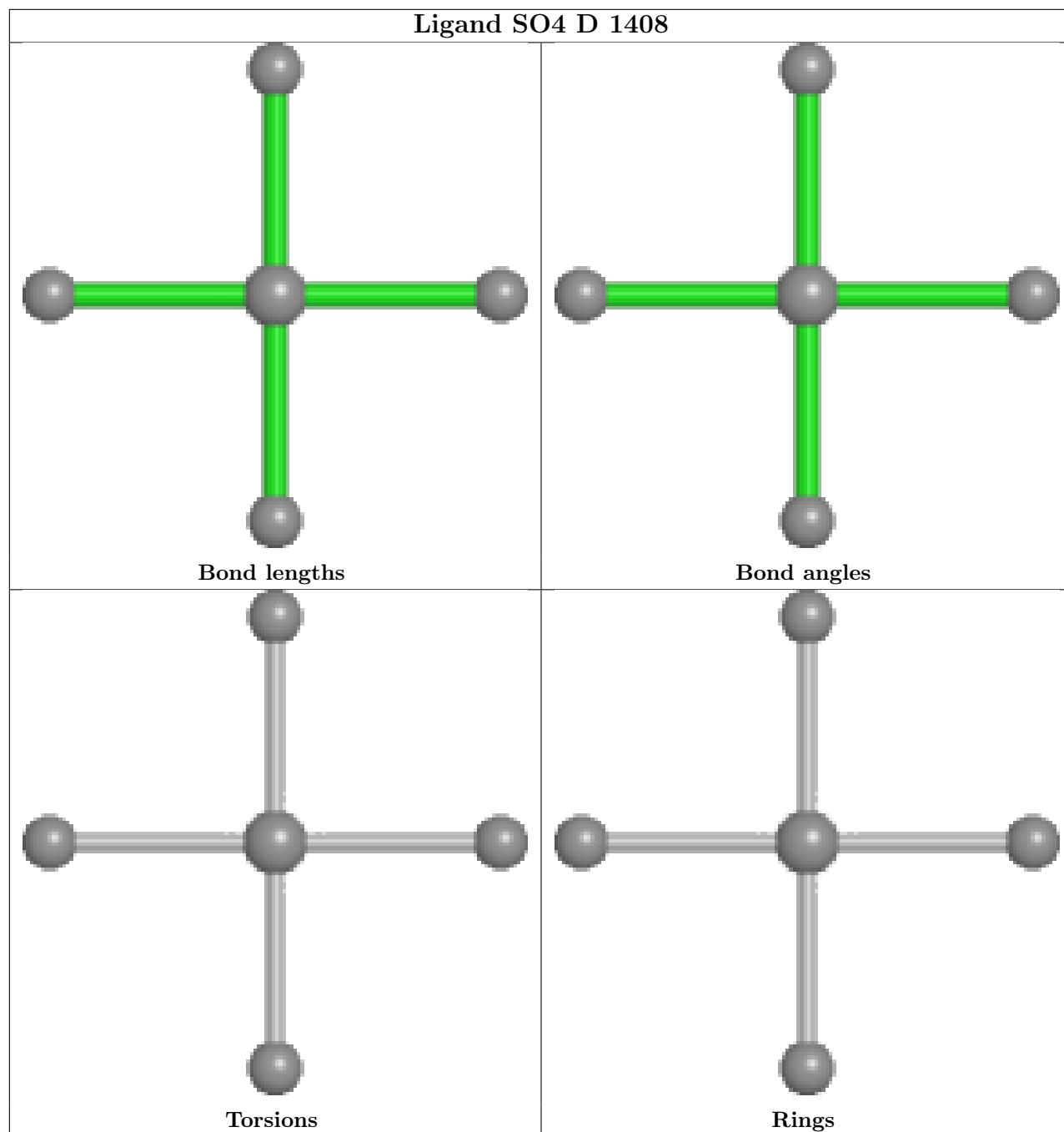


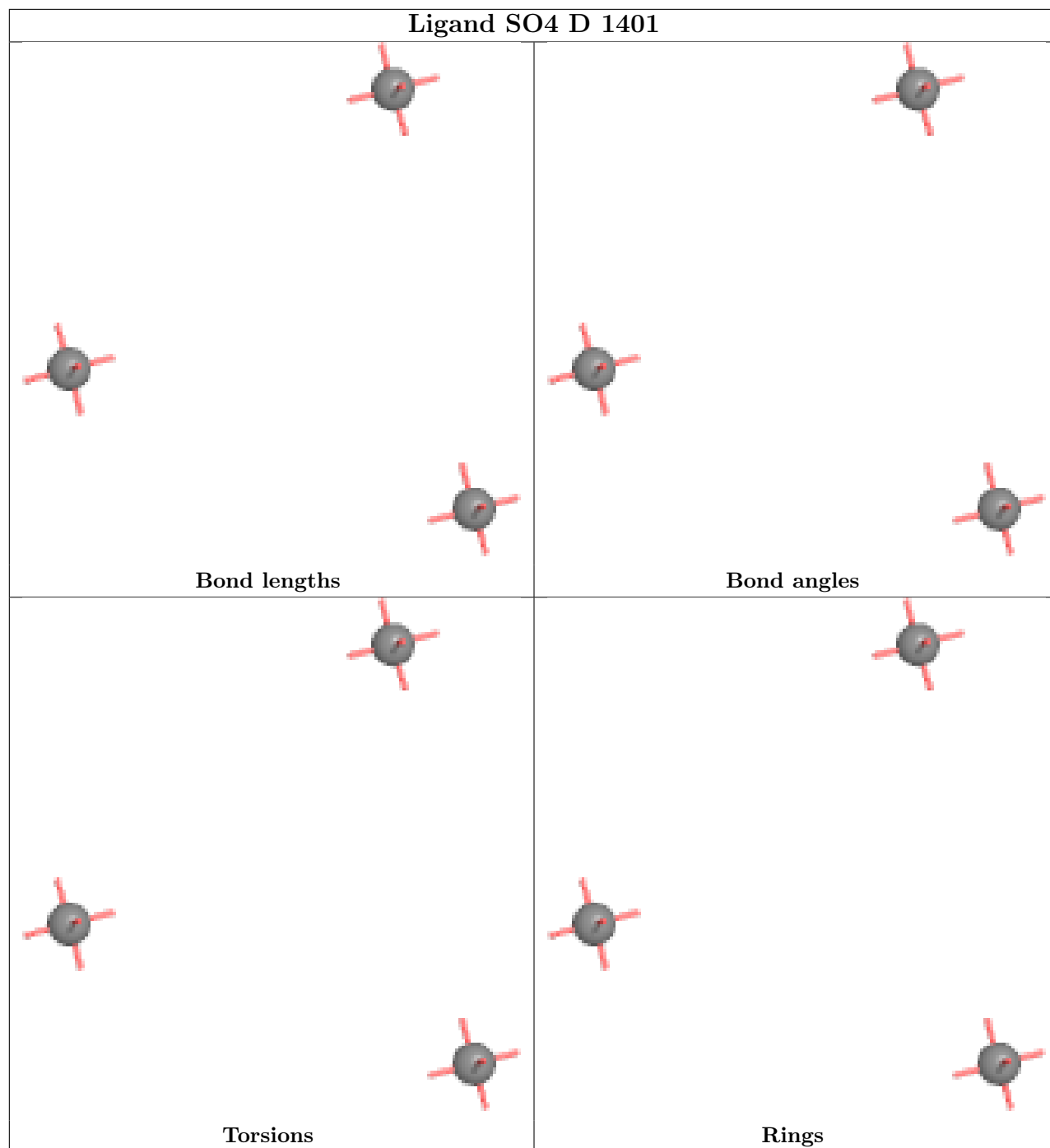












5.7 Other polymers [i](#)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	J	88/114 (77%)	-0.17	1 (1%) 80 69	76, 128, 174, 187	0
2	A	223/350 (63%)	-0.04	1 (0%) 92 89	82, 115, 150, 177	0
2	B	235/350 (67%)	0.18	15 (6%) 19 11	86, 136, 167, 206	0
2	T	53/350 (15%)	3.61	41 (77%) 0 0	170, 212, 225, 234	0
3	C	790/1169 (67%)	0.19	27 (3%) 45 29	63, 116, 174, 201	0
4	D	1174/1317 (89%)	0.22	59 (5%) 28 16	53, 107, 180, 215	0
5	E	77/107 (71%)	0.42	6 (7%) 13 7	80, 112, 164, 184	0
6	F	302/466 (64%)	0.01	3 (0%) 82 72	64, 104, 146, 189	0
7	O	31/31 (100%)	-0.79	0 100 100	81, 107, 150, 162	0
8	P	26/26 (100%)	-0.74	0 100 100	95, 107, 150, 162	0
All	All	2999/4280 (70%)	0.20	153 (5%) 28 16	53, 115, 179, 234	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	289	PHE	8.6
5	E	106	GLY	7.5
4	D	766	HIS	7.1
2	T	283	LEU	7.0
4	D	739	PRO	6.5
2	T	253	ASP	6.4
2	T	263	CYS	6.2
4	D	754	ALA	6.1
2	T	262	ASN	5.8
2	T	261	TYR	5.5
2	T	268	GLY	5.4
2	T	275	LEU	5.3
2	T	255	ASP	5.2

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Mol	Chain	Res	Type	RSRZ
2	T	294	ILE	5.2
2	T	285	ASP	5.2
2	T	297	VAL	5.2
2	T	264	LEU	5.2
2	T	256	LEU	5.2
2	T	254	LEU	5.2
3	C	1132	ASP	4.8
2	T	267	GLU	4.8
5	E	105	GLU	4.8
2	T	274	GLU	4.7
2	T	266	ARG	4.5
2	T	286	ILE	4.2
4	D	1027	GLY	4.2
4	D	782	GLU	4.2
2	T	260	SER	4.2
2	T	301	LEU	4.1
2	T	293	SER	4.0
4	D	750	ALA	3.9
4	D	738	PRO	3.9
2	T	251	ILE	3.7
4	D	755	ILE	3.7
4	D	764	LEU	3.7
2	T	252	ASP	3.7
2	T	291	GLN	3.7
3	C	167	VAL	3.6
2	T	269	VAL	3.6
2	T	259	ARG	3.6
2	T	288	ASN	3.6
4	D	751	GLU	3.5
5	E	29	PRO	3.5
4	D	768	GLU	3.5
4	D	773	LEU	3.4
2	T	281	SER	3.4
2	T	296	GLU	3.4
4	D	758	LYS	3.4
4	D	742	GLN	3.4
2	T	273	GLY	3.4
4	D	765	ASN	3.4
3	C	80	VAL	3.3
3	C	497	VAL	3.3
4	D	753	ASP	3.3
2	T	277	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	138	LEU	3.3
2	T	284	LEU	3.3
3	C	525	ASP	3.2
4	D	685	GLU	3.2
4	D	767	THR	3.2
4	D	925	ALA	3.2
3	C	169	GLN	3.2
4	D	748	HIS	3.2
4	D	784	VAL	3.2
3	C	1133	GLY	3.1
2	T	282	ASP	3.1
3	C	369	LEU	3.1
3	C	86	PRO	3.1
4	D	740	GLN	3.1
4	D	866	THR	3.0
4	D	760	GLN	3.0
3	C	399	ASP	3.0
5	E	104	THR	3.0
2	T	270	HIS	3.0
4	D	412	ARG	2.9
4	D	780	ALA	2.9
4	D	409	LYS	2.9
2	B	107	ALA	2.9
4	D	1282	ALA	2.9
4	D	410	GLN	2.9
4	D	747	ARG	2.9
2	T	280	GLU	2.8
6	F	351	ILE	2.8
3	C	529	ARG	2.8
4	D	772	SER	2.8
2	B	2	LEU	2.8
2	B	140	VAL	2.8
4	D	749	GLU	2.7
5	E	53	TYR	2.7
4	D	769	ARG	2.7
4	D	1063	PHE	2.7
3	C	503	ILE	2.6
2	B	202	ILE	2.6
6	F	461	LEU	2.6
4	D	234	LEU	2.6
3	C	854	ALA	2.6
3	C	765	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	1182	THR	2.5
3	C	500	PHE	2.5
2	B	104	VAL	2.5
2	B	127	THR	2.5
4	D	283	SER	2.5
4	D	774	VAL	2.5
3	C	812	LEU	2.5
3	C	523	THR	2.5
4	D	743	GLU	2.5
3	C	106	VAL	2.4
3	C	528	ASP	2.4
3	C	530	HIS	2.4
2	B	118	VAL	2.4
2	B	71	GLU	2.4
4	D	752	ALA	2.4
2	T	299	ILE	2.4
6	F	173	ILE	2.4
4	D	781	THR	2.4
2	B	139	VAL	2.3
2	B	195	ASP	2.3
2	T	276	VAL	2.3
1	J	69	VAL	2.3
2	T	298	LYS	2.3
2	B	70	LYS	2.3
4	D	900	LEU	2.3
4	D	1113	MET	2.2
4	D	1060	ASP	2.2
3	C	447	LEU	2.2
3	C	383	GLY	2.2
5	E	28	THR	2.2
4	D	1082	SER	2.2
3	C	427	LEU	2.2
4	D	460	LEU	2.2
2	T	295	ASP	2.2
2	T	302	HIS	2.2
4	D	776	ILE	2.2
2	A	85	VAL	2.2
3	C	823	VAL	2.2
2	B	196	VAL	2.1
4	D	771	GLU	2.1
4	D	312	MET	2.1
4	D	136	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	270	ILE	2.1
2	B	204	PRO	2.1
2	B	102	PRO	2.1
4	D	763	ALA	2.1
4	D	1128	PRO	2.1
3	C	124	LEU	2.1
3	C	173	SER	2.1
4	D	264	LEU	2.0
4	D	3	ASP	2.0
4	D	124	ASP	2.0
4	D	1028	GLY	2.0
4	D	107	PHE	2.0
4	D	783	GLU	2.0
3	C	379	GLN	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(\AA^2)	Q<0.9
9	SO4	D	1408	5/5	0.54	0.31	197,200,219,408	0
9	SO4	D	1405	5/5	0.77	0.27	129,140,169,242	0
9	SO4	F	1204	5/5	0.79	0.65	181,184,229,383	0
9	SO4	F	1203	5/5	0.86	0.24	114,121,134,176	0
9	SO4	D	1406	5/5	0.86	0.23	145,154,158,235	0
9	SO4	D	1407	5/5	0.87	0.18	132,144,164,224	0
9	SO4	D	1404	5/5	0.89	0.30	134,138,153,204	0
9	SO4	D	1403	5/5	0.90	0.13	154,154,189,244	0
9	SO4	F	1201	5/5	0.91	0.20	94,96,132,149	0

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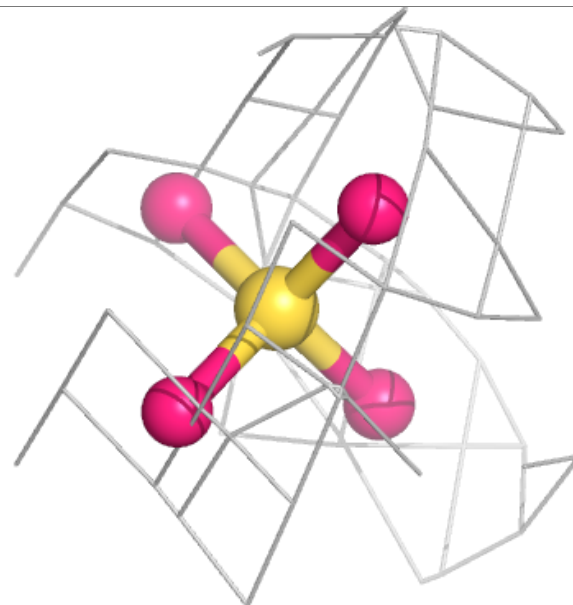
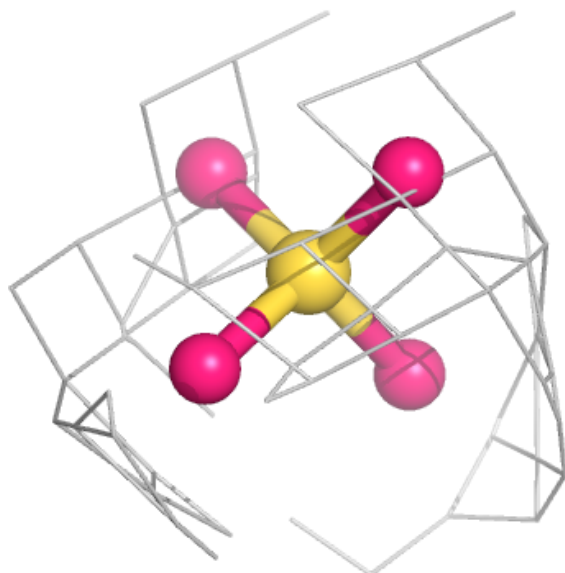
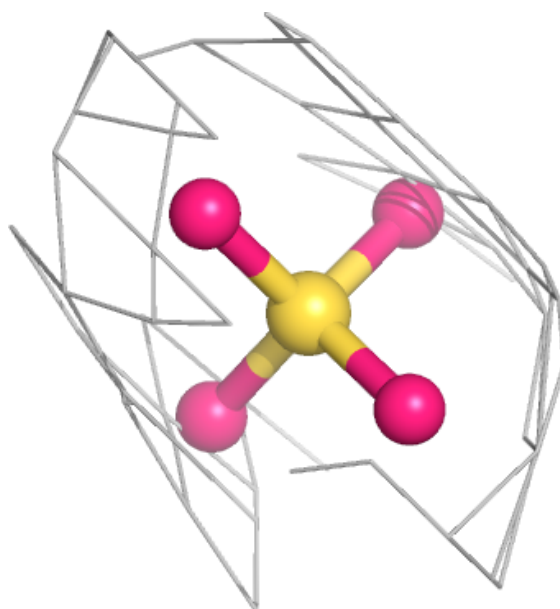
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	F	1202	5/5	0.91	0.12	113,115,129,138	0
9	SO4	D	1401	3/5	0.93	0.21	107,107,111,117	0
9	SO4	D	1402	2/5	0.96	0.15	131,131,131,153	0
10	ZN	D	1409	1/1	0.98	0.33	161,161,161,161	0
10	ZN	D	1410	1/1	0.99	0.23	149,149,149,149	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.

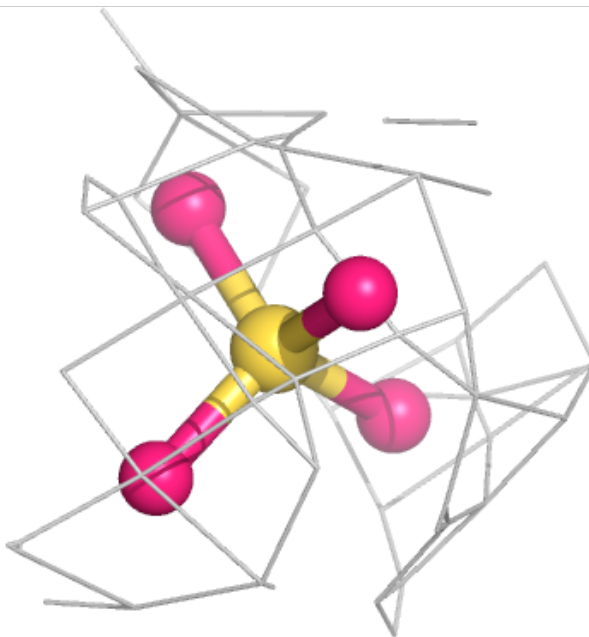
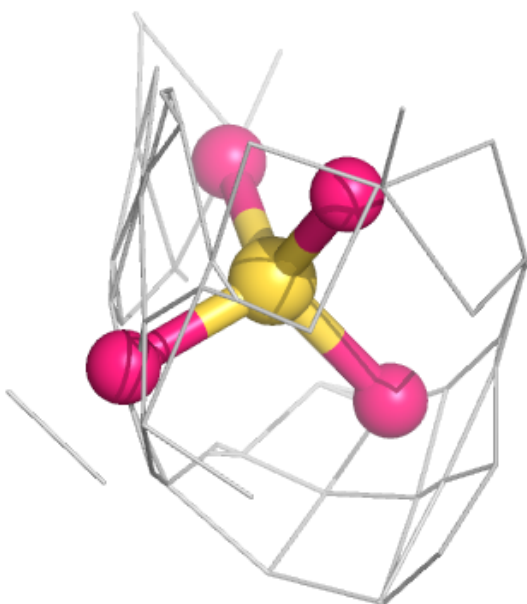
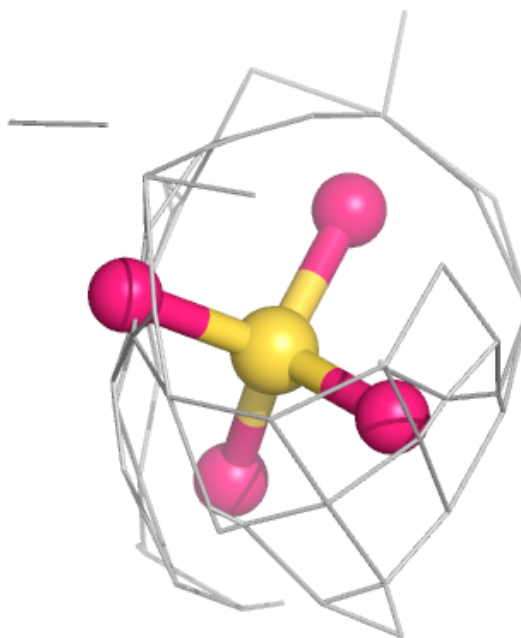
Electron density around SO4 D 1408:

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



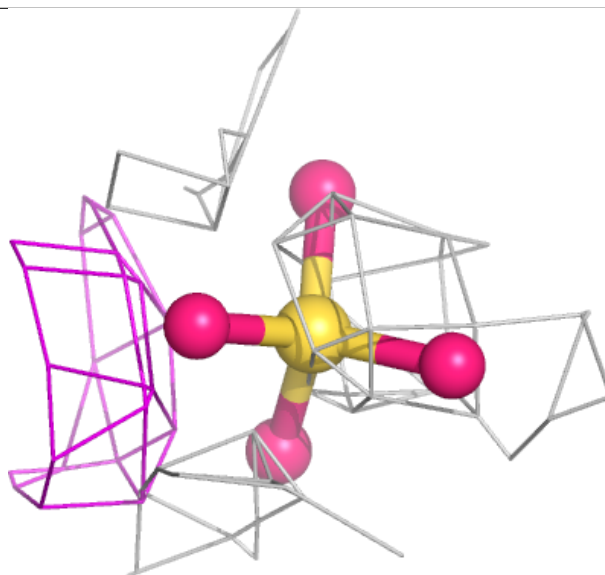
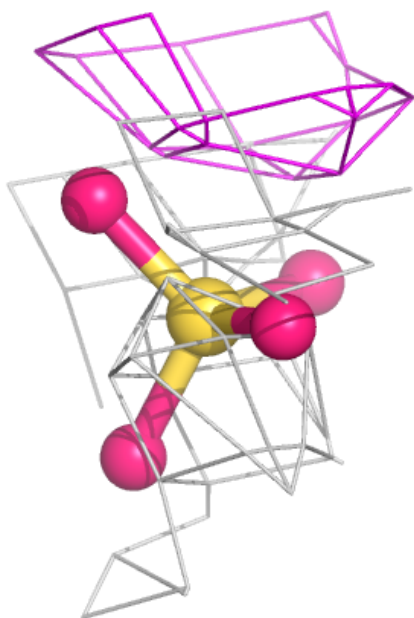
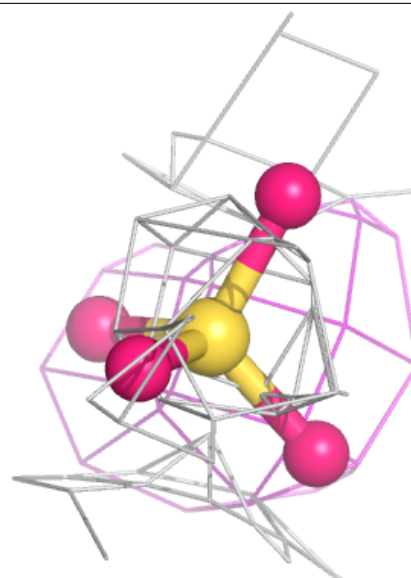
Electron density around SO4 D 1405:

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



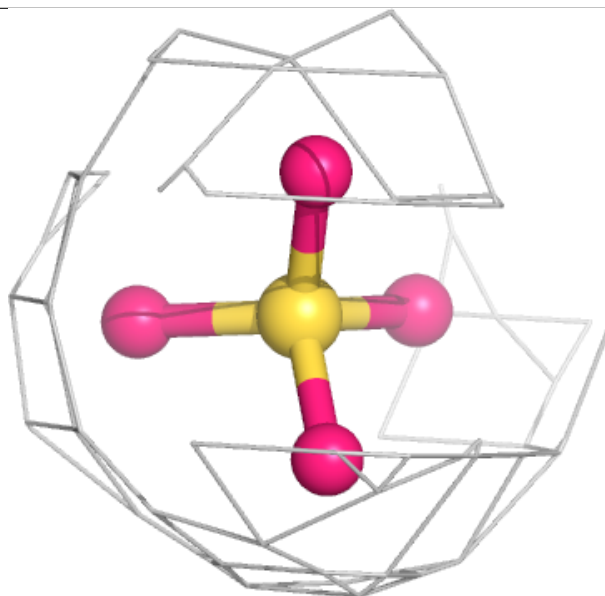
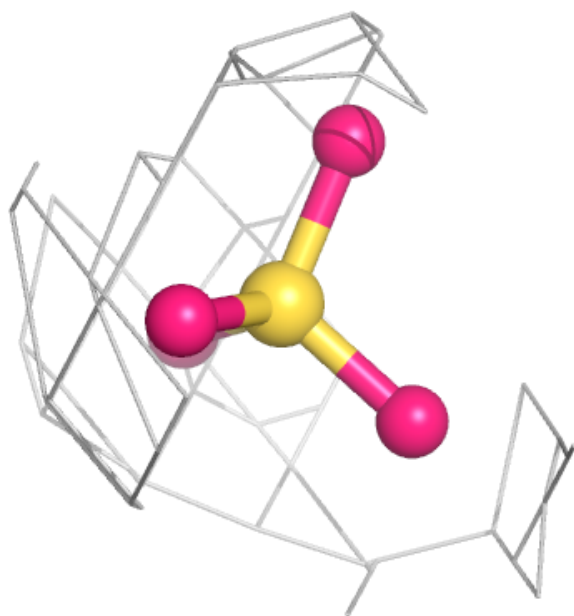
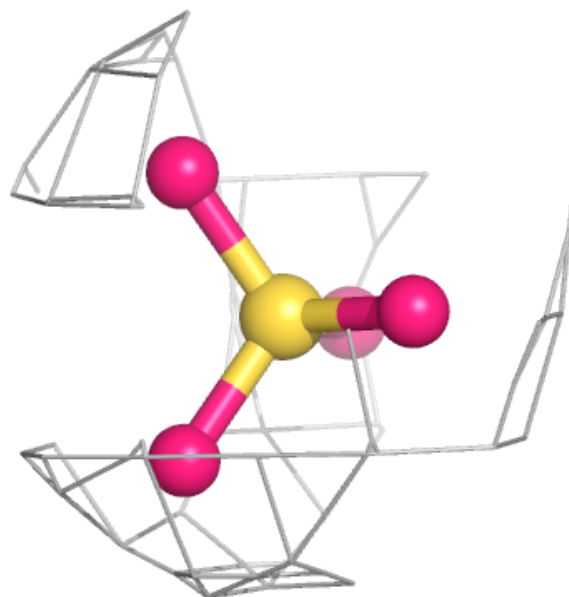
Electron density around SO4 F 1204:

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



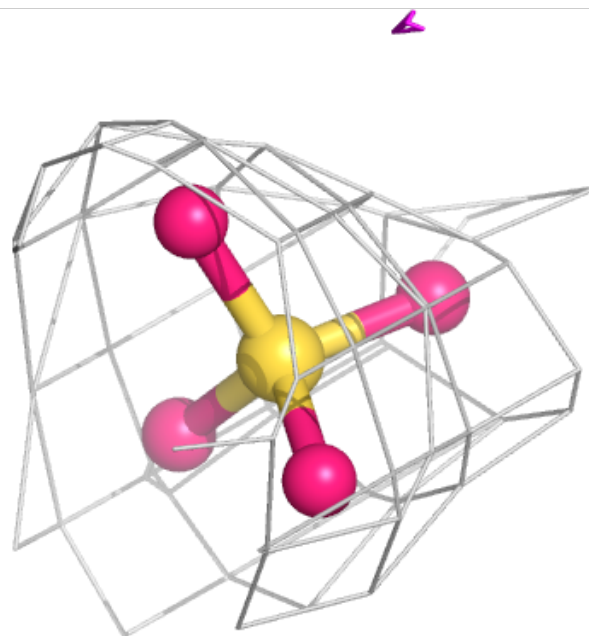
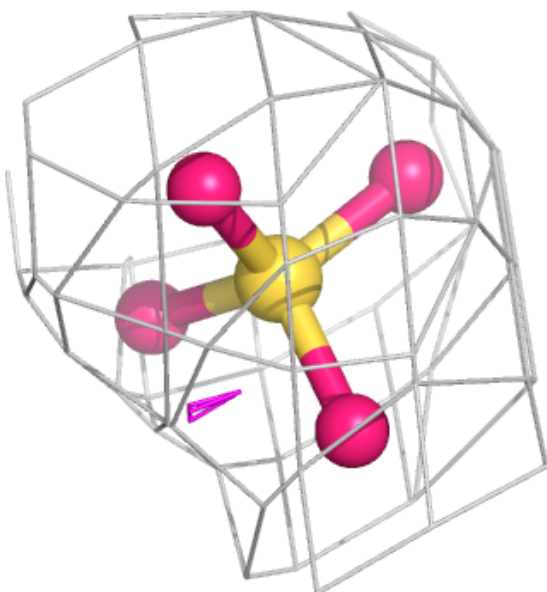
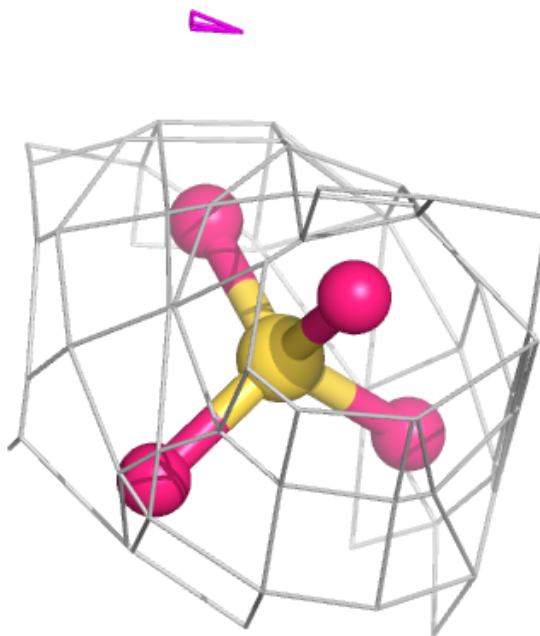
Electron density around SO4 F 1203:

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



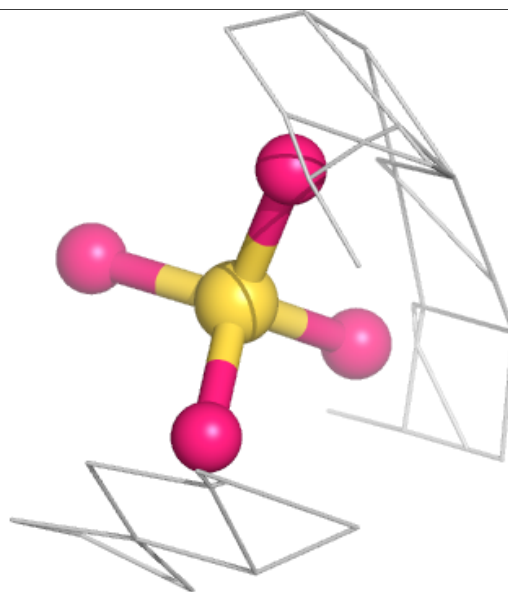
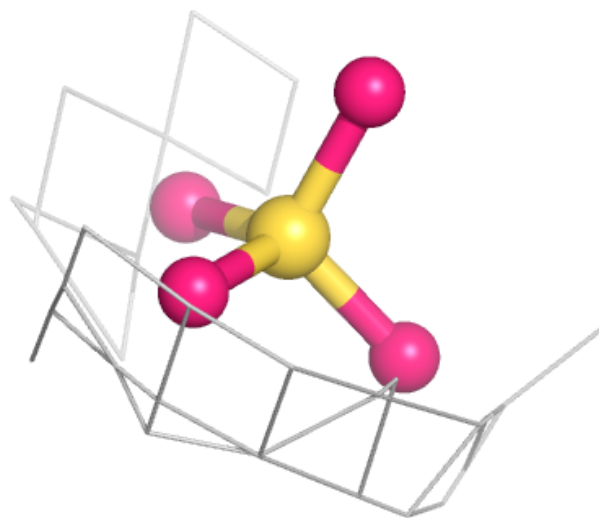
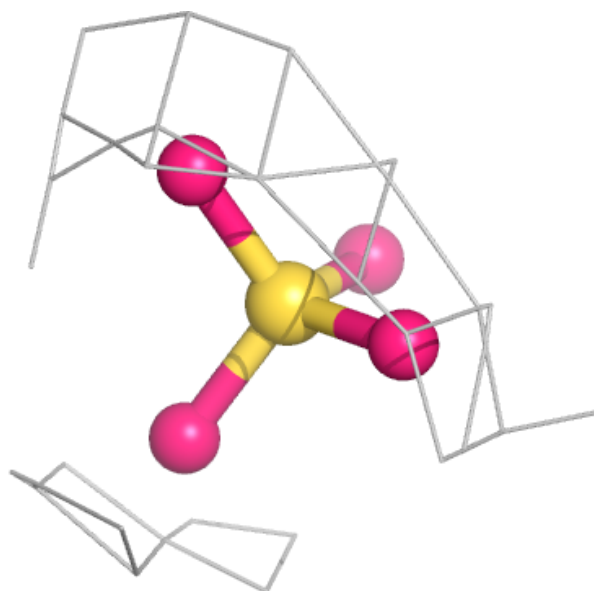
Electron density around SO4 D 1406:

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



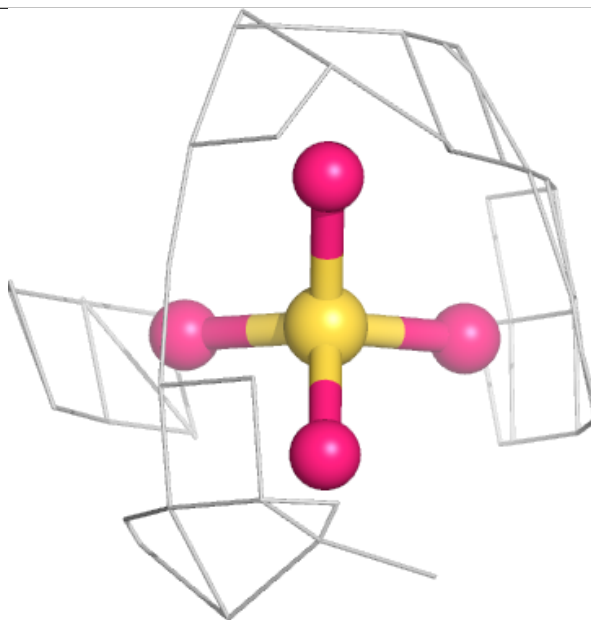
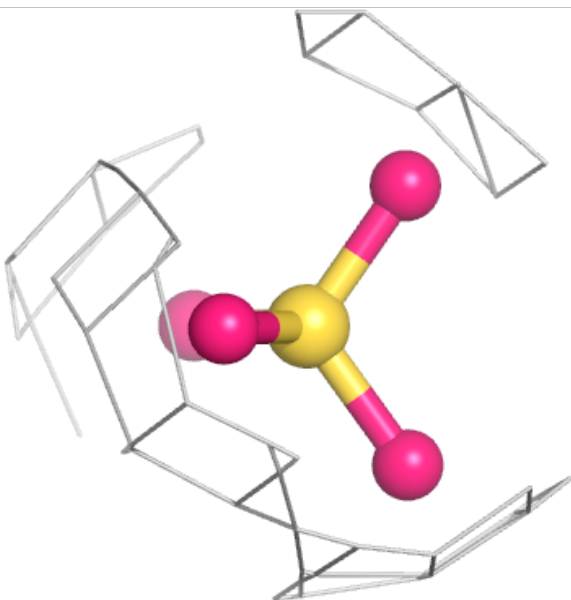
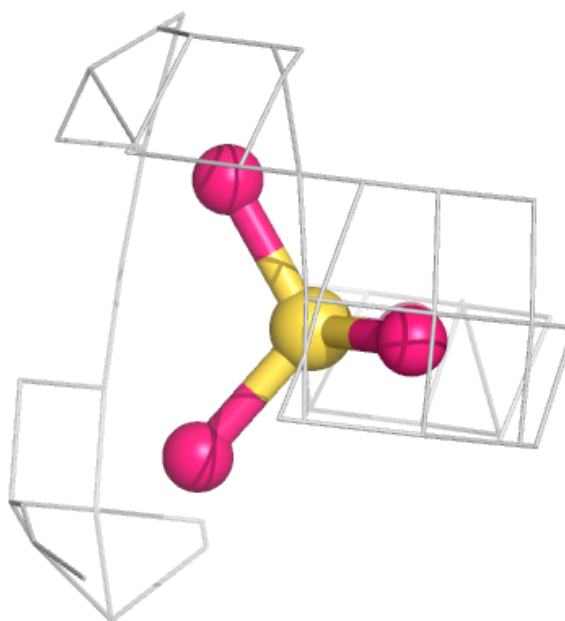
Electron density around SO4 D 1407:

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



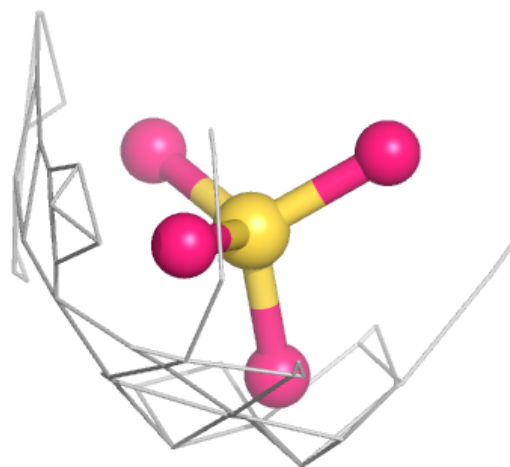
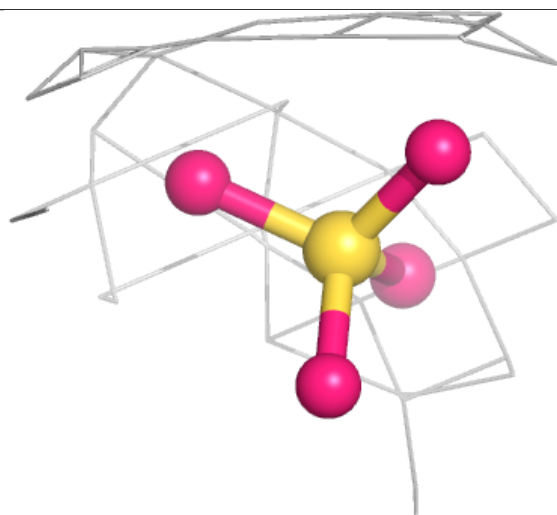
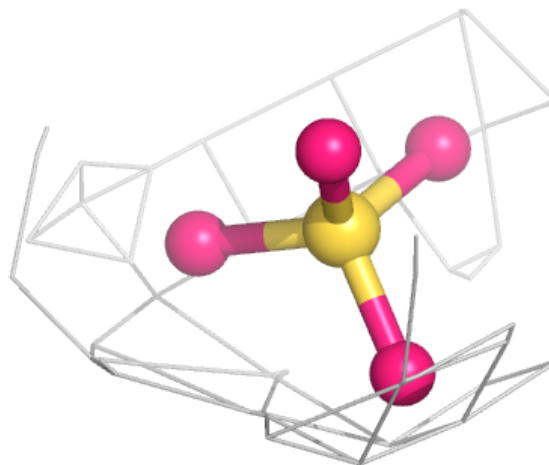
Electron density around SO4 D 1404:

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



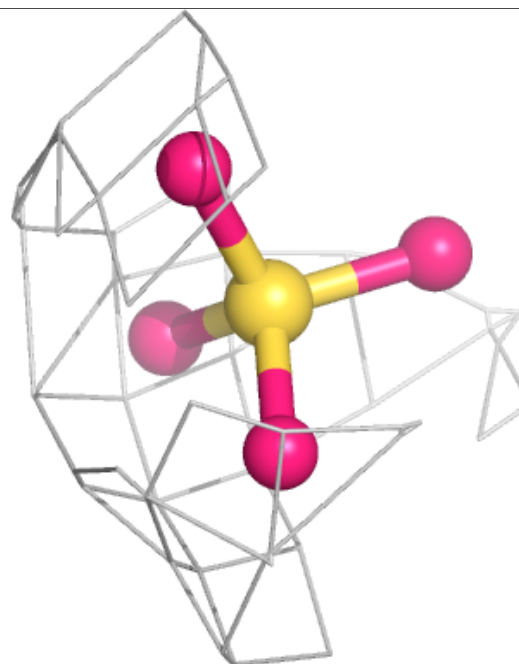
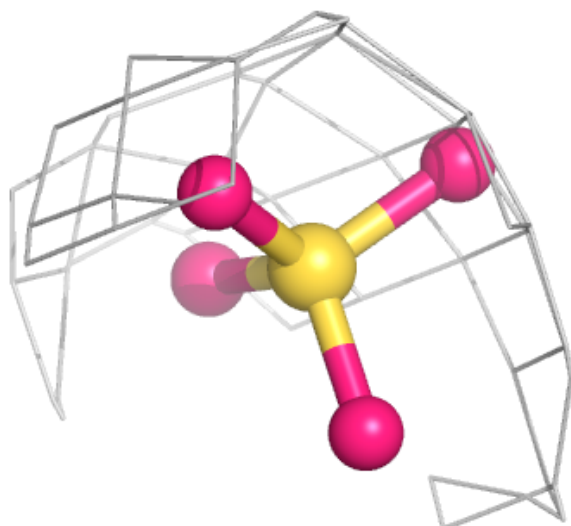
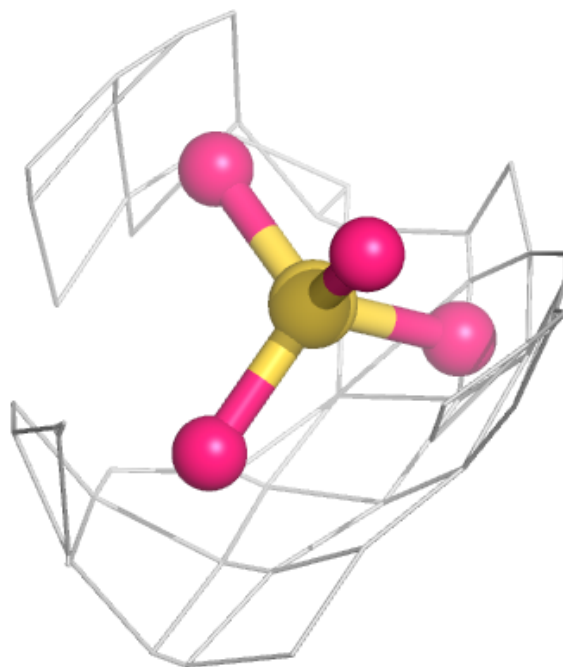
Electron density around SO4 D 1403:

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



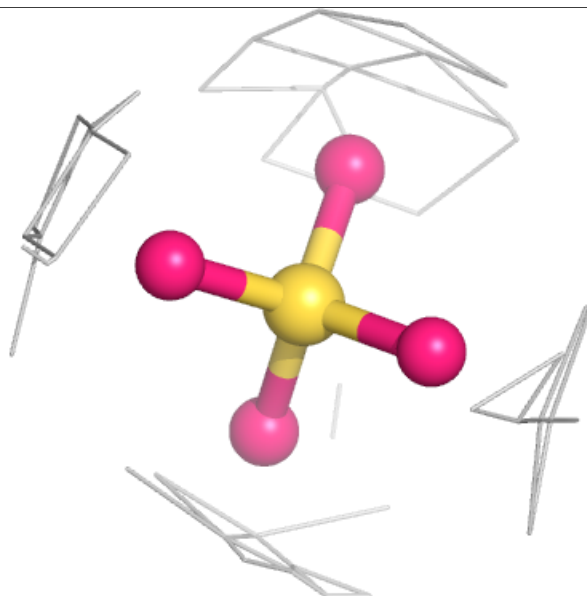
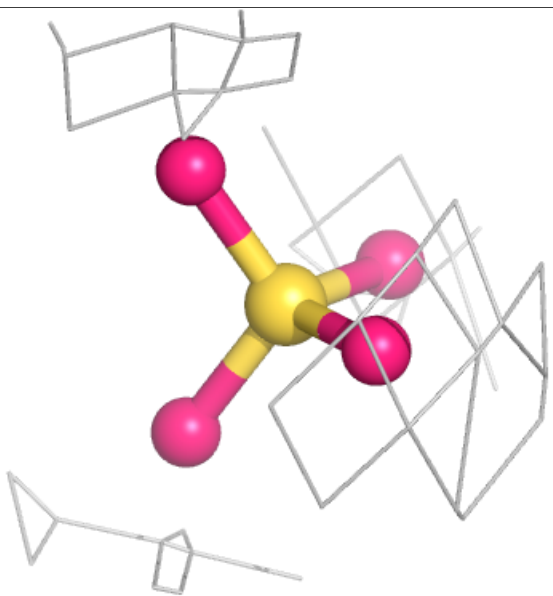
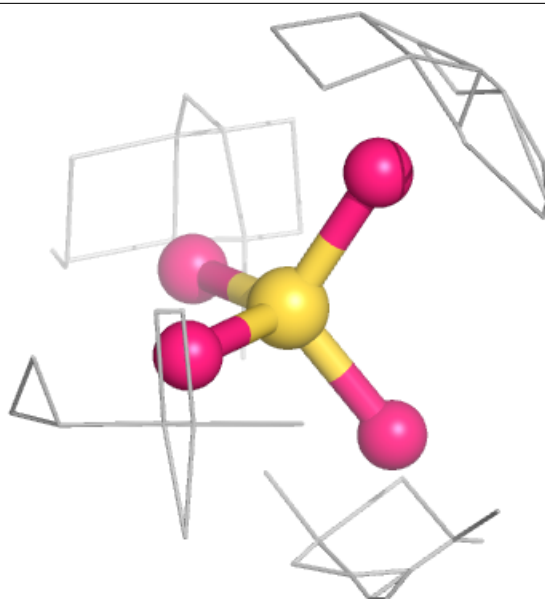
Electron density around SO4 F 1201:

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



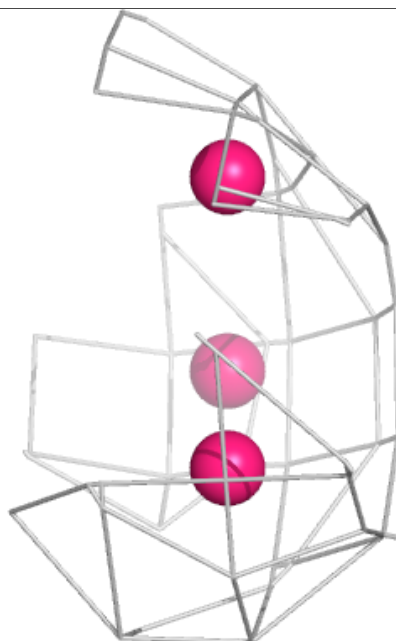
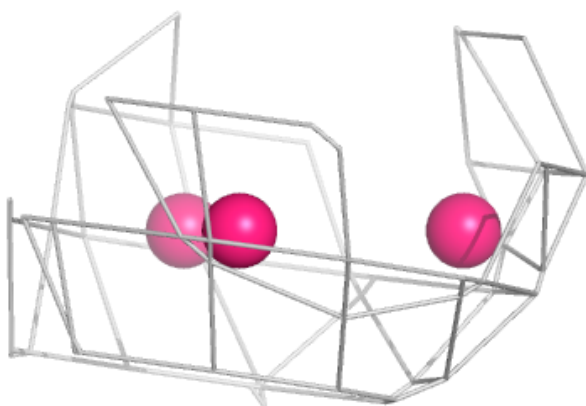
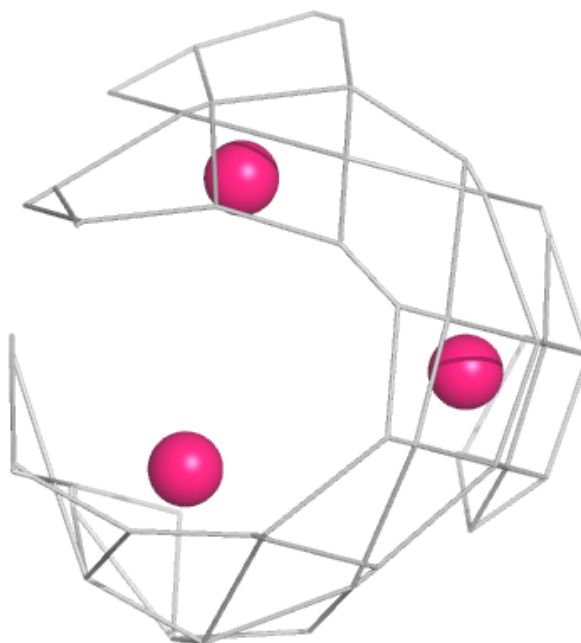
Electron density around SO4 F 1202:

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



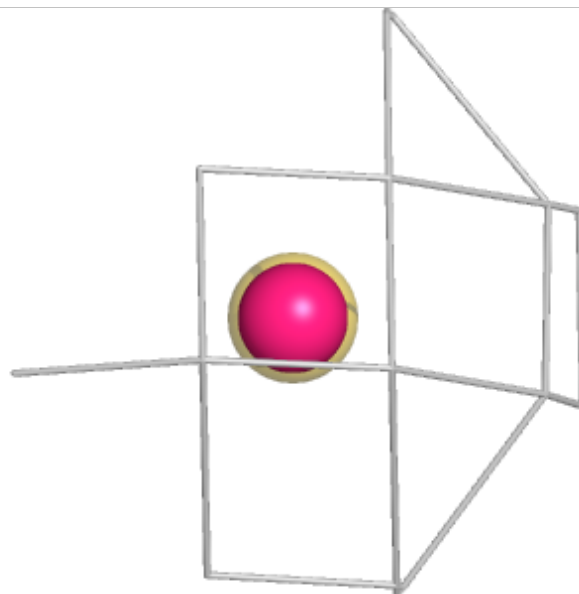
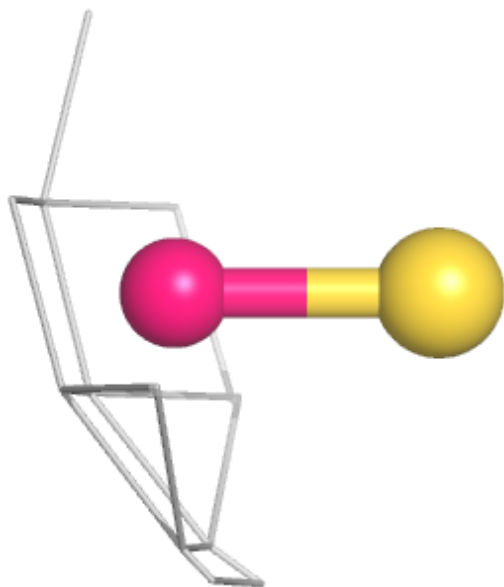
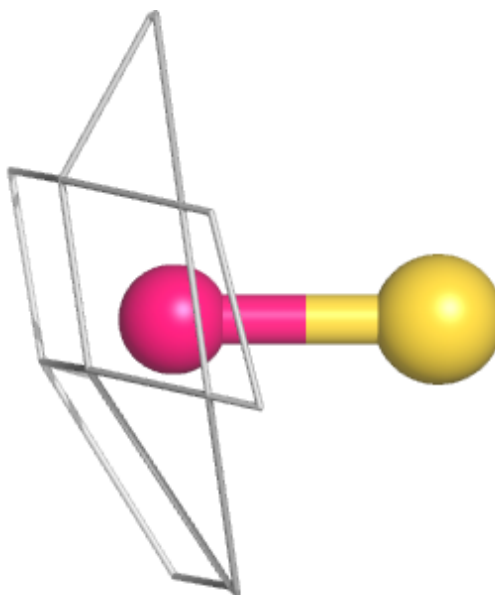
Electron density around SO4 D 1401:

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



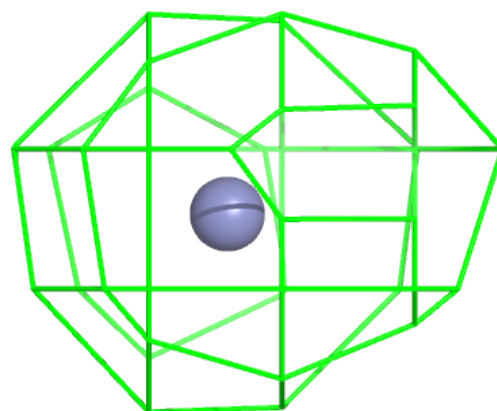
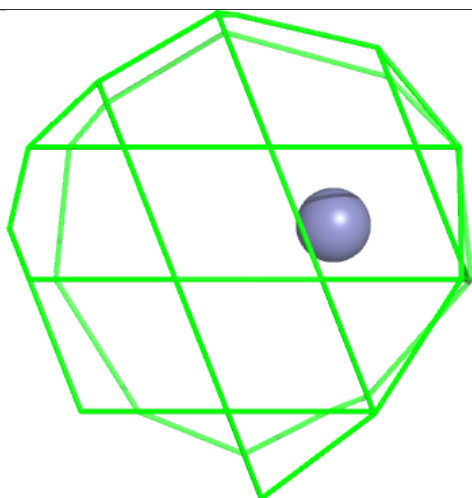
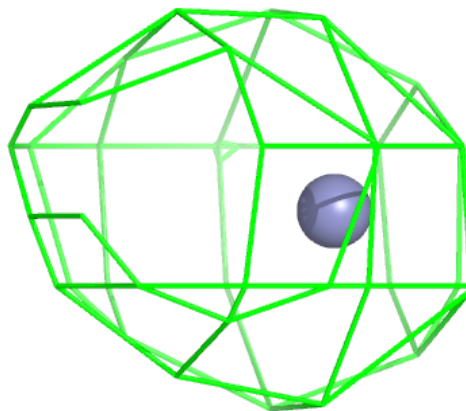
Electron density around SO4 D 1402:

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



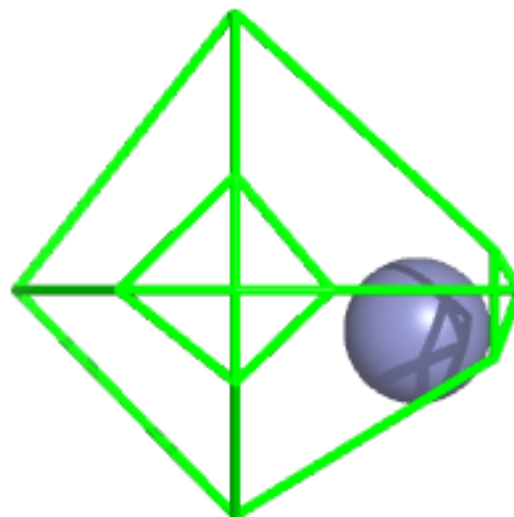
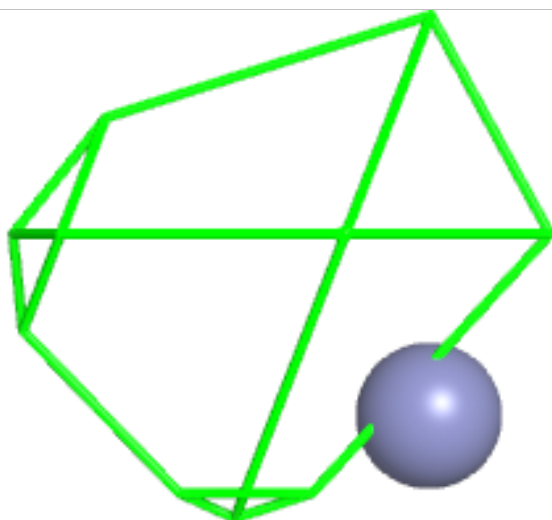
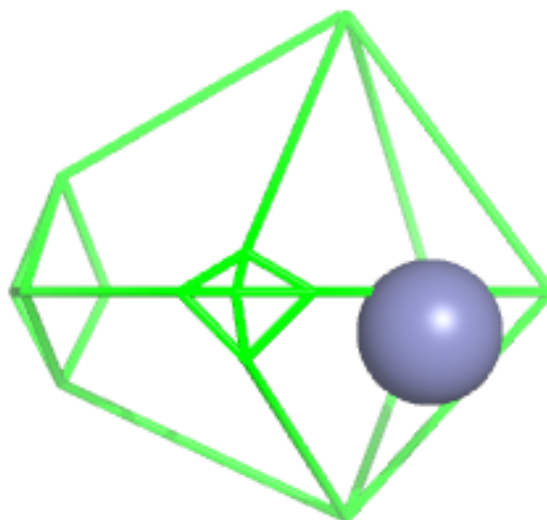
Electron density around ZN D 1409:

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



Electron density around ZN D 1410:

$2mF_o-DF_c$ (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.