



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2020 – 12:34 PM EDT

PDB ID : 6VVT
Title : Crystal structure of a Mycobacterium smegmatis transcription initiation complex with Rifampicin-resistant RNA polymerase and antibiotic Sorangicin
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

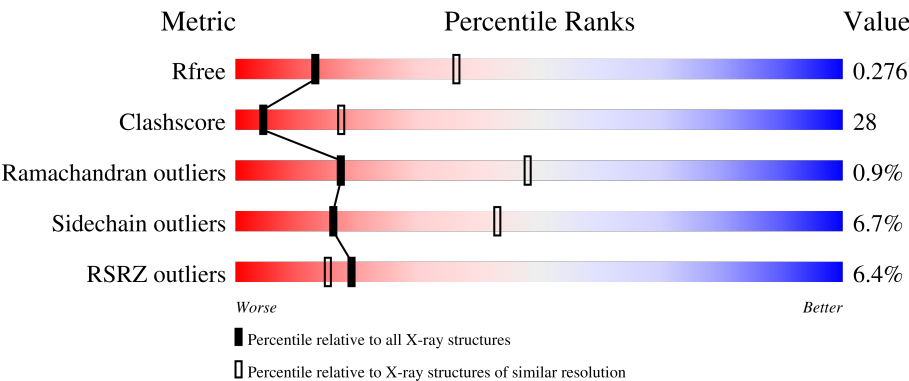
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & 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 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
3	C	1169	
4	D	1317	

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Mol	Chain	Length	Quality of chain
5	E	107	<div><div></div><div>10%</div><div>35%</div><div>35%</div><div>7%</div><div>23%</div></div>
6	F	466	<div><div></div><div>2%</div><div>38%</div><div>25%</div><div></div><div>35%</div></div>
7	O	31	<div><div></div><div>35%</div><div>65%</div></div>
8	P	26	<div><div></div><div>50%</div><div>50%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23757 atoms, of which 10 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	84	Total	C	N	O	S	0	0	0
			672	421	122	127	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	222	Total	C	N	O	S	0	0	0
			1641	1040	277	321	3			
2	B	225	Total	C	N	O	S	0	0	0
			1616	1018	283	313	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	883	Total	C	N	O	S	0	0	0
			6474	4060	1130	1255	29			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1200	Total	C	N	O	S	0	0	0
			9053	5669	1623	1722	39			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			613	388	106	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	303	Total	C	N	O	S	0	0	0
			2393	1501	433	452	7			

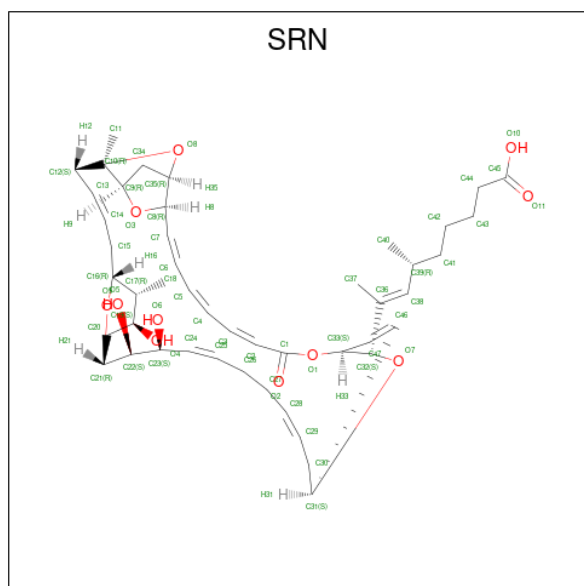
- Molecule 7 is a DNA chain called DNA (31-MER).

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).

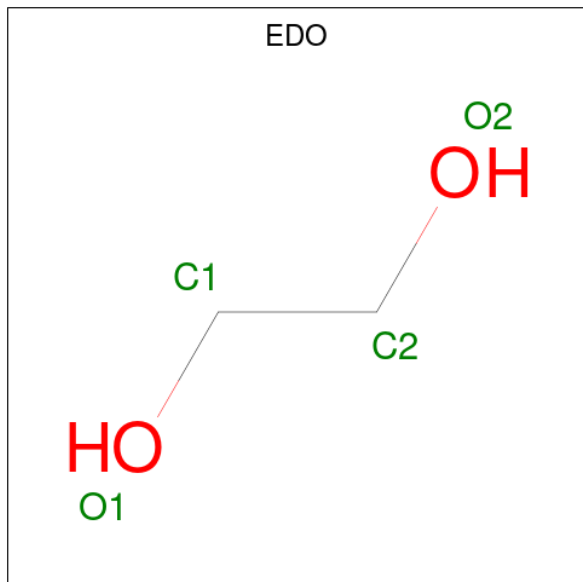
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is SORANGICIN A (three-letter code: SRN) (formula: C₄₇H₆₆O₁₁) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			58	47	11		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

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

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by author).



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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	J	1	Total	O		0	0
			1	1			
13	B	1	Total	O		0	0
			1	1			
13	C	2	Total	H	O	0	0
			4	2	2		

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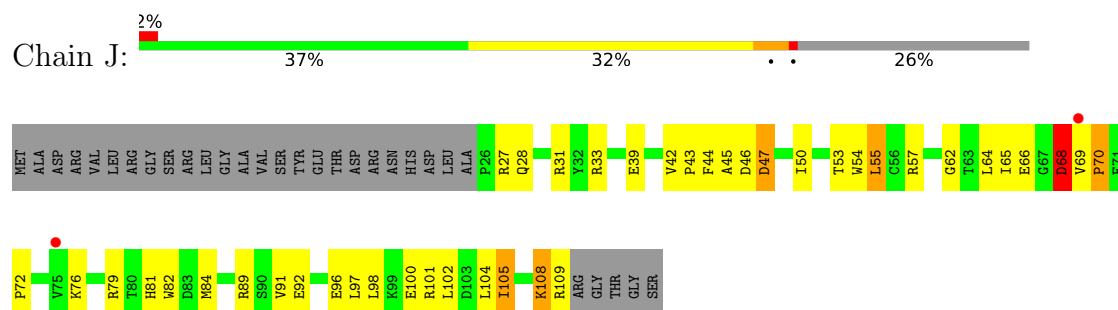
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	8	Total H O 10 2 8	0	0
13	F	1	Total O 1 1	0	0
13	O	1	Total O 1 1	0	0
13	P	1	Total O 1 1	0	0

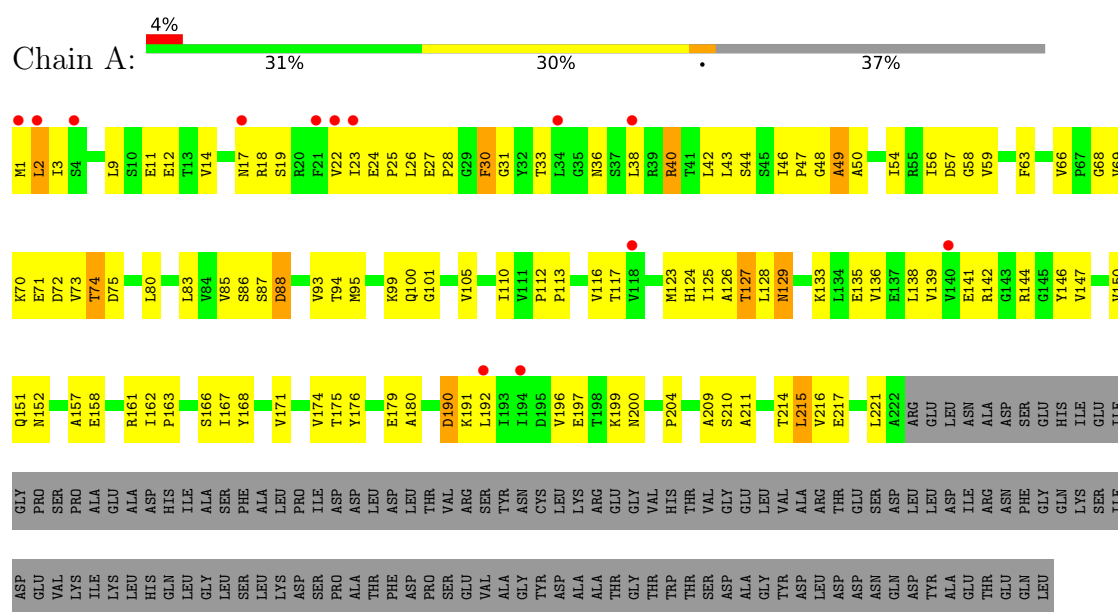
3 Residue-property plots

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.

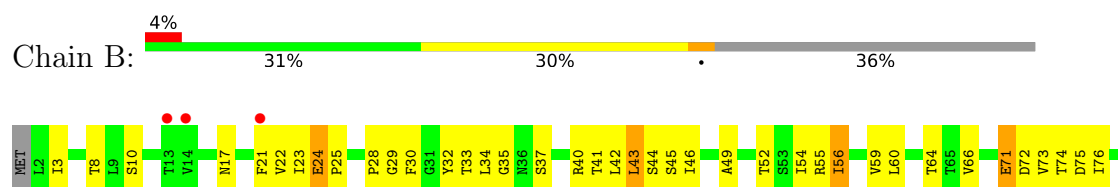
- Molecule 1: RNA polymerase-binding protein RbpA

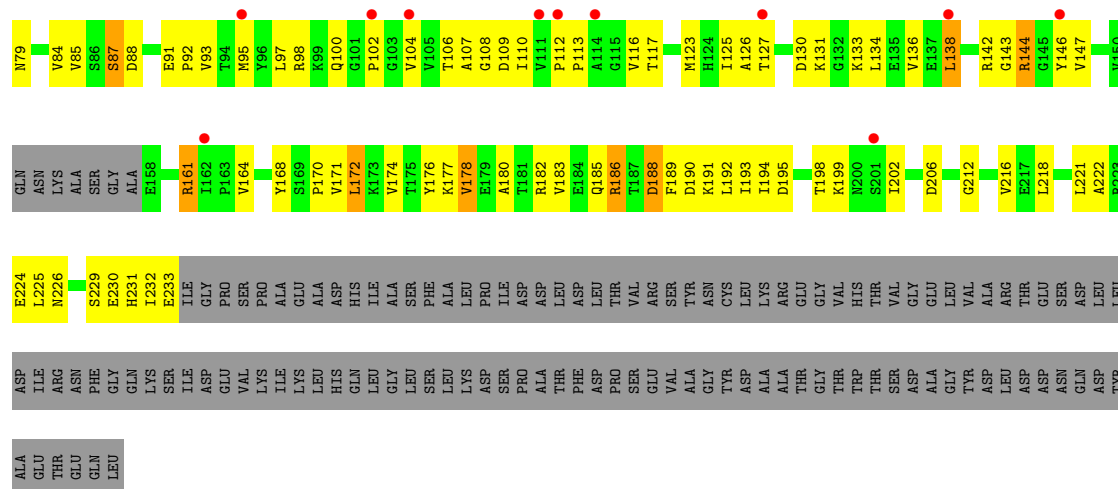


- Molecule 2: DNA-directed RNA polymerase subunit alpha

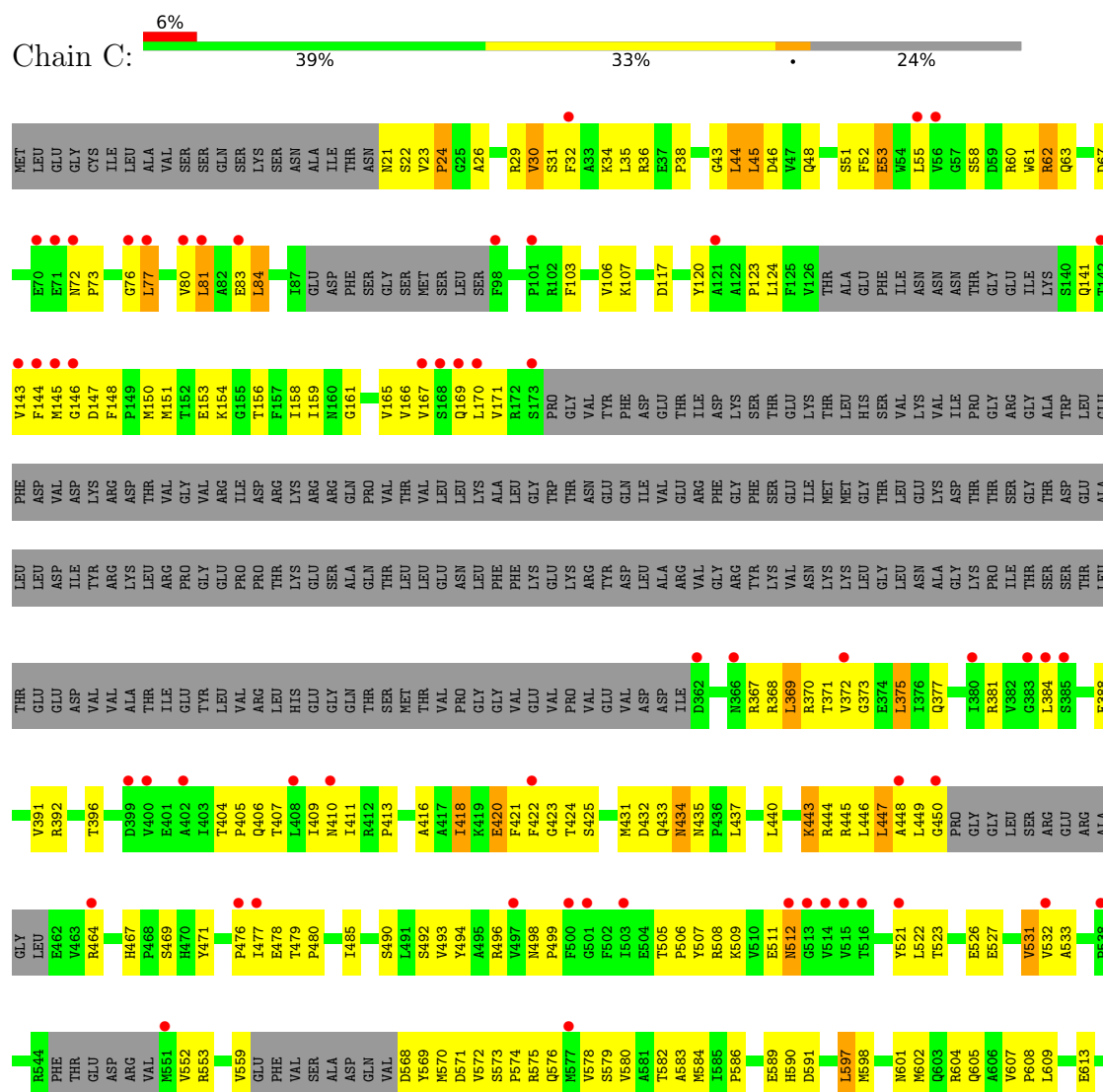


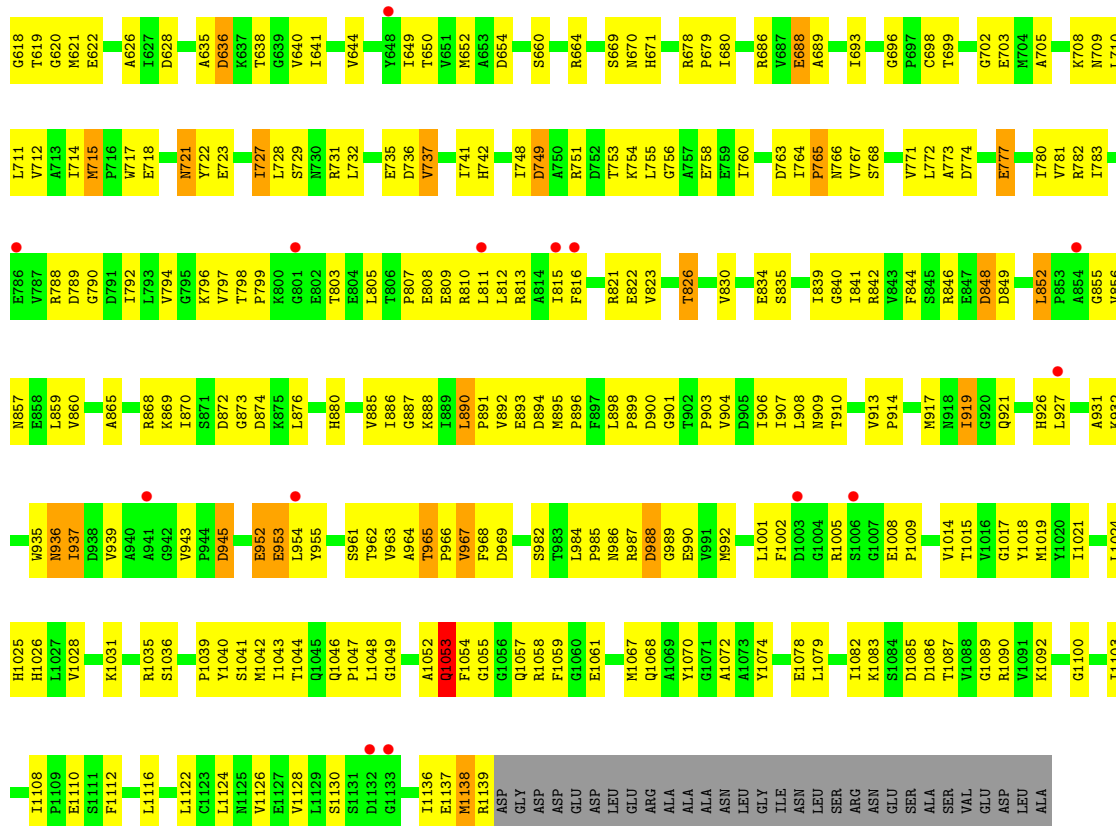
- Molecule 2: DNA-directed RNA polymerase subunit alpha

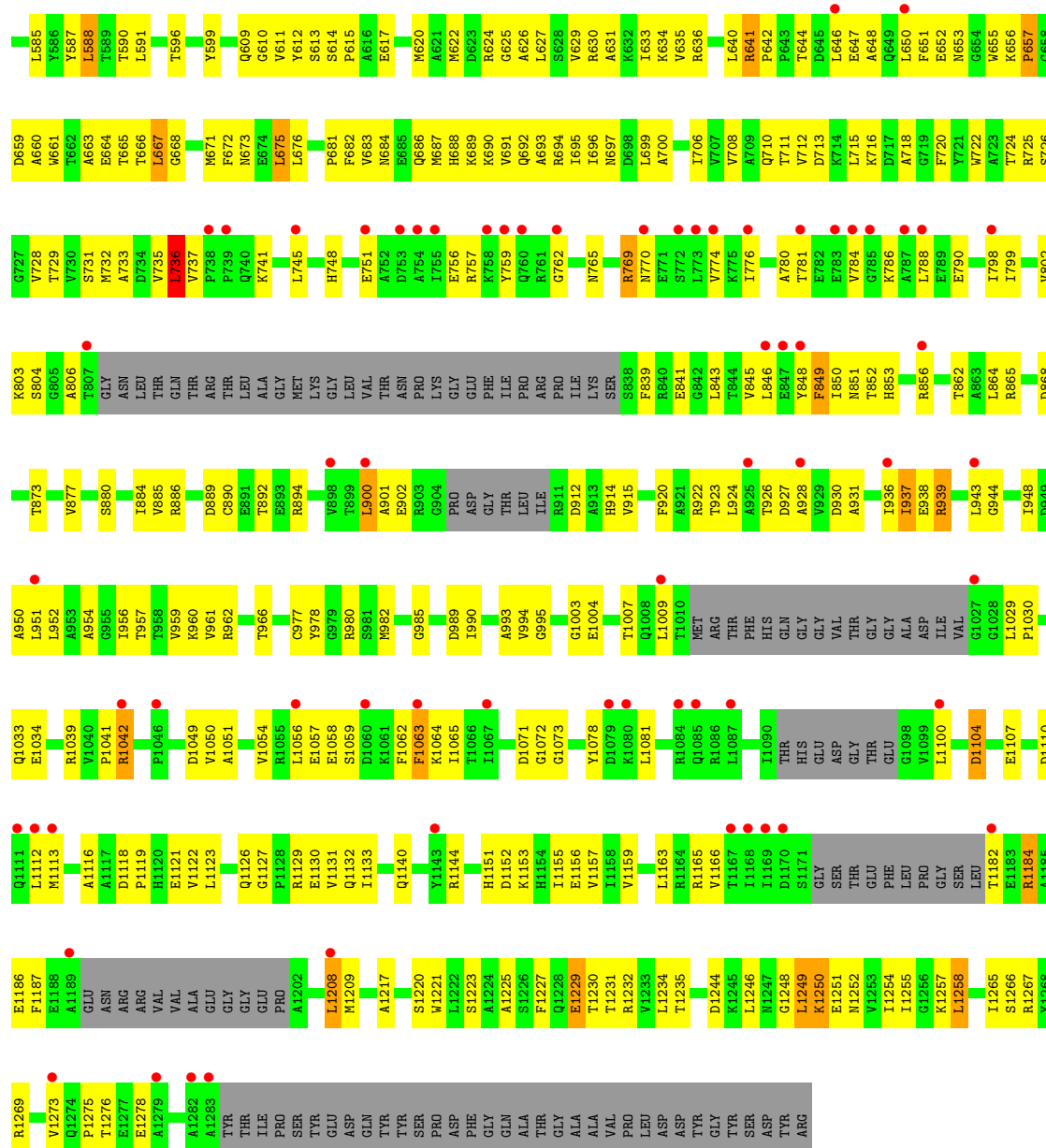




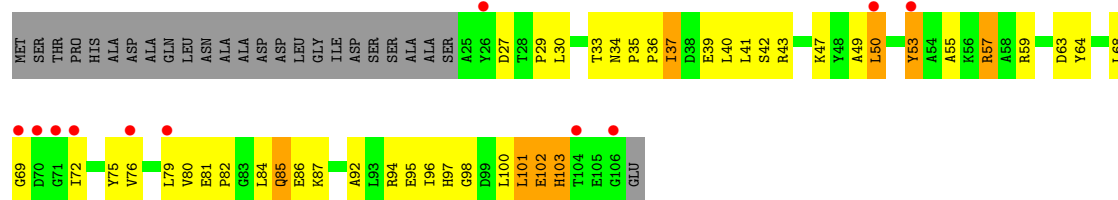
• Molecule 3: DNA-directed RNA polymerase subunit beta





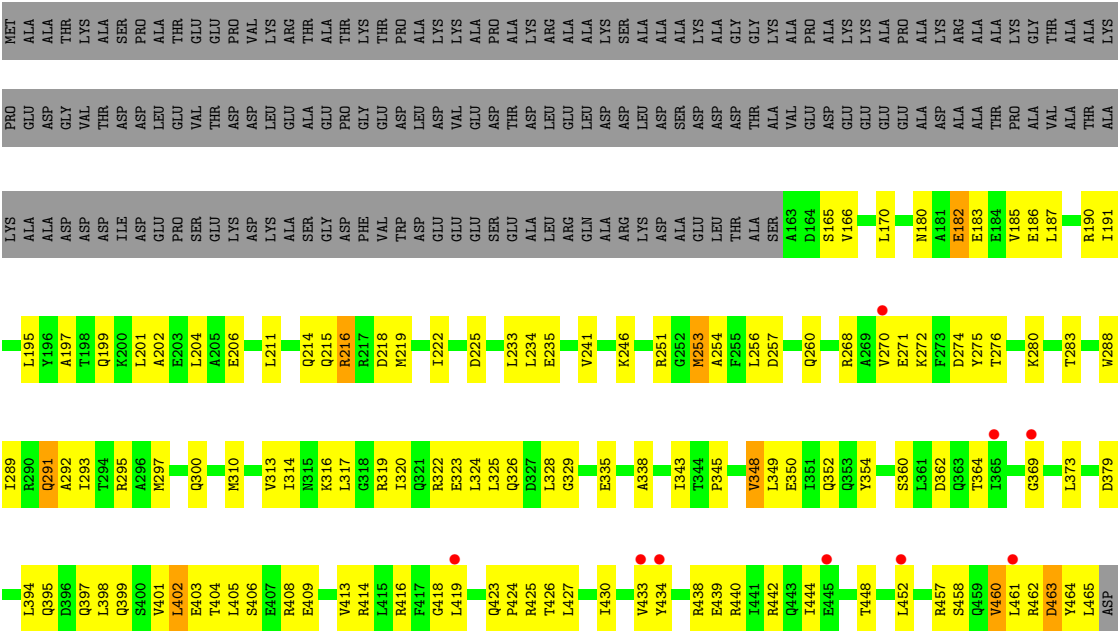


- Molecule 5: DNA-directed RNA polymerase subunit omega

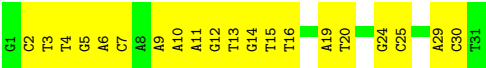


- Molecule 6: RNA polymerase sigma factor SigA





• 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	129.22Å 162.21Å 136.29Å 90.00° 111.36° 90.00°	Depositor
Resolution (Å)	49.75 – 2.90 49.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	82.6 (49.75-2.90) 82.4 (49.75-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.91Å)	Xtriage
Refinement program	PHENIX v0	Depositor
R, R_{free}	0.240 , 0.275 0.243 , 0.276	Depositor DCC
R_{free} test set	1709 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	101.7	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23757	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/686	0.39	0/929
2	A	0.24	0/1667	0.46	0/2275
2	B	0.23	0/1640	0.43	1/2244 (0.0%)
3	C	0.25	0/6584	0.42	0/8959
4	D	0.24	0/9191	0.40	0/12467
5	E	0.23	0/625	0.41	0/852
6	F	0.23	0/2424	0.39	0/3271
7	O	0.54	0/712	0.94	0/1098
8	P	0.55	0/589	0.93	0/906
All	All	0.26	0/24118	0.46	1/33001 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	ASP	CB-CG-OD2	5.14	122.93	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	672	0	651	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1641	0	1663	135	0
2	B	1616	0	1578	138	0
3	C	6474	0	6202	454	1
4	D	9053	0	8845	472	1
5	E	613	0	591	46	0
6	F	2393	0	2417	120	0
7	O	635	0	354	20	0
8	P	526	0	296	16	0
9	C	58	0	65	16	0
10	C	4	6	6	0	0
11	D	2	0	0	0	0
12	D	25	0	0	1	0
12	F	20	0	0	2	0
13	B	1	0	0	0	0
13	C	2	2	0	1	0
13	D	8	2	0	3	0
13	F	1	0	0	0	0
13	J	1	0	0	0	0
13	O	1	0	0	0	0
13	P	1	0	0	0	0
All	All	23747	10	22668	1316	1

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

All (1316) 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)
9:C:1201:SRN:C10	9:C:1201:SRN:C12	1.77	1.54
9:C:1201:SRN:O3	9:C:1201:SRN:C9	1.81	1.29
9:C:1201:SRN:O3	9:C:1201:SRN:C8	1.80	1.28
2:B:102:PRO:HG3	2:B:130:ASP:HA	1.30	1.12
2:A:2:LEU:HD11	2:B:142:ARG:HB2	1.30	1.11
2:B:87:SER:HB2	2:B:116:VAL:HG12	1.33	1.05
4:D:706:ILE:HD12	5:E:36:PRO:HB3	1.39	1.03
4:D:912:ASP:HB3	4:D:915:VAL:HG13	1.38	1.00
4:D:951:LEU:HB3	4:D:956:ILE:HD11	1.38	1.00
3:C:533:ALA:HA	3:C:552:VAL:HG12	1.39	0.99
4:D:622:MET:HE3	4:D:667:LEU:HD13	1.45	0.99
1:J:28:GLN:HG3	1:J:46:ASP:HA	1.45	0.98
4:D:725:ARG:NH1	13:D:2101:HOH:O	1.95	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:ILE:HD13	4:D:318:PRO:HD3	1.46	0.97
3:C:506:PRO:HB2	3:C:572:VAL:HG11	1.43	0.96
3:C:715:MET:HG2	3:C:1014:VAL:HG11	1.46	0.96
4:D:275:GLU:HA	4:D:278:ARG:HG3	1.48	0.95
2:A:216:VAL:HG13	2:B:216:VAL:HG23	1.46	0.95
3:C:756:GLY:HA3	3:C:799:PRO:HG3	1.49	0.94
6:F:216:ARG:HG2	6:F:216:ARG:HH21	1.34	0.92
3:C:1058:ARG:HH11	4:D:415:GLN:HG2	1.34	0.91
4:D:641:ARG:NH2	4:D:656:LYS:O	2.04	0.91
3:C:754:LYS:HB3	4:D:39:LEU:HD12	1.53	0.91
3:C:807:PRO:HB2	6:F:419:LEU:HD23	1.53	0.90
3:C:710:LEU:HD22	3:C:1021:ILE:HD11	1.52	0.90
9:C:1201:SRN:C10	9:C:1201:SRN:C13	2.51	0.88
2:B:95:MET:HG2	2:B:113:PRO:HD2	1.56	0.87
3:C:478:GLU:OE2	3:C:604:ARG:NH2	2.07	0.87
4:D:47:PHE:O	4:D:88:ARG:NH2	2.08	0.87
2:A:40:ARG:HB3	2:A:40:ARG:HH11	1.40	0.86
3:C:433:GLN:NE2	3:C:670:ASN:OD1	2.08	0.86
3:C:936:ASN:N	3:C:982:SER:OG	2.08	0.86
4:D:119:ASP:HB2	4:D:295:ARG:HH12	1.40	0.86
2:A:48:GLY:HA2	2:A:49:ALA:HB3	1.55	0.86
3:C:1043:ILE:H	3:C:1043:ILE:HD12	1.41	0.86
2:A:54:ILE:HD11	2:A:162:ILE:HD11	1.56	0.85
4:D:128:ILE:HD11	4:D:234:LEU:HD11	1.58	0.85
4:D:633:ILE:HD13	4:D:635:VAL:HG13	1.59	0.85
2:B:107:ALA:O	2:B:110:ILE:HG22	1.77	0.84
3:C:432:ASP:HB2	9:C:1201:SRN:H182	1.59	0.84
2:B:56:ILE:HG22	2:B:59:VAL:HG22	1.58	0.84
3:C:728:LEU:HD22	3:C:906:ILE:HG22	1.59	0.84
3:C:717:TRP:H	3:C:721:ASN:HD21	1.26	0.83
5:E:84:LEU:HB2	5:E:85:GLN:HE21	1.41	0.83
3:C:649:ILE:HD11	3:C:679:PRO:HB3	1.61	0.83
3:C:170:LEU:HA	3:C:369:LEU:HA	1.57	0.83
4:D:924:LEU:HD21	4:D:943:LEU:HD11	1.59	0.82
2:A:99:LYS:HG2	2:A:105:VAL:HG22	1.60	0.82
3:C:372:VAL:HA	3:C:375:LEU:HD11	1.59	0.82
4:D:111:PRO:O	4:D:113:ARG:NH1	2.11	0.82
3:C:641:ILE:HG21	3:C:644:VAL:HG13	1.61	0.82
3:C:63:GLN:O	3:C:67:ASP:OD2	1.97	0.81
3:C:1040:TYR:HD1	3:C:1047:PRO:HA	1.46	0.81
6:F:438:ARG:NH1	8:P:20:DG:N7	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:444:ARG:NH2	3:C:492:SER:O	2.13	0.81
2:A:47:PRO:HG2	2:B:230:GLU:HB3	1.62	0.81
4:D:927:ASP:OD1	4:D:939:ARG:N	2.13	0.80
6:F:401:VAL:O	6:F:404:THR:HG22	1.82	0.80
3:C:123:PRO:HB3	3:C:144:PHE:HE1	1.46	0.80
3:C:467:HIS:HD2	3:C:469:SER:H	1.27	0.80
3:C:124:LEU:HD21	3:C:145:MET:HB2	1.61	0.80
3:C:607:VAL:O	13:C:1301:HOH:O	1.98	0.79
2:A:2:LEU:HD11	2:B:142:ARG:CB	2.09	0.79
1:J:31:ARG:NH2	1:J:39:GLU:OE1	2.15	0.79
4:D:894:ARG:HB3	4:D:966:THR:HB	1.63	0.78
3:C:783:ILE:H	3:C:783:ILE:HD12	1.48	0.78
3:C:51:SER:OG	3:C:373:GLY:N	2.17	0.78
8:P:11:DA:H2''	8:P:12:DA:C5'	2.14	0.78
6:F:319:ARG:NH1	8:P:2:DG:OP1	2.15	0.78
2:A:48:GLY:CA	2:A:49:ALA:HB3	2.12	0.78
2:B:110:ILE:HD11	2:B:138:LEU:HD11	1.66	0.78
3:C:799:PRO:HA	3:C:823:VAL:CG1	2.13	0.78
3:C:937:ILE:HD11	3:C:955:TYR:HB3	1.65	0.77
2:B:107:ALA:HB2	2:B:125:ILE:HD11	1.66	0.77
5:E:84:LEU:H	5:E:84:LEU:HD12	1.48	0.77
3:C:584:MET:HA	3:C:619:THR:HG21	1.66	0.77
3:C:844:PHE:HD2	3:C:859:LEU:HD12	1.50	0.77
5:E:40:LEU:HB3	5:E:50:LEU:HD11	1.67	0.77
3:C:742:HIS:HD2	3:C:868:ARG:HG3	1.48	0.76
2:A:1:MET:N	2:B:142:ARG:O	2.19	0.76
2:A:24:GLU:HB3	2:A:191:LYS:HG3	1.67	0.76
3:C:1130:SER:HB2	3:C:1136:ILE:HD11	1.67	0.76
6:F:280:LYS:HG2	7:O:30:DC:OP2	1.86	0.76
2:B:71:GLU:OE2	2:B:127:THR:N	2.19	0.76
3:C:598:MET:O	3:C:602:MET:HG3	1.86	0.75
4:D:936:ILE:HG12	4:D:937:ILE:HD13	1.66	0.75
6:F:216:ARG:CG	6:F:216:ARG:HH21	1.98	0.75
1:J:92:GLU:OE1	1:J:92:GLU:N	2.18	0.75
4:D:442:GLY:HA3	4:D:523:GLN:HB2	1.68	0.75
3:C:171:VAL:HG12	3:C:450:GLY:HA3	1.67	0.75
4:D:799:ILE:HG22	4:D:803:LYS:HE2	1.68	0.75
2:A:24:GLU:HB3	2:A:191:LYS:CG	2.17	0.75
3:C:764:ILE:HB	3:C:767:VAL:HG21	1.68	0.75
4:D:1165:ARG:HD2	4:D:1209:MET:HE1	1.69	0.75
4:D:407:LYS:HA	4:D:413:PHE:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1058:ARG:NH1	4:D:415:GLN:HG2	2.00	0.75
4:D:573:PRO:HD3	4:D:697:ASN:OD1	1.86	0.75
2:B:75:ASP:O	2:B:79:ASN:ND2	2.20	0.74
3:C:790:GLY:H	3:C:830:VAL:HG22	1.53	0.74
3:C:751:ARG:NH1	4:D:332:GLY:O	2.20	0.74
4:D:119:ASP:HB2	4:D:295:ARG:NH1	2.02	0.74
4:D:951:LEU:HB3	4:D:956:ILE:CD1	2.17	0.74
1:J:109:ARG:NH2	6:F:214:GLN:OE1	2.20	0.74
4:D:690:LYS:O	4:D:694:ARG:N	2.15	0.73
3:C:1049:GLY:HA2	3:C:1055:GLY:HA2	1.70	0.73
3:C:478:GLU:OE1	3:C:490:SER:OG	2.06	0.73
3:C:732:LEU:HA	3:C:737:VAL:CG1	2.18	0.73
4:D:417:LEU:HD21	4:D:1254:ILE:HG23	1.71	0.73
4:D:641:ARG:HB3	4:D:681:PRO:HA	1.71	0.73
3:C:711:LEU:HD23	3:C:904:VAL:HA	1.71	0.73
4:D:237:ASP:HB3	4:D:240:LEU:HB3	1.70	0.73
3:C:1078:GLU:HG3	3:C:1082:ILE:HD11	1.68	0.72
3:C:1015:THR:H	4:D:729:THR:HG21	1.54	0.72
3:C:635:ALA:HB2	3:C:693:ILE:HD11	1.72	0.72
2:A:26:LEU:HD22	2:B:218:LEU:HD11	1.71	0.72
4:D:978:TYR:CE1	4:D:994:VAL:HG11	2.25	0.72
3:C:968:PHE:CD2	4:D:845:VAL:HG22	2.25	0.71
6:F:408:ARG:HG3	6:F:434:TYR:CE1	2.25	0.71
3:C:404:THR:HG22	3:C:407:THR:HG23	1.70	0.71
4:D:365:ILE:HD12	4:D:365:ILE:H	1.54	0.71
3:C:650:THR:HG22	3:C:660:SER:OG	1.90	0.71
4:D:397:ARG:NH2	6:F:360:SER:OG	2.22	0.71
3:C:574:PRO:O	3:C:575:ARG:HG2	1.90	0.71
3:C:578:VAL:HG13	3:C:582:THR:HB	1.72	0.71
2:A:40:ARG:HH21	3:C:894:ASP:HB3	1.53	0.71
4:D:1056:LEU:HD23	4:D:1065:ILE:HG12	1.72	0.70
4:D:1165:ARG:HD2	4:D:1209:MET:CE	2.21	0.70
4:D:1275:PRO:HG3	5:E:76:VAL:HG11	1.71	0.70
2:A:2:LEU:CD1	2:B:142:ARG:HB2	2.16	0.70
4:D:1248:GLY:O	4:D:1252:ASN:ND2	2.24	0.70
2:B:56:ILE:HD11	2:B:136:VAL:HB	1.73	0.70
2:B:107:ALA:N	2:B:125:ILE:HD13	2.07	0.70
2:B:43:LEU:HA	2:B:171:VAL:HG21	1.74	0.70
4:D:277:LEU:HD11	4:D:295:ARG:HG2	1.74	0.70
2:A:133:LYS:NZ	2:A:135:GLU:OE2	2.19	0.70
4:D:535:ASP:HB2	13:D:2104:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:622:MET:CE	4:D:629:VAL:HG22	2.22	0.70
4:D:21:ARG:NE	4:D:96:GLU:OE2	2.20	0.70
4:D:901:ALA:HA	4:D:912:ASP:N	2.06	0.69
3:C:1042:MET:HA	6:F:379:ASP:HB2	1.75	0.69
3:C:508:ARG:HD2	3:C:570:MET:HG3	1.74	0.69
8:P:11:DA:H2''	8:P:12:DA:O5'	1.92	0.69
6:F:185:VAL:HG13	6:F:275:TYR:HB2	1.74	0.69
3:C:169:GLN:O	3:C:370:ARG:N	2.25	0.69
3:C:966:PRO:HG2	3:C:969:ASP:O	1.93	0.69
4:D:737:VAL:HG11	4:D:841:GLU:OE2	1.93	0.69
2:A:83:LEU:HG	2:A:123:MET:HE1	1.73	0.69
3:C:935:TRP:NE1	3:C:954:LEU:O	2.21	0.69
4:D:444:PRO:HD2	4:D:447:MET:HE2	1.74	0.69
4:D:499:ASN:HB2	4:D:509:ILE:HG12	1.75	0.69
4:D:733:ALA:HA	4:D:736:LEU:HD23	1.74	0.69
3:C:967:VAL:HG23	3:C:968:PHE:H	1.56	0.69
4:D:1041:PRO:HB3	4:D:1116:ALA:HB3	1.74	0.69
3:C:388:GLU:HA	3:C:391:VAL:HG22	1.75	0.69
3:C:83:GLU:OE2	3:C:381:ARG:NH2	2.26	0.69
2:B:93:VAL:HG11	2:B:116:VAL:HG11	1.73	0.68
2:B:74:THR:HG23	4:D:611:VAL:HG21	1.75	0.68
4:D:1063:PHE:O	4:D:1081:LEU:HB2	1.92	0.68
6:F:190:ARG:HD2	6:F:225:ASP:OD2	1.93	0.68
2:A:94:THR:HG22	2:A:139:VAL:HG22	1.76	0.68
3:C:51:SER:HB3	3:C:372:VAL:HG12	1.73	0.68
4:D:951:LEU:CB	4:D:956:ILE:HD11	2.21	0.68
3:C:30:VAL:HB	3:C:954:LEU:HD21	1.76	0.68
4:D:284:GLY:HA2	4:D:289:LYS:CB	2.24	0.68
4:D:944:GLY:HA2	4:D:980:ARG:HH22	1.58	0.68
6:F:216:ARG:HG2	6:F:216:ARG:NH2	2.06	0.68
2:A:152:ASN:HB2	2:A:157:ALA:HB3	1.76	0.68
4:D:880:SER:O	4:D:995:GLY:HA3	1.94	0.68
4:D:912:ASP:HB3	4:D:915:VAL:CG1	2.18	0.68
4:D:928:ALA:HB3	4:D:936:ILE:O	1.94	0.68
2:A:152:ASN:CB	2:A:157:ALA:HB3	2.24	0.67
4:D:138:SER:HB3	4:D:253:THR:OG1	1.93	0.67
4:D:614:SER:HB2	4:D:615:PRO:HD2	1.74	0.67
9:C:1201:SRN:C12	9:C:1201:SRN:C11	2.66	0.67
3:C:573:SER:HB2	3:C:574:PRO:HD2	1.76	0.67
3:C:654:ASP:OD2	3:C:686:ARG:NH2	2.25	0.67
4:D:885:VAL:HB	4:D:990:ILE:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:MET:HG2	2:B:113:PRO:CD	2.23	0.67
3:C:952:GLU:OE1	3:C:953:GLU:N	2.28	0.67
3:C:773:ALA:O	3:C:782:ARG:NH2	2.28	0.67
4:D:31:PRO:HB3	4:D:348:ILE:HG23	1.76	0.67
4:D:741:LYS:O	4:D:745:LEU:HG	1.94	0.67
4:D:799:ILE:CG2	4:D:803:LYS:HE2	2.25	0.67
3:C:601:ASN:HA	3:C:604:ARG:NH1	2.10	0.67
6:F:409:GLU:CG	6:F:448:THR:HG22	2.25	0.67
5:E:35:PRO:HG2	5:E:40:LEU:HD11	1.76	0.67
2:A:14:VAL:HG13	2:A:18:ARG:HG3	1.77	0.67
1:J:64:LEU:HD23	1:J:65:ILE:H	1.60	0.67
3:C:619:THR:OG1	3:C:620:GLY:N	2.28	0.67
4:D:214:ARG:O	4:D:218:ARG:HG3	1.95	0.66
4:D:330:LEU:N	4:D:334:ARG:O	2.25	0.66
3:C:808:GLU:HG2	6:F:395:GLN:HG2	1.77	0.66
4:D:688:HIS:O	4:D:692:GLN:HG3	1.94	0.66
6:F:234:LEU:HD23	6:F:270:VAL:HG21	1.78	0.66
8:P:11:DA:H4'	8:P:12:DA:OP1	1.95	0.66
2:A:66:VAL:O	2:A:69:VAL:HG22	1.95	0.66
2:B:49:ALA:HA	2:B:142:ARG:HA	1.76	0.66
4:D:1230:THR:HG22	4:D:1234:LEU:HD22	1.77	0.66
4:D:735:VAL:O	4:D:736:LEU:HD12	1.95	0.66
1:J:64:LEU:HD23	1:J:65:ILE:N	2.10	0.66
2:B:100:GLN:HA	2:B:133:LYS:HA	1.78	0.66
4:D:386:ARG:HH12	4:D:1231:THR:HG21	1.59	0.66
3:C:718:GLU:H	4:D:724:THR:CG2	2.09	0.66
2:A:56:ILE:HB	2:A:59:VAL:HG22	1.77	0.66
4:D:1071:ASP:N	4:D:1072:GLY:HA2	2.10	0.66
4:D:733:ALA:HA	4:D:736:LEU:CD2	2.25	0.66
5:E:29:PRO:CG	5:E:34:ASN:HB2	2.25	0.66
3:C:936:ASN:H	3:C:982:SER:HG	1.40	0.66
4:D:647:GLU:HG3	4:D:655:TRP:CD1	2.30	0.66
3:C:377:GLN:OE1	3:C:381:ARG:NH1	2.28	0.66
3:C:527:GLU:OE1	3:C:553:ARG:NH2	2.29	0.66
2:B:198:THR:HG21	2:B:202:ILE:HD12	1.77	0.66
7:O:14:DG:H2''	7:O:15:DT:OP2	1.95	0.66
4:D:1251:GLU:OE1	4:D:1251:GLU:N	2.22	0.65
2:B:17:ASN:HB3	2:B:198:THR:O	1.95	0.65
3:C:1112:PHE:CE2	4:D:1255:ILE:HG22	2.32	0.65
2:A:56:ILE:HG12	2:A:136:VAL:HB	1.78	0.65
3:C:423:GLY:O	3:C:424:THR:OG1	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:622:GLU:HB3	3:C:703:GLU:HB2	1.79	0.65
3:C:751:ARG:CD	3:C:856:VAL:HG22	2.26	0.65
3:C:952:GLU:O	3:C:953:GLU:HB2	1.97	0.65
4:D:480:ARG:HB3	4:D:482:GLN:OE1	1.97	0.65
4:D:579:LEU:HA	4:D:806:ALA:HB1	1.78	0.65
9:C:1201:SRN:H401	9:C:1201:SRN:C3	2.27	0.65
3:C:480:PRO:HB3	9:C:1201:SRN:O10	1.97	0.65
4:D:200:SER:O	4:D:204:GLU:HG3	1.97	0.65
4:D:642:PRO:HG2	4:D:647:GLU:HB2	1.77	0.65
4:D:786:LYS:O	4:D:790:GLU:HG2	1.95	0.65
2:B:97:LEU:HB2	2:B:110:ILE:HG13	1.77	0.65
3:C:29:ARG:HG2	3:C:964:ALA:HB2	1.79	0.65
3:C:771:VAL:HG23	3:C:772:LEU:CD1	2.27	0.65
2:B:24:GLU:OE2	2:B:191:LYS:HD3	1.97	0.65
3:C:774:ASP:HA	3:C:782:ARG:HH21	1.62	0.65
6:F:254:ALA:HB3	6:F:257:ASP:OD2	1.96	0.65
3:C:751:ARG:HG2	3:C:856:VAL:HG22	1.79	0.65
4:D:1249:LEU:HD12	4:D:1250:LYS:N	2.12	0.65
4:D:612:TYR:HB2	4:D:635:VAL:HG12	1.79	0.64
3:C:848:ASP:N	3:C:848:ASP:OD1	2.30	0.64
6:F:409:GLU:OE1	6:F:448:THR:HG22	1.97	0.64
6:F:444:ILE:O	6:F:448:THR:HG23	1.96	0.64
4:D:1127:GLY:O	4:D:1131:VAL:HG23	1.97	0.64
4:D:444:PRO:HG3	4:D:521:ALA:O	1.97	0.64
4:D:936:ILE:HD11	4:D:950:ALA:HB1	1.78	0.64
4:D:1126:GLN:OE1	4:D:1130:GLU:HG2	1.97	0.64
4:D:295:ARG:O	4:D:298:VAL:HG22	1.97	0.64
3:C:509:LYS:HA	3:C:569:TYR:HA	1.79	0.64
4:D:12:ILE:HD11	4:D:1221:TRP:CD2	2.33	0.64
2:B:95:MET:HB2	2:B:138:LEU:CD1	2.27	0.64
4:D:1071:ASP:HB2	4:D:1073:GLY:N	2.12	0.64
4:D:550:GLU:O	4:D:554:GLU:HG3	1.98	0.64
1:J:47:ASP:N	1:J:47:ASP:OD1	2.31	0.64
3:C:1079:LEU:HD23	3:C:1083:LYS:HD2	1.80	0.64
9:C:1201:SRN:O1	9:C:1201:SRN:H4	1.98	0.64
3:C:809:GLU:O	3:C:813:ARG:HG2	1.98	0.63
3:C:508:ARG:HG3	3:C:570:MET:O	1.97	0.63
3:C:760:ILE:HA	3:C:796:LYS:HA	1.79	0.63
3:C:76:GLY:O	3:C:80:VAL:HG23	1.98	0.63
6:F:460:VAL:HG22	6:F:461:LEU:HD23	1.80	0.63
3:C:507:TYR:OH	3:C:527:GLU:OE2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:939:VAL:CG1	3:C:943:VAL:HG12	2.28	0.63
4:D:1050:VAL:HG22	4:D:1051:ALA:H	1.63	0.63
4:D:611:VAL:HA	4:D:634:LYS:O	1.99	0.63
2:B:30:PHE:HA	2:B:33:THR:HG23	1.81	0.63
3:C:717:TRP:N	3:C:721:ASN:HD21	1.95	0.63
2:A:31:GLY:HA2	2:A:192:LEU:HD23	1.80	0.63
3:C:494:TYR:HB3	3:C:506:PRO:HG3	1.80	0.63
3:C:873:GLY:HA3	3:C:1028:VAL:HG11	1.80	0.63
3:C:171:VAL:O	3:C:368:ARG:N	2.19	0.63
4:D:421:ARG:NH2	12:D:2006:SO4:O4	2.25	0.63
4:D:633:ILE:HD13	4:D:635:VAL:CG1	2.29	0.63
2:A:129:ASN:H	2:A:129:ASN:HD22	1.44	0.63
4:D:104:ILE:HD12	4:D:379:ASP:HB3	1.81	0.63
4:D:641:ARG:NE	4:D:641:ARG:HA	2.13	0.63
7:O:19:DA:H2''	7:O:20:DT:O5'	1.99	0.63
2:A:40:ARG:NH2	3:C:894:ASP:HB3	2.14	0.63
2:B:143:GLY:HA3	2:B:168:TYR:CD1	2.34	0.63
3:C:1087:THR:O	3:C:1090:ARG:NH1	2.32	0.63
4:D:444:PRO:HD2	4:D:447:MET:CE	2.29	0.63
6:F:409:GLU:HG3	6:F:448:THR:HG22	1.80	0.63
5:E:29:PRO:HG2	5:E:34:ASN:HB2	1.80	0.62
3:C:143:VAL:HG21	3:C:409:ILE:HD12	1.82	0.62
3:C:416:ALA:O	3:C:420:GLU:HB2	2.00	0.62
3:C:618:GLY:O	3:C:964:ALA:HA	2.00	0.62
4:D:751:GLU:HB3	4:D:776:ILE:HD13	1.81	0.62
6:F:335:GLU:OE1	6:F:335:GLU:N	2.31	0.62
2:A:9:LEU:HD23	2:B:221:LEU:O	2.00	0.62
3:C:1085:ASP:HB3	3:C:1110:GLU:H	1.63	0.62
3:C:937:ILE:HD11	3:C:955:TYR:CB	2.29	0.62
4:D:748:HIS:CG	4:D:780:ALA:HB2	2.34	0.62
3:C:816:PHE:CE2	6:F:462:ARG:HG3	2.34	0.62
7:O:19:DA:H4'	7:O:20:DT:OP1	1.98	0.62
4:D:1275:PRO:HB3	5:E:79:LEU:HD11	1.80	0.62
3:C:742:HIS:CD2	3:C:868:ARG:HG3	2.31	0.62
3:C:888:LYS:HD3	3:C:890:LEU:HD11	1.81	0.62
4:D:901:ALA:H	4:D:912:ASP:HB2	1.64	0.62
2:A:48:GLY:HA2	2:A:49:ALA:CB	2.27	0.62
2:A:40:ARG:NH1	2:B:33:THR:HG22	2.15	0.62
3:C:898:LEU:HD23	3:C:1001:LEU:CD2	2.30	0.62
2:A:2:LEU:HD12	2:A:2:LEU:H	1.62	0.62
3:C:80:VAL:HG12	3:C:384:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:SER:HB3	3:C:372:VAL:CG1	2.30	0.62
2:B:106:THR:O	2:B:108:GLY:N	2.30	0.62
4:D:320:ILE:HG12	4:D:321:PRO:HD2	1.82	0.62
3:C:80:VAL:CG1	3:C:384:LEU:HD12	2.30	0.61
2:A:162:ILE:HG13	2:A:162:ILE:O	2.00	0.61
4:D:409:LYS:HA	4:D:414:ARG:NH1	2.14	0.61
8:P:13:DC:H2"	8:P:14:DA:C8	2.36	0.61
4:D:930:ASP:OD1	4:D:931:ALA:N	2.33	0.61
2:B:97:LEU:O	2:B:136:VAL:HG12	1.99	0.61
3:C:727:ILE:HG13	3:C:907:ILE:HB	1.81	0.61
4:D:687:MET:HE3	4:D:695:ILE:HD12	1.81	0.61
6:F:364:THR:HG21	6:F:369:GLY:HA2	1.81	0.61
3:C:124:LEU:CD2	3:C:145:MET:HB2	2.31	0.61
3:C:638:THR:HG23	3:C:688:GLU:HA	1.82	0.61
4:D:1153:LYS:O	4:D:1157:VAL:HG23	1.99	0.61
6:F:187:LEU:O	6:F:191:ILE:HG13	2.01	0.61
3:C:1041:SER:HB3	3:C:1044:THR:O	2.00	0.61
3:C:1103:ILE:HD12	4:D:548:SER:HA	1.81	0.61
4:D:1186:GLU:N	4:D:1186:GLU:OE1	2.34	0.61
4:D:396:ASN:ND2	4:D:396:ASN:O	2.32	0.61
4:D:567:SER:HB2	4:D:574:LEU:CD1	2.31	0.61
6:F:233:LEU:HD23	6:F:270:VAL:HG13	1.81	0.61
3:C:479:THR:O	3:C:597:LEU:HD21	1.99	0.61
4:D:1059:SER:OG	4:D:1062:PHE:O	2.18	0.61
2:A:28:PRO:HA	2:A:190:ASP:CG	2.21	0.60
2:A:49:ALA:HB1	2:A:85:VAL:O	2.01	0.60
2:A:40:ARG:HD3	2:B:33:THR:HG22	1.81	0.60
4:D:344:TYR:O	4:D:348:ILE:HG22	2.00	0.60
3:C:803:THR:HB	3:C:805:LEU:HD23	1.83	0.60
4:D:936:ILE:HG12	4:D:937:ILE:CD1	2.31	0.60
3:C:756:GLY:CA	3:C:799:PRO:HG3	2.27	0.60
3:C:77:LEU:O	3:C:81:LEU:HD22	2.01	0.60
4:D:1107:GLU:HB2	4:D:1110:ASP:OD1	2.02	0.60
6:F:345:PRO:O	6:F:348:VAL:HG13	2.00	0.60
3:C:731:ARG:NH1	3:C:735:GLU:OE1	2.35	0.60
3:C:771:VAL:HG23	3:C:772:LEU:HD12	1.84	0.60
3:C:876:LEU:HD11	3:C:886:ILE:HD11	1.84	0.60
4:D:409:LYS:HA	4:D:414:ARG:HH11	1.65	0.60
4:D:622:MET:HE1	4:D:629:VAL:HG22	1.82	0.60
3:C:404:THR:HG23	3:C:406:GLN:H	1.65	0.60
3:C:728:LEU:HD22	3:C:906:ILE:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1165:ARG:NH2	4:D:1217:ALA:O	2.34	0.60
4:D:890:CYS:SG	4:D:892:THR:HG22	2.42	0.60
2:B:186:ARG:HG3	2:B:188:ASP:OD2	2.01	0.60
3:C:410:ASN:O	3:C:413:PRO:HD2	2.01	0.60
4:D:103:HIS:HB3	4:D:106:TYR:HD2	1.66	0.60
6:F:402:LEU:HD23	6:F:414:ARG:CZ	2.31	0.60
4:D:1225:ALA:HB1	4:D:1230:THR:HG23	1.84	0.60
2:A:50:ALA:HB3	2:A:168:TYR:CE1	2.37	0.60
3:C:1085:ASP:HB3	3:C:1110:GLU:N	2.16	0.60
2:A:63:PHE:HE1	3:C:741:ILE:HD13	1.66	0.60
3:C:796:LYS:HB3	3:C:826:THR:O	2.01	0.60
4:D:938:GLU:OE1	4:D:938:GLU:N	2.33	0.60
3:C:106:VAL:HG11	3:C:120:TYR:CE1	2.37	0.60
4:D:1140:GLN:HG3	4:D:1144:ARG:NE	2.17	0.60
4:D:143:MET:HG2	4:D:251:TYR:CE1	2.37	0.60
3:C:1036:SER:HB3	4:D:450:GLU:O	2.01	0.60
3:C:1053:GLN:HE21	3:C:1054:PHE:H	1.47	0.59
2:B:97:LEU:HB3	2:B:136:VAL:CG1	2.32	0.59
2:A:30:PHE:HZ	2:B:41:THR:HA	1.66	0.59
3:C:783:ILE:HG13	3:C:841:ILE:HD13	1.84	0.59
4:D:588:LEU:O	4:D:588:LEU:HD22	2.01	0.59
3:C:55:LEU:HD13	3:C:373:GLY:O	2.03	0.59
3:C:372:VAL:O	3:C:375:LEU:HD12	2.02	0.59
1:J:102:LEU:HA	1:J:105:ILE:CG2	2.32	0.59
2:A:30:PHE:CE2	2:B:40:ARG:HG3	2.37	0.59
3:C:732:LEU:HA	3:C:737:VAL:HG13	1.84	0.59
4:D:277:LEU:HD21	4:D:292:ALA:O	2.02	0.59
6:F:426:THR:O	6:F:430:ILE:HG13	2.03	0.59
2:A:48:GLY:O	2:A:142:ARG:HG3	2.01	0.59
2:B:32:TYR:CE2	2:B:178:VAL:HG21	2.38	0.59
3:C:872:ASP:N	3:C:872:ASP:OD1	2.34	0.59
3:C:1068:GLN:NE2	4:D:1249:LEU:HD13	2.16	0.59
4:D:128:ILE:HD11	4:D:234:LEU:CD1	2.31	0.59
3:C:476:PRO:O	4:D:856:ARG:NH2	2.36	0.59
2:A:18:ARG:HB2	2:A:196:VAL:O	2.02	0.59
2:A:33:THR:CG2	2:B:37:SER:HA	2.33	0.59
7:O:16:DT:H6	7:O:16:DT:H5'	1.67	0.59
4:D:1123:LEU:HA	4:D:1131:VAL:CG2	2.32	0.59
3:C:812:LEU:HD11	6:F:398:LEU:HD21	1.85	0.59
3:C:404:THR:OG1	3:C:405:PRO:HD2	2.02	0.59
5:E:41:LEU:HD23	5:E:50:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:714:ILE:O	4:D:729:THR:HG23	2.02	0.59
4:D:687:MET:CE	4:D:695:ILE:HD12	2.33	0.59
6:F:452:LEU:O	6:F:458:SER:HB3	2.01	0.59
2:A:210:SER:HB3	2:B:229:SER:HB3	1.84	0.58
3:C:589:GLU:OE1	3:C:589:GLU:N	2.25	0.58
3:C:77:LEU:H	3:C:77:LEU:HD22	1.68	0.58
2:A:36:ASN:HD21	2:A:40:ARG:HD2	1.68	0.58
3:C:170:LEU:HD11	3:C:367:ARG:CB	2.33	0.58
3:C:531:VAL:HG12	3:C:568:ASP:N	2.18	0.58
6:F:406:SER:HB3	6:F:409:GLU:CB	2.33	0.58
6:F:464:TYR:C	6:F:465:LEU:HD23	2.24	0.58
2:A:24:GLU:HB3	2:A:191:LYS:CD	2.33	0.58
3:C:888:LYS:HD3	3:C:890:LEU:CD1	2.34	0.58
1:J:42:VAL:HG13	4:D:74:ILE:HD12	1.85	0.58
6:F:272:LYS:HE3	7:O:25:DC:OP1	2.03	0.58
3:C:77:LEU:H	3:C:77:LEU:HD13	1.68	0.58
4:D:1166:VAL:O	4:D:1182:THR:N	2.37	0.58
4:D:400:LYS:HG3	6:F:362:ASP:HB3	1.85	0.58
2:A:24:GLU:HB3	2:A:191:LYS:HD3	1.86	0.58
2:A:66:VAL:HB	2:A:69:VAL:CG2	2.33	0.58
3:C:447:LEU:HD23	3:C:448:ALA:H	1.69	0.58
3:C:798:THR:O	3:C:823:VAL:HB	2.02	0.58
6:F:316:LYS:O	6:F:320:ILE:HG12	2.03	0.58
3:C:718:GLU:H	4:D:724:THR:HG22	1.68	0.58
2:A:11:GLU:OE2	2:B:225:LEU:HD22	2.04	0.58
3:C:1124:LEU:HD11	4:D:105:TRP:HZ3	1.67	0.58
3:C:931:ALA:HB1	3:C:961:SER:O	2.03	0.58
4:D:273:GLU:OE1	4:D:295:ARG:NH2	2.37	0.58
2:A:50:ALA:HB3	2:A:168:TYR:CD1	2.39	0.58
2:B:10:SER:HB3	2:B:22:VAL:CG2	2.33	0.58
1:J:81:HIS:ND1	6:F:195:LEU:HD11	2.19	0.58
3:C:1035:ARG:NH1	3:C:1054:PHE:O	2.27	0.58
3:C:107:LYS:HE2	3:C:123:PRO:HG3	1.86	0.58
3:C:480:PRO:O	3:C:485:ILE:HG12	2.04	0.58
2:A:12:GLU:O	2:A:19:SER:HB2	2.04	0.57
3:C:932:LYS:HG2	3:C:1018:TYR:CE2	2.39	0.57
3:C:154:LYS:HE2	3:C:664:ARG:NH2	2.18	0.57
4:D:28:VAL:HG21	4:D:46:LEU:HD23	1.86	0.57
3:C:968:PHE:HD2	4:D:845:VAL:HG22	1.65	0.57
1:J:81:HIS:CE1	6:F:195:LEU:HD11	2.39	0.57
7:O:15:DT:H1'	7:O:16:DT:H5''	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:811:LEU:HD22	6:F:419:LEU:HD11	1.84	0.57
3:C:789:ASP:HA	3:C:830:VAL:CG2	2.34	0.57
3:C:580:VAL:HG13	3:C:621:MET:HE2	1.86	0.57
4:D:865:ARG:HD2	4:D:1007:THR:O	2.03	0.57
6:F:405:LEU:HD11	6:F:452:LEU:HD11	1.85	0.57
3:C:613:GLU:O	3:C:705:ALA:HB1	2.04	0.57
3:C:1040:TYR:CD1	3:C:1047:PRO:HA	2.35	0.57
4:D:103:HIS:CE1	4:D:105:TRP:HB2	2.40	0.57
4:D:665:THR:HG22	4:D:684:ASN:HD22	1.69	0.57
4:D:948:ILE:O	4:D:952:LEU:HD13	2.04	0.57
6:F:399:GLN:O	6:F:403:GLU:HG2	2.04	0.57
2:A:42:LEU:HD23	2:A:211:ALA:HB2	1.86	0.57
3:C:945:ASP:OD1	3:C:945:ASP:N	2.38	0.57
4:D:1081:LEU:HD13	4:D:1113:MET:CE	2.33	0.57
5:E:86:GLU:OE2	5:E:94:ARG:NH1	2.37	0.57
3:C:1087:THR:HA	3:C:1090:ARG:NH1	2.18	0.57
3:C:34:LYS:C	3:C:35:LEU:HD12	2.24	0.57
3:C:899:PRO:HD2	3:C:992:MET:SD	2.44	0.57
3:C:952:GLU:HA	3:C:955:TYR:CD1	2.40	0.57
4:D:118:LEU:HB2	4:D:120:LEU:HD13	1.86	0.57
4:D:641:ARG:O	4:D:682:PHE:HB2	2.05	0.57
3:C:437:LEU:O	3:C:437:LEU:HD23	2.05	0.57
4:D:357:LEU:HD13	4:D:366:ILE:HG22	1.86	0.57
3:C:766:ASN:HB3	6:F:465:LEU:HD12	1.86	0.57
3:C:435:ASN:HD21	3:C:604:ARG:HA	1.69	0.57
4:D:17:ALA:O	4:D:21:ARG:HG3	2.04	0.57
1:J:57:ARG:NH1	4:D:24:SER:O	2.38	0.57
2:B:54:ILE:HG22	2:B:138:LEU:HB3	1.87	0.56
3:C:165:VAL:HG23	3:C:431:MET:HB2	1.86	0.56
3:C:768:SER:O	3:C:771:VAL:HG22	2.05	0.56
3:C:1074:TYR:CZ	4:D:1258:LEU:HD21	2.40	0.56
2:A:36:ASN:HB2	2:A:176:TYR:OH	2.04	0.56
3:C:749:ASP:O	3:C:796:LYS:NZ	2.24	0.56
3:C:852:LEU:N	3:C:852:LEU:HD12	2.20	0.56
2:B:34:LEU:HD11	2:B:192:LEU:HD22	1.87	0.56
2:B:46:ILE:C	2:B:144:ARG:HD2	2.26	0.56
3:C:123:PRO:HB3	3:C:144:PHE:CE1	2.35	0.56
3:C:937:ILE:H	3:C:937:ILE:HD12	1.69	0.56
4:D:376:GLU:OE2	6:F:165:SER:OG	2.20	0.56
4:D:415:GLN:O	4:D:419:GLY:N	2.37	0.56
1:J:27:ARG:N	1:J:46:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:79:ARG:NH2	7:O:25:DC:OP1	2.38	0.56
3:C:143:VAL:HG13	6:F:326:GLN:OE1	2.06	0.56
3:C:141:GLN:HB3	3:C:405:PRO:CG	2.35	0.56
4:D:596:THR:HG22	4:D:626:ALA:O	2.04	0.56
5:E:63:ASP:HB3	5:E:68:LEU:CB	2.35	0.56
6:F:180:ASN:OD1	6:F:182:GLU:HG2	2.05	0.56
3:C:170:LEU:HB3	3:C:447:LEU:O	2.06	0.56
3:C:433:GLN:O	3:C:669:SER:OG	2.18	0.56
3:C:799:PRO:HA	3:C:823:VAL:HG11	1.86	0.56
4:D:269:ASP:HB3	4:D:272:ALA:HB3	1.86	0.56
4:D:432:VAL:HG22	4:D:434:PRO:HD3	1.86	0.56
2:B:64:THR:O	2:B:73:VAL:HG23	2.05	0.56
4:D:956:ILE:HD12	4:D:956:ILE:O	2.05	0.56
4:D:581:MET:HE2	4:D:716:LYS:HA	1.88	0.56
3:C:842:ARG:O	3:C:860:VAL:HA	2.05	0.56
6:F:180:ASN:OD1	6:F:183:GLU:HG3	2.06	0.56
1:J:70:PRO:O	1:J:72:PRO:HD3	2.05	0.56
3:C:51:SER:HB2	3:C:371:THR:HB	1.87	0.56
3:C:870:ILE:HD11	3:C:886:ILE:HD11	1.88	0.56
4:D:386:ARG:NH1	4:D:1231:THR:HG21	2.21	0.56
4:D:277:LEU:HD22	4:D:296:LEU:HB2	1.86	0.56
3:C:901:GLY:O	3:C:903:PRO:HD3	2.06	0.56
4:D:129:ILE:HG22	4:D:261:ILE:HG13	1.88	0.56
4:D:282:ARG:O	4:D:283:SER:OG	2.16	0.56
5:E:98:GLY:O	5:E:100:LEU:HD12	2.06	0.56
2:B:170:PRO:HA	2:B:199:LYS:HD2	1.87	0.55
3:C:985:PRO:HB2	3:C:989:GLY:HA2	1.88	0.55
3:C:1103:ILE:HD12	4:D:548:SER:CA	2.36	0.55
4:D:567:SER:HB2	4:D:574:LEU:HD13	1.88	0.55
2:A:157:ALA:O	2:A:161:ARG:HD3	2.06	0.55
4:D:459:ARG:NE	4:D:489:GLU:OE2	2.39	0.55
4:D:781:THR:O	4:D:784:VAL:HG12	2.06	0.55
6:F:405:LEU:HD23	6:F:457:ARG:HH12	1.70	0.55
2:A:40:ARG:HH11	2:B:33:THR:HG22	1.70	0.55
2:A:63:PHE:CE1	3:C:741:ILE:HD13	2.41	0.55
3:C:167:VAL:HG11	9:C:1201:SRN:H29	1.88	0.55
3:C:44:LEU:O	3:C:444:ARG:HD2	2.06	0.55
3:C:792:ILE:HD12	3:C:792:ILE:H	1.70	0.55
4:D:1081:LEU:HD13	4:D:1113:MET:HE3	1.87	0.55
2:A:30:PHE:CD2	2:B:40:ARG:HG3	2.42	0.55
4:D:183:GLU:O	4:D:187:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:453:LYS:HB3	4:D:454:PRO:HD3	1.89	0.55
4:D:527:LEU:HD21	4:D:581:MET:CE	2.36	0.55
2:A:48:GLY:CA	2:A:49:ALA:CB	2.81	0.55
2:B:104:VAL:HG22	2:B:106:THR:HG23	1.87	0.55
2:B:29:GLY:HA2	2:B:190:ASP:OD2	2.06	0.55
3:C:507:TYR:CD1	3:C:522:LEU:HB2	2.41	0.55
4:D:1132:GLN:HG3	4:D:1163:LEU:HD12	1.88	0.55
2:B:30:PHE:HA	2:B:33:THR:CG2	2.36	0.55
2:B:71:GLU:OE2	2:B:127:THR:HG22	2.07	0.55
4:D:48:CYS:HB3	4:D:51:ILE:HD11	1.89	0.55
4:D:581:MET:HE3	4:D:716:LYS:HB2	1.89	0.55
7:O:13:DT:H2''	7:O:14:DG:C8	2.41	0.55
2:A:66:VAL:HB	2:A:69:VAL:HG21	1.88	0.55
2:B:56:ILE:HG12	2:B:136:VAL:HG23	1.89	0.55
8:P:11:DA:H2''	8:P:12:DA:H5'	1.89	0.55
3:C:751:ARG:CG	3:C:856:VAL:HG22	2.37	0.55
4:D:865:ARG:HD3	4:D:1009:LEU:O	2.06	0.55
4:D:647:GLU:O	4:D:650:LEU:N	2.39	0.55
6:F:402:LEU:HD23	6:F:414:ARG:NH2	2.22	0.55
2:A:27:GLU:O	2:A:30:PHE:HB2	2.06	0.55
3:C:764:ILE:HB	3:C:767:VAL:CG2	2.37	0.55
4:D:1265:ILE:CG2	4:D:1267:ARG:HG2	2.37	0.55
4:D:339:ASP:OD2	4:D:397:ARG:NH2	2.39	0.55
4:D:460:LEU:HD11	4:D:472:ALA:CB	2.36	0.55
4:D:590:THR:CG2	4:D:630:ARG:HE	2.20	0.55
9:C:1201:SRN:C12	9:C:1201:SRN:C9	2.60	0.54
2:B:74:THR:HG21	4:D:611:VAL:HG11	1.89	0.54
4:D:613:SER:N	4:D:617:GLU:OE1	2.34	0.54
4:D:647:GLU:HG3	4:D:655:TRP:HD1	1.71	0.54
2:B:33:THR:OG1	2:B:34:LEU:N	2.40	0.54
3:C:635:ALA:CB	3:C:693:ILE:HD11	2.36	0.54
4:D:1056:LEU:HD22	4:D:1063:PHE:HE1	1.73	0.54
4:D:211:ARG:NH1	4:D:214:ARG:HH22	2.05	0.54
1:J:54:TRP:CH2	4:D:79:GLY:HA2	2.42	0.54
2:B:212:GLY:O	2:B:216:VAL:HG12	2.07	0.54
6:F:364:THR:CG2	6:F:369:GLY:HA2	2.38	0.54
3:C:894:ASP:HB2	3:C:1005:ARG:CG	2.38	0.54
6:F:406:SER:HB3	6:F:409:GLU:HB2	1.89	0.54
1:J:91:VAL:HG22	1:J:92:GLU:OE1	2.08	0.54
4:D:1056:LEU:CD2	4:D:1065:ILE:HG12	2.38	0.54
5:E:29:PRO:HB2	5:E:34:ASN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:439:GLU:OE1	8:P:22:DC:N4	2.37	0.54
4:D:1276:THR:HG22	5:E:102:GLU:HG3	1.88	0.54
1:J:81:HIS:CG	6:F:195:LEU:HD11	2.42	0.54
8:P:5:DC:H2"	8:P:6:DA:C8	2.43	0.54
4:D:599:TYR:HA	4:D:610:GLY:HA3	1.88	0.54
6:F:338:ALA:HB1	6:F:343:ILE:O	2.07	0.54
1:J:102:LEU:HA	1:J:105:ILE:HG22	1.90	0.54
3:C:1070:TYR:CD1	4:D:559:MET:HG2	2.43	0.54
3:C:826:THR:OG1	3:C:826:THR:O	2.21	0.54
4:D:263:LYS:HD2	4:D:266:GLU:OE1	2.08	0.54
4:D:401:SER:OG	4:D:404:ASP:OD2	2.13	0.54
4:D:1118:ASP:HB3	4:D:1121:GLU:HB2	1.90	0.53
4:D:765:ASN:ND2	4:D:765:ASN:O	2.41	0.53
2:B:97:LEU:HD13	2:B:110:ILE:N	2.23	0.53
3:C:992:MET:HA	3:C:992:MET:CE	2.38	0.53
7:O:15:DT:H2"	7:O:16:DT:OP2	2.09	0.53
2:A:14:VAL:HG12	2:A:19:SER:HA	1.91	0.53
2:A:40:ARG:HB3	2:A:40:ARG:NH1	2.18	0.53
4:D:1151:HIS:ND1	4:D:1153:LYS:HG2	2.23	0.53
4:D:487:LEU:O	4:D:491:ILE:HD13	2.07	0.53
2:A:70:LYS:HB3	2:A:71:GLU:OE1	2.09	0.53
2:B:43:LEU:HA	2:B:171:VAL:CG2	2.38	0.53
3:C:729:SER:HA	3:C:895:MET:HE1	1.90	0.53
4:D:289:LYS:O	4:D:293:LEU:N	2.39	0.53
4:D:527:LEU:HD21	4:D:581:MET:HE1	1.89	0.53
5:E:57:ARG:HD3	5:E:57:ARG:O	2.07	0.53
4:D:417:LEU:HD21	4:D:1254:ILE:CG2	2.38	0.53
3:C:1100:GLY:HA3	4:D:458:LYS:HE3	1.91	0.53
3:C:496:ARG:HH22	3:C:521:TYR:CB	2.21	0.53
2:A:105:VAL:HG23	2:A:128:LEU:HD13	1.90	0.53
3:C:449:LEU:HD13	3:C:450:GLY:N	2.24	0.53
3:C:464:ARG:NH1	3:C:485:ILE:O	2.39	0.53
4:D:665:THR:HG22	4:D:684:ASN:ND2	2.23	0.53
6:F:253:MET:HE3	6:F:300:GLN:HB2	1.90	0.53
1:J:98:LEU:HD21	6:F:219:MET:CE	2.38	0.53
2:A:24:GLU:CD	2:A:191:LYS:HD3	2.29	0.53
2:B:95:MET:HE2	2:B:138:LEU:HD13	1.90	0.53
3:C:103:PHE:HE1	3:C:148:PHE:HB3	1.73	0.53
3:C:839:ILE:CD1	3:C:865:ALA:HB2	2.38	0.53
2:A:42:LEU:O	2:A:46:ILE:HG12	2.07	0.53
2:B:22:VAL:HG12	2:B:193:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLU:HB3	2:B:92:PRO:HD2	1.90	0.53
3:C:144:PHE:N	6:F:326:GLN:OE1	2.40	0.53
3:C:810:ARG:O	3:C:813:ARG:HB2	2.09	0.53
3:C:937:ILE:HD11	3:C:955:TYR:CA	2.38	0.53
4:D:1049:ASP:HB2	4:D:1078:TYR:OH	2.08	0.53
4:D:430:ILE:HG21	4:D:541:MET:SD	2.48	0.53
4:D:49:GLU:CG	4:D:88:ARG:HH21	2.21	0.53
6:F:234:LEU:CD2	6:F:270:VAL:HG21	2.38	0.53
1:J:101:ARG:O	1:J:105:ILE:HG22	2.08	0.53
2:A:197:GLU:OE1	3:C:987:ARG:NH2	2.35	0.53
2:A:33:THR:HG21	2:B:37:SER:HA	1.91	0.53
2:B:71:GLU:CD	2:B:127:THR:HG22	2.28	0.53
2:B:95:MET:HB2	2:B:138:LEU:HD11	1.90	0.53
3:C:1052:ALA:O	3:C:1053:GLN:HB2	2.08	0.53
3:C:1072:ALA:HB1	4:D:554:GLU:OE2	2.09	0.53
4:D:978:TYR:CE1	4:D:1153:LYS:HD3	2.44	0.53
4:D:900:LEU:HB3	4:D:957:THR:O	2.09	0.53
4:D:901:ALA:N	4:D:912:ASP:HB2	2.23	0.53
4:D:923:THR:OG1	4:D:962:ARG:HB2	2.09	0.53
3:C:815:ILE:HG12	6:F:452:LEU:HD23	1.90	0.53
2:B:85:VAL:HG23	2:B:117:THR:C	2.29	0.52
4:D:622:MET:HE1	4:D:629:VAL:HG13	1.91	0.52
2:A:27:GLU:HB2	2:A:30:PHE:CD1	2.44	0.52
3:C:1053:GLN:NE2	3:C:1054:PHE:H	2.07	0.52
3:C:404:THR:HG23	3:C:406:GLN:N	2.25	0.52
3:C:570:MET:SD	3:C:571:ASP:N	2.83	0.52
4:D:237:ASP:O	4:D:239:VAL:N	2.42	0.52
2:A:124:HIS:NE2	2:A:127:THR:HG22	2.23	0.52
2:B:34:LEU:HD12	2:B:35:GLY:N	2.23	0.52
4:D:1071:ASP:HB2	4:D:1072:GLY:CA	2.40	0.52
6:F:463:ASP:OD1	6:F:463:ASP:N	2.43	0.52
2:A:80:LEU:HD21	2:A:125:ILE:HD13	1.92	0.52
2:B:42:LEU:O	2:B:171:VAL:HG21	2.10	0.52
3:C:479:THR:H	3:C:597:LEU:HD21	1.73	0.52
2:B:170:PRO:O	2:B:199:LYS:HG2	2.10	0.52
2:B:41:THR:O	2:B:45:SER:HB3	2.10	0.52
3:C:388:GLU:O	3:C:391:VAL:HG22	2.09	0.52
3:C:433:GLN:HG3	3:C:669:SER:OG	2.10	0.52
3:C:584:MET:HA	3:C:619:THR:CG2	2.37	0.52
4:D:1229:GLU:OE2	4:D:1231:THR:HB	2.10	0.52
4:D:330:LEU:HD23	4:D:336:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ARG:HA	2:B:134:LEU:O	2.09	0.52
3:C:641:ILE:HG21	3:C:644:VAL:CG1	2.37	0.52
4:D:218:ARG:O	4:D:222:ILE:HG13	2.09	0.52
4:D:24:SER:HB2	4:D:94:HIS:HB3	1.92	0.52
4:D:405:LEU:HD12	4:D:405:LEU:O	2.10	0.52
2:A:190:ASP:OD1	2:A:190:ASP:N	2.42	0.52
2:A:9:LEU:HD13	2:A:23:ILE:CG1	2.39	0.52
3:C:965:THR:O	3:C:965:THR:OG1	2.22	0.52
4:D:1057:GLU:HB2	4:D:1064:LYS:HB3	1.90	0.52
6:F:310:MET:HA	6:F:313:VAL:HG12	1.90	0.52
6:F:440:ARG:O	6:F:444:ILE:HG13	2.10	0.52
2:B:97:LEU:HB2	2:B:110:ILE:CG1	2.40	0.52
2:A:24:GLU:OE1	2:A:191:LYS:HD3	2.09	0.52
2:B:22:VAL:HG12	2:B:193:ILE:CD1	2.40	0.52
2:A:30:PHE:CZ	2:B:41:THR:HA	2.45	0.52
3:C:578:VAL:HG13	3:C:582:THR:CB	2.38	0.52
3:C:84:LEU:HD13	3:C:84:LEU:O	2.10	0.52
3:C:751:ARG:HG2	3:C:856:VAL:HA	1.91	0.52
4:D:248:TYR:HA	4:D:251:TYR:CD2	2.45	0.52
4:D:901:ALA:HA	4:D:912:ASP:H	1.73	0.52
3:C:120:TYR:HB2	3:C:158:ILE:HB	1.92	0.52
4:D:170:LEU:HD12	4:D:209:ARG:NH2	2.25	0.52
6:F:253:MET:CE	6:F:300:GLN:HB2	2.40	0.52
2:A:100:GLN:OE1	2:A:101:GLY:N	2.43	0.51
2:A:113:PRO:HD2	2:A:116:VAL:HG21	1.92	0.51
3:C:1103:ILE:HD12	4:D:548:SER:N	2.26	0.51
3:C:987:ARG:O	3:C:988:ASP:CB	2.58	0.51
4:D:277:LEU:HD21	4:D:292:ALA:HB1	1.92	0.51
4:D:88:ARG:O	4:D:322:PRO:HD2	2.10	0.51
6:F:324:LEU:HD23	6:F:328:LEU:HD13	1.92	0.51
1:J:108:LYS:HD2	1:J:108:LYS:O	2.10	0.51
2:A:42:LEU:O	2:A:171:VAL:HG11	2.11	0.51
2:B:95:MET:CE	2:B:138:LEU:HD13	2.41	0.51
4:D:12:ILE:HG12	4:D:1221:TRP:CZ2	2.44	0.51
4:D:137:THR:HG23	4:D:253:THR:OG1	2.11	0.51
2:A:157:ALA:O	2:A:158:GLU:HB2	2.11	0.51
2:A:2:LEU:N	2:A:2:LEU:HD12	2.24	0.51
2:B:76:ILE:HA	2:B:79:ASN:HD22	1.75	0.51
3:C:31:SER:HA	3:C:964:ALA:O	2.11	0.51
5:E:37:ILE:O	5:E:41:LEU:HG	2.10	0.51
3:C:1086:ASP:O	3:C:1090:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:840:GLY:C	3:C:841:ILE:HD12	2.30	0.51
4:D:590:THR:HG23	4:D:630:ARG:HE	1.74	0.51
4:D:720:PHE:O	4:D:724:THR:HG23	2.10	0.51
4:D:930:ASP:OD2	4:D:954:ALA:HB1	2.10	0.51
3:C:117:ASP:HA	3:C:161:GLY:HA3	1.92	0.51
3:C:839:ILE:HD11	3:C:865:ALA:HB2	1.91	0.51
1:J:28:GLN:O	1:J:43:PRO:HA	2.11	0.51
4:D:962:ARG:NH1	4:D:977:CYS:SG	2.84	0.51
2:A:88:ASP:N	2:A:88:ASP:OD1	2.44	0.51
3:C:371:THR:O	3:C:375:LEU:HG	2.11	0.51
4:D:268:PHE:CE1	4:D:273:GLU:HG3	2.46	0.51
4:D:277:LEU:CD2	4:D:292:ALA:HB1	2.41	0.51
3:C:1128:VAL:HG11	3:C:1138:MET:HE1	1.91	0.51
3:C:44:LEU:HD13	3:C:440:LEU:HD21	1.93	0.51
4:D:404:ASP:N	4:D:404:ASP:OD2	2.38	0.51
3:C:1026:HIS:ND1	3:C:1031:LYS:HE3	2.26	0.50
3:C:372:VAL:HA	3:C:375:LEU:CD1	2.34	0.50
3:C:467:HIS:CD2	3:C:469:SER:H	2.18	0.50
3:C:613:GLU:HB3	3:C:708:LYS:HD3	1.93	0.50
3:C:718:GLU:H	4:D:724:THR:HG21	1.77	0.50
4:D:1034:GLU:OE2	4:D:1042:ARG:HG2	2.10	0.50
4:D:1265:ILE:HG21	4:D:1267:ARG:HG2	1.93	0.50
4:D:190:LYS:HB2	4:D:193:VAL:HB	1.92	0.50
3:C:443:LYS:O	3:C:444:ARG:HB2	2.11	0.50
3:C:578:VAL:HG13	3:C:582:THR:CG2	2.41	0.50
3:C:780:ILE:HD12	3:C:781:VAL:O	2.11	0.50
4:D:7:PHE:O	4:D:1246:LEU:HD12	2.12	0.50
4:D:28:VAL:HG11	4:D:319:VAL:HG21	1.92	0.50
4:D:486:VAL:O	4:D:490:VAL:HG22	2.12	0.50
4:D:587:TYR:O	4:D:590:THR:HG22	2.11	0.50
2:A:28:PRO:HA	2:A:190:ASP:OD1	2.11	0.50
2:B:34:LEU:CD1	2:B:192:LEU:HD22	2.41	0.50
3:C:24:PRO:HG2	3:C:689:ALA:O	2.11	0.50
4:D:1275:PRO:HG3	5:E:76:VAL:CG1	2.40	0.50
4:D:231:PRO:O	4:D:232:LYS:HB2	2.11	0.50
4:D:76:GLU:H	4:D:76:GLU:CD	2.14	0.50
4:D:922:ARG:HD2	4:D:961:VAL:HG11	1.94	0.50
6:F:251:ARG:HB2	6:F:297:MET:HE3	1.93	0.50
6:F:373:LEU:HD23	6:F:373:LEU:O	2.11	0.50
2:B:102:PRO:CG	2:B:130:ASP:HA	2.22	0.50
3:C:447:LEU:HD12	9:C:1201:SRN:H301	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:619:THR:N	3:C:622:GLU:OE2	2.41	0.50
4:D:6:PHE:CD1	4:D:1257:LYS:HE3	2.47	0.50
2:A:138:LEU:HD12	2:A:138:LEU:N	2.26	0.50
3:C:890:LEU:H	3:C:890:LEU:HD22	1.77	0.50
4:D:868:ASP:CB	4:D:1029:LEU:HD21	2.41	0.50
4:D:395:GLY:N	13:D:2102:HOH:O	2.22	0.50
4:D:58:TRP:HA	4:D:82:VAL:HG23	1.93	0.50
1:J:98:LEU:HD21	6:F:219:MET:HE2	1.94	0.50
3:C:1137:GLU:OE1	3:C:1139:ARG:NE	2.44	0.50
3:C:492:SER:HB3	3:C:576:GLN:O	2.11	0.50
3:C:885:VAL:HG13	4:D:538:GLY:H	1.77	0.50
4:D:565:ILE:HG23	4:D:575:ALA:HB3	1.93	0.50
4:D:647:GLU:OE2	4:D:651:PHE:HB2	2.11	0.50
4:D:924:LEU:HD21	4:D:943:LEU:CD1	2.37	0.50
3:C:532:VAL:O	3:C:552:VAL:HB	2.11	0.50
4:D:443:LEU:HD22	4:D:514:PRO:HB3	1.92	0.50
4:D:527:LEU:CD1	4:D:712:VAL:HG12	2.41	0.50
4:D:527:LEU:HD22	4:D:575:ALA:O	2.11	0.50
7:O:9:DA:H2"	7:O:10:DA:C8	2.47	0.50
3:C:479:THR:CG2	3:C:597:LEU:HD11	2.42	0.50
4:D:461:VAL:HG23	4:D:472:ALA:HB2	1.94	0.50
4:D:686:GLN:O	4:D:686:GLN:HG3	2.11	0.50
3:C:141:GLN:HB3	3:C:405:PRO:HG2	1.93	0.50
3:C:727:ILE:CG1	3:C:907:ILE:HB	2.42	0.50
4:D:1071:ASP:HB2	4:D:1072:GLY:C	2.31	0.50
4:D:695:ILE:HG22	4:D:699:LEU:HD23	1.92	0.50
4:D:699:LEU:HD12	4:D:708:VAL:HG22	1.93	0.50
4:D:474:ARG:HH22	4:D:480:ARG:HD3	1.77	0.49
5:E:39:GLU:OE1	5:E:97:HIS:NE2	2.29	0.49
5:E:80:VAL:HG23	5:E:95:GLU:HG2	1.95	0.49
6:F:406:SER:OG	12:F:504:SO4:O1	2.16	0.49
2:B:72:ASP:OD1	2:B:72:ASP:N	2.43	0.49
3:C:758:GLU:CB	3:C:798:THR:HG22	2.42	0.49
4:D:26:GLY:HA3	4:D:51:ILE:CG2	2.41	0.49
6:F:423:GLN:O	6:F:425:ARG:NE	2.44	0.49
3:C:1059:PHE:HZ	3:C:1067:MET:HE3	1.77	0.49
3:C:909:ASN:OD1	3:C:910:THR:N	2.40	0.49
3:C:1015:THR:OG1	4:D:731:SER:OG	2.30	0.49
4:D:884:ILE:HG22	4:D:993:ALA:HA	1.95	0.49
5:E:92:ALA:O	5:E:96:ILE:HG13	2.12	0.49
2:A:112:PRO:HB2	2:A:116:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:72:ASP:OD1	2:A:74:THR:HG22	2.12	0.49
2:A:9:LEU:HD23	2:B:221:LEU:C	2.33	0.49
2:B:54:ILE:HG22	2:B:138:LEU:CB	2.42	0.49
3:C:1128:VAL:HA	4:D:10:LEU:HD12	1.94	0.49
3:C:141:GLN:HB3	3:C:405:PRO:HB2	1.93	0.49
3:C:508:ARG:CD	3:C:570:MET:HG3	2.40	0.49
3:C:572:VAL:HG22	3:C:576:GLN:CD	2.32	0.49
3:C:874:ASP:OD1	3:C:1028:VAL:HG22	2.13	0.49
3:C:943:VAL:HG11	3:C:955:TYR:HE2	1.77	0.49
4:D:1034:GLU:OE2	4:D:1042:ARG:N	2.36	0.49
4:D:708:VAL:O	4:D:712:VAL:HG23	2.12	0.49
1:J:89:ARG:NH2	6:F:276:THR:HG23	2.28	0.49
3:C:445:ARG:HA	3:C:490:SER:HA	1.95	0.49
3:C:533:ALA:HA	3:C:552:VAL:CG1	2.28	0.49
3:C:870:ILE:HD11	3:C:876:LEU:HD11	1.93	0.49
4:D:706:ILE:HD12	5:E:36:PRO:CB	2.28	0.49
2:A:26:LEU:HD22	2:B:218:LEU:CD1	2.41	0.49
3:C:51:SER:CB	3:C:373:GLY:H	2.26	0.49
3:C:572:VAL:O	3:C:573:SER:HB3	2.12	0.49
3:C:729:SER:HA	3:C:895:MET:CE	2.42	0.49
5:E:29:PRO:CB	5:E:34:ASN:HB2	2.43	0.49
2:A:152:ASN:HB3	2:A:157:ALA:HB3	1.94	0.49
2:A:146:TYR:HD2	2:A:167:ILE:HG12	1.78	0.49
3:C:636:ASP:N	3:C:636:ASP:OD1	2.46	0.49
3:C:926:HIS:CD2	4:D:732:MET:HG3	2.48	0.49
2:A:43:LEU:HD11	2:A:174:VAL:HB	1.95	0.49
4:D:636:ARG:HD3	4:D:660:ALA:HB1	1.95	0.49
1:J:82:TRP:CZ2	6:F:199:GLN:HG2	2.48	0.49
4:D:1034:GLU:OE2	4:D:1041:PRO:HA	2.12	0.49
4:D:1123:LEU:HD22	4:D:1208:LEU:HB2	1.94	0.49
4:D:1220:SER:OG	4:D:1244:ASP:OD2	2.14	0.49
4:D:691:VAL:O	4:D:695:ILE:HG13	2.13	0.49
4:D:839:PHE:HD1	4:D:843:LEU:HD13	1.78	0.49
4:D:1132:GLN:CG	4:D:1163:LEU:HD12	2.43	0.49
4:D:1184:ARG:HH11	4:D:1187:PHE:CB	2.25	0.49
4:D:980:ARG:HD3	4:D:985:GLY:O	2.12	0.49
2:A:158:GLU:HA	2:A:158:GLU:OE1	2.13	0.48
3:C:144:PHE:O	3:C:411:ILE:HD13	2.13	0.48
3:C:899:PRO:HB2	3:C:992:MET:HE1	1.95	0.48
4:D:430:ILE:HG21	4:D:541:MET:HG3	1.95	0.48
4:D:588:LEU:HG	4:D:722:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:LYS:HG3	4:D:79:GLY:O	2.13	0.48
4:D:924:LEU:HD22	4:D:959:VAL:CG1	2.43	0.48
6:F:310:MET:O	6:F:314:ILE:HG13	2.13	0.48
3:C:21:ASN:O	3:C:22:SER:OG	2.22	0.48
4:D:951:LEU:C	4:D:956:ILE:HD11	2.33	0.48
6:F:348:VAL:O	6:F:352:GLN:HG3	2.13	0.48
2:B:97:LEU:HB2	2:B:110:ILE:CB	2.44	0.48
3:C:421:PHE:O	3:C:425:SER:HB3	2.14	0.48
3:C:61:TRP:CH2	3:C:73:PRO:HB2	2.49	0.48
4:D:1152:ASP:O	4:D:1156:GLU:HG3	2.14	0.48
4:D:656:LYS:CB	4:D:659:ASP:HB2	2.44	0.48
4:D:1275:PRO:CG	5:E:76:VAL:HG11	2.40	0.48
7:O:12:DG:O6	8:P:14:DA:N6	2.47	0.48
2:B:32:TYR:CZ	2:B:178:VAL:HG21	2.49	0.48
5:E:95:GLU:HB3	5:E:101:LEU:CD2	2.43	0.48
6:F:180:ASN:ND2	6:F:183:GLU:OE2	2.45	0.48
4:D:369:ASN:ND2	6:F:260:GLN:OE1	2.43	0.48
2:B:146:TYR:HB2	4:D:620:MET:CE	2.44	0.48
3:C:53:GLU:HG2	3:C:58:SER:HB3	1.96	0.48
3:C:641:ILE:CG2	3:C:644:VAL:HG13	2.38	0.48
4:D:177:LEU:O	4:D:177:LEU:HD23	2.12	0.48
4:D:631:ALA:O	4:D:666:THR:HG22	2.13	0.48
4:D:700:ALA:HA	4:D:708:VAL:HG21	1.96	0.48
1:J:84:MET:HE3	6:F:272:LYS:HE2	1.95	0.48
8:P:11:DA:H2'	8:P:12:DA:C8	2.48	0.48
2:B:8:THR:O	2:B:23:ILE:HA	2.14	0.48
3:C:77:LEU:N	3:C:77:LEU:HD13	2.28	0.48
2:B:102:PRO:HG3	2:B:130:ASP:CA	2.21	0.48
2:B:56:ILE:HD13	2:B:136:VAL:HA	1.96	0.48
3:C:894:ASP:HB2	3:C:1005:ARG:HG3	1.94	0.48
3:C:148:PHE:HD2	3:C:150:MET:HE1	1.77	0.48
3:C:696:GLY:N	3:C:699:THR:OG1	2.46	0.48
3:C:77:LEU:N	3:C:77:LEU:HD22	2.28	0.48
3:C:811:LEU:O	3:C:815:ILE:HG13	2.13	0.48
5:E:49:ALA:O	5:E:53:TYR:HB2	2.14	0.48
2:B:112:PRO:HB2	2:B:116:VAL:HG23	1.95	0.48
3:C:601:ASN:O	3:C:605:GLN:HG3	2.14	0.48
4:D:1029:LEU:N	4:D:1030:PRO:HD2	2.29	0.48
4:D:673:ASN:HA	4:D:676:LEU:HD13	1.95	0.48
3:C:144:PHE:CD2	6:F:329:GLY:HA2	2.48	0.48
3:C:728:LEU:HB3	3:C:732:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:590:THR:HG21	4:D:630:ARG:HH21	1.79	0.48
6:F:416:ARG:HA	6:F:430:ILE:HD11	1.94	0.48
2:A:27:GLU:HG3	2:B:44:SER:O	2.14	0.47
3:C:434:ASN:O	3:C:608:PRO:HD3	2.14	0.47
3:C:447:LEU:HD23	3:C:448:ALA:N	2.29	0.47
3:C:717:TRP:H	3:C:721:ASN:ND2	2.03	0.47
4:D:102:THR:OG1	4:D:129:ILE:HD12	2.14	0.47
4:D:726:SER:OG	4:D:728:VAL:HG23	2.13	0.47
6:F:404:THR:HG23	6:F:457:ARG:NH1	2.29	0.47
1:J:28:GLN:OE1	1:J:50:ILE:HD11	2.14	0.47
2:A:18:ARG:HA	2:A:204:PRO:HG3	1.96	0.47
2:B:180:ALA:HA	2:B:189:PHE:O	2.14	0.47
3:C:635:ALA:CA	3:C:693:ILE:HD11	2.44	0.47
3:C:753:THR:OG1	3:C:756:GLY:O	2.22	0.47
4:D:914:HIS:CG	4:D:1144:ARG:HH21	2.33	0.47
1:J:54:TRP:HH2	4:D:79:GLY:HA2	1.78	0.47
4:D:848:TYR:O	4:D:852:THR:HG23	2.13	0.47
2:A:150:VAL:O	2:A:150:VAL:HG13	2.13	0.47
4:D:321:PRO:HD2	4:D:324:LEU:HD12	1.97	0.47
4:D:550:GLU:OE1	4:D:550:GLU:N	2.43	0.47
4:D:588:LEU:HD22	4:D:668:GLY:HA3	1.97	0.47
6:F:268:ARG:HD3	6:F:288:TRP:CZ3	2.49	0.47
1:J:69:VAL:N	1:J:70:PRO:HD2	2.30	0.47
2:A:71:GLU:OE2	2:A:126:ALA:HA	2.14	0.47
3:C:722:TYR:CE2	3:C:723:GLU:HG3	2.50	0.47
2:A:3:ILE:O	2:A:3:ILE:HG23	2.14	0.47
2:B:174:VAL:HA	2:B:195:ASP:O	2.14	0.47
3:C:602:MET:CE	3:C:1024:LEU:HD21	2.44	0.47
3:C:939:VAL:HG11	3:C:943:VAL:HG12	1.96	0.47
4:D:936:ILE:O	4:D:937:ILE:HB	2.15	0.47
6:F:430:ILE:O	6:F:433:VAL:HG12	2.14	0.47
2:B:107:ALA:HB2	2:B:125:ILE:CD1	2.42	0.47
3:C:505:THR:CG2	3:C:506:PRO:HD2	2.44	0.47
4:D:430:ILE:HG21	4:D:541:MET:CG	2.44	0.47
1:J:89:ARG:NH2	6:F:274:ASP:OD1	2.37	0.47
2:B:125:ILE:N	2:B:125:ILE:HD12	2.29	0.47
3:C:1048:LEU:HD12	3:C:1049:GLY:N	2.30	0.47
3:C:144:PHE:CG	6:F:329:GLY:HA2	2.50	0.47
5:E:80:VAL:O	5:E:82:PRO:HD3	2.14	0.47
6:F:180:ASN:CG	6:F:183:GLU:HG3	2.34	0.47
6:F:204:LEU:HD13	6:F:211:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:MET:O	2:A:1:MET:HG2	2.15	0.47
3:C:167:VAL:HG13	3:C:445:ARG:O	2.15	0.47
3:C:758:GLU:CB	3:C:796:LYS:HE3	2.44	0.47
4:D:1071:ASP:H	4:D:1072:GLY:HA2	1.79	0.47
5:E:81:GLU:OE1	5:E:81:GLU:HA	2.14	0.47
5:E:85:GLN:NE2	5:E:85:GLN:H	2.12	0.47
6:F:322:ARG:HB2	6:F:322:ARG:NH2	2.30	0.47
2:B:59:VAL:HG23	2:B:59:VAL:O	2.15	0.47
3:C:35:LEU:N	3:C:35:LEU:HD12	2.30	0.47
4:D:661:TRP:HZ3	4:D:663:ALA:HB2	1.79	0.47
4:D:901:ALA:H	4:D:912:ASP:CB	2.26	0.47
6:F:397:GLN:O	6:F:401:VAL:HG23	2.14	0.47
3:C:1002:PHE:HA	3:C:1009:PRO:HA	1.97	0.47
3:C:892:VAL:CG2	3:C:903:PRO:HG2	2.45	0.47
3:C:890:LEU:HB2	3:C:895:MET:HE2	1.97	0.47
3:C:906:ILE:HD13	3:C:1021:ILE:HD13	1.97	0.47
3:C:913:VAL:HB	3:C:914:PRO:HD2	1.97	0.47
4:D:28:VAL:CG1	4:D:319:VAL:HG21	2.45	0.47
4:D:500:ARG:HB2	4:D:541:MET:HG2	1.96	0.47
6:F:405:LEU:HD23	6:F:457:ARG:NH1	2.29	0.47
2:A:27:GLU:OE1	2:A:27:GLU:HA	2.14	0.47
3:C:1110:GLU:OE2	4:D:89:ARG:HD3	2.15	0.47
3:C:591:ASP:OD2	3:C:880:HIS:ND1	2.41	0.47
4:D:473:LYS:HE2	4:D:477:GLU:OE2	2.14	0.47
4:D:644:THR:HG22	4:D:655:TRP:CZ2	2.50	0.47
4:D:588:LEU:HD21	4:D:671:MET:HE3	1.97	0.47
4:D:675:LEU:HD21	4:D:718:ALA:HB2	1.97	0.47
1:J:64:LEU:HD22	1:J:66:GLU:O	2.14	0.47
2:B:56:ILE:HG22	2:B:59:VAL:CG2	2.37	0.46
3:C:1128:VAL:O	3:C:1128:VAL:HG13	2.14	0.46
3:C:609:LEU:HD12	3:C:708:LYS:HE3	1.96	0.46
4:D:1119:PRO:HA	4:D:1122:VAL:HG12	1.97	0.46
4:D:48:CYS:HB3	4:D:51:ILE:CG1	2.44	0.46
4:D:585:LEU:HD13	4:D:672:PHE:HE1	1.79	0.46
4:D:582:VAL:HG12	4:D:804:SER:HB2	1.95	0.46
6:F:409:GLU:O	6:F:413:VAL:HG23	2.15	0.46
1:J:28:GLN:CG	1:J:46:ASP:HA	2.32	0.46
3:C:671:HIS:HB3	3:C:1025:HIS:HE1	1.81	0.46
3:C:608:PRO:HA	3:C:698:CYS:SG	2.56	0.46
4:D:1129:ARG:O	4:D:1133:ILE:HG12	2.15	0.46
4:D:129:ILE:HG13	4:D:130:TYR:CD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:407:LYS:O	4:D:411:GLY:HA3	2.16	0.46
2:A:157:ALA:O	2:A:161:ARG:NH1	2.48	0.46
3:C:729:SER:OG	3:C:904:VAL:O	2.31	0.46
4:D:567:SER:HB2	4:D:574:LEU:HD11	1.97	0.46
4:D:924:LEU:HD12	4:D:937:ILE:HG22	1.97	0.46
6:F:406:SER:HB3	6:F:409:GLU:HB3	1.97	0.46
2:A:9:LEU:HD13	2:A:23:ILE:HG12	1.96	0.46
2:A:95:MET:HG2	2:A:113:PRO:HD2	1.98	0.46
2:B:10:SER:HB3	2:B:22:VAL:HG22	1.96	0.46
3:C:477:ILE:O	3:C:597:LEU:HG	2.16	0.46
3:C:755:LEU:HD12	3:C:799:PRO:HG2	1.96	0.46
3:C:763:ASP:HB3	3:C:821:ARG:HH22	1.81	0.46
4:D:612:TYR:HE1	4:D:633:ILE:HG21	1.79	0.46
5:E:42:SER:OG	5:E:43:ARG:NH1	2.48	0.46
6:F:202:ALA:O	6:F:206:GLU:HG3	2.15	0.46
4:D:1054:VAL:HG23	4:D:1065:ILE:HG23	1.97	0.46
4:D:1123:LEU:HA	4:D:1131:VAL:HG21	1.97	0.46
4:D:117:LEU:O	4:D:117:LEU:HD22	2.14	0.46
4:D:373:MET:SD	6:F:256:LEU:HB3	2.55	0.46
4:D:634:LYS:HA	4:D:664:GLU:HA	1.97	0.46
4:D:759:TYR:CD2	4:D:769:ARG:HB2	2.51	0.46
3:C:170:LEU:HD13	3:C:369:LEU:CB	2.46	0.46
3:C:159:ILE:HG13	3:C:422:PHE:HB3	1.97	0.46
3:C:792:ILE:HD12	3:C:792:ILE:N	2.31	0.46
3:C:846:ARG:HB2	3:C:857:ASN:O	2.16	0.46
3:C:876:LEU:CD1	3:C:886:ILE:HD11	2.45	0.46
3:C:937:ILE:HD11	3:C:955:TYR:C	2.35	0.46
4:D:667:LEU:HD22	4:D:671:MET:HG3	1.97	0.46
7:O:2:DC:H2''	7:O:3:DT:H5'	1.97	0.46
2:A:59:VAL:HG11	2:A:73:VAL:HG21	1.98	0.46
3:C:771:VAL:HG23	3:C:772:LEU:HD13	1.97	0.46
4:D:181:LEU:HD22	4:D:184:LEU:HD12	1.98	0.46
4:D:61:TYR:HB3	4:D:78:CYS:CB	2.46	0.46
5:E:53:TYR:CE1	5:E:103:HIS:HB3	2.51	0.46
2:B:54:ILE:CG2	2:B:138:LEU:HB3	2.46	0.46
2:B:60:LEU:HD22	2:B:60:LEU:N	2.31	0.46
2:B:71:GLU:OE2	2:B:126:ALA:HA	2.16	0.46
3:C:626:ALA:HB3	3:C:702:GLY:O	2.15	0.46
7:O:6:DA:H2''	7:O:7:DC:H5'	1.98	0.46
2:A:214:THR:HG23	2:B:232:ILE:HG13	1.98	0.46
3:C:844:PHE:O	3:C:859:LEU:N	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:952:GLU:HA	3:C:955:TYR:CE1	2.50	0.46
4:D:1252:ASN:OD1	4:D:1257:LYS:HD3	2.16	0.46
4:D:640:LEU:O	4:D:641:ARG:NH2	2.49	0.46
4:D:672:PHE:CE2	4:D:676:LEU:HD11	2.50	0.46
4:D:527:LEU:HD13	4:D:712:VAL:HG12	1.98	0.46
1:J:45:ALA:HB2	4:D:73:ILE:HD12	1.97	0.46
4:D:181:LEU:O	4:D:181:LEU:HD13	2.16	0.46
6:F:166:VAL:O	6:F:170:LEU:HG	2.15	0.46
2:B:22:VAL:HA	2:B:192:LEU:O	2.16	0.45
3:C:708:LYS:HG3	3:C:737:VAL:HG23	1.97	0.45
4:D:1056:LEU:HD22	4:D:1063:PHE:CE1	2.50	0.45
4:D:1132:GLN:NE2	4:D:1163:LEU:HD12	2.31	0.45
4:D:474:ARG:NH2	4:D:478:ARG:HD3	2.31	0.45
4:D:759:TYR:HD2	4:D:769:ARG:HB2	1.80	0.45
5:E:30:LEU:O	5:E:33:THR:HG22	2.16	0.45
6:F:197:ALA:O	6:F:201:LEU:HG	2.15	0.45
3:C:914:PRO:HG3	4:D:802:VAL:HG22	1.98	0.45
4:D:1220:SER:HB3	4:D:1223:SER:HB3	1.98	0.45
4:D:330:LEU:HD12	4:D:331:ASP:H	1.82	0.45
4:D:693:ALA:O	4:D:697:ASN:ND2	2.49	0.45
5:E:64:TYR:HB2	5:E:75:TYR:CB	2.46	0.45
6:F:394:LEU:HB2	6:F:464:TYR:CE1	2.51	0.45
2:A:22:VAL:CG2	2:A:191:LYS:HD2	2.46	0.45
2:A:33:THR:HG22	2:B:37:SER:HA	1.98	0.45
2:B:28:PRO:HA	2:B:29:GLY:HA2	1.45	0.45
3:C:1103:ILE:CD1	4:D:547:LEU:HB3	2.47	0.45
3:C:36:ARG:O	3:C:38:PRO:HD3	2.16	0.45
3:C:493:VAL:HG23	3:C:578:VAL:O	2.15	0.45
3:C:844:PHE:N	3:C:859:LEU:O	2.38	0.45
4:D:234:LEU:HD22	4:D:234:LEU:N	2.31	0.45
4:D:622:MET:CE	4:D:667:LEU:HD13	2.32	0.45
5:E:55:ALA:O	5:E:59:ARG:HG2	2.16	0.45
6:F:218:ASP:O	6:F:222:ILE:HG12	2.16	0.45
2:B:21:PHE:HB2	2:B:194:ILE:HG22	1.99	0.45
2:B:55:ARG:HD2	2:B:161:ARG:NH1	2.31	0.45
3:C:640:VAL:O	3:C:652:MET:N	2.42	0.45
4:D:177:LEU:HD23	4:D:177:LEU:C	2.36	0.45
4:D:262:LYS:HG3	4:D:310:MET:HE3	1.99	0.45
4:D:920:PHE:O	4:D:1151:HIS:NE2	2.30	0.45
7:O:16:DT:C6	7:O:16:DT:H5'	2.50	0.45
2:B:32:TYR:CG	3:C:1005:ARG:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1137:GLU:HG2	3:C:1138:MET:H	1.82	0.45
3:C:619:THR:HG23	3:C:620:GLY:N	2.31	0.45
4:D:1062:PHE:HB3	4:D:1081:LEU:O	2.17	0.45
4:D:236:VAL:O	4:D:236:VAL:HG12	2.16	0.45
4:D:48:CYS:SG	4:D:50:LYS:HB3	2.57	0.45
4:D:873:THR:O	4:D:877:VAL:HG23	2.16	0.45
2:B:232:ILE:HG22	2:B:233:GLU:N	2.31	0.45
4:D:1050:VAL:HG22	4:D:1051:ALA:N	2.30	0.45
4:D:460:LEU:HD11	4:D:472:ALA:HB1	1.98	0.45
4:D:647:GLU:HG2	4:D:651:PHE:CD2	2.51	0.45
4:D:884:ILE:HD11	4:D:886:ARG:CZ	2.47	0.45
6:F:241:VAL:HG22	6:F:289:ILE:HD13	1.98	0.45
2:A:180:ALA:HA	2:A:190:ASP:HA	1.99	0.45
2:A:24:GLU:HA	2:A:25:PRO:HA	1.73	0.45
3:C:790:GLY:N	3:C:830:VAL:HG22	2.25	0.45
4:D:367:VAL:HG12	4:D:371:LYS:HE2	1.98	0.45
4:D:1104:ASP:N	4:D:1104:ASP:OD1	2.50	0.45
4:D:1249:LEU:HD12	4:D:1250:LYS:H	1.80	0.45
4:D:92:MET:HG2	4:D:321:PRO:HD3	1.98	0.45
6:F:322:ARG:HB2	6:F:322:ARG:CZ	2.46	0.45
2:A:14:VAL:CG1	2:A:18:ARG:HG3	2.45	0.45
2:B:97:LEU:HD11	2:B:109:ASP:HB2	1.99	0.45
3:C:51:SER:O	3:C:373:GLY:HA3	2.17	0.45
3:C:578:VAL:CG1	3:C:582:THR:HB	2.44	0.45
4:D:240:LEU:C	4:D:240:LEU:HD23	2.37	0.45
6:F:186:GLU:O	6:F:190:ARG:HG3	2.16	0.45
1:J:104:LEU:O	1:J:104:LEU:HD23	2.17	0.45
2:B:198:THR:HG21	2:B:202:ILE:CD1	2.45	0.45
3:C:496:ARG:HH12	3:C:521:TYR:CB	2.30	0.45
3:C:870:ILE:HG23	3:C:870:ILE:O	2.17	0.45
4:D:23:TRP:HB3	4:D:92:MET:HE3	1.98	0.45
4:D:710:GLN:OE1	5:E:27:ASP:HB2	2.17	0.45
3:C:479:THR:HG23	3:C:597:LEU:HD11	1.99	0.44
3:C:523:THR:HG23	3:C:526:GLU:H	1.82	0.44
3:C:586:PRO:O	3:C:880:HIS:HE1	2.01	0.44
3:C:680:ILE:HG12	3:C:693:ILE:O	2.17	0.44
4:D:403:SER:O	4:D:407:LYS:HG2	2.17	0.44
2:B:74:THR:CG2	4:D:611:VAL:HG21	2.46	0.44
4:D:692:GLN:O	4:D:696:ILE:HG13	2.17	0.44
5:E:29:PRO:HB2	5:E:33:THR:HG23	2.00	0.44
5:E:29:PRO:CB	5:E:33:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1039:PRO:HG2	3:C:1048:LEU:O	2.16	0.44
3:C:388:GLU:CA	3:C:391:VAL:HG22	2.46	0.44
3:C:887:GLY:HA2	4:D:431:VAL:HB	1.99	0.44
3:C:728:LEU:CD2	3:C:906:ILE:HG22	2.39	0.44
4:D:262:LYS:HG3	4:D:310:MET:CE	2.46	0.44
4:D:644:THR:HG22	4:D:655:TRP:HZ2	1.81	0.44
2:A:217:GLU:HG2	2:B:233:GLU:C	2.38	0.44
3:C:418:ILE:HG12	3:C:418:ILE:H	1.60	0.44
3:C:799:PRO:HA	3:C:823:VAL:HG12	1.95	0.44
3:C:939:VAL:HG12	3:C:943:VAL:HG12	1.99	0.44
4:D:43:LYS:NZ	4:D:50:LYS:HE2	2.31	0.44
4:D:900:LEU:O	4:D:901:ALA:HB3	2.16	0.44
1:J:33:ARG:NH2	1:J:39:GLU:OE2	2.44	0.44
2:A:40:ARG:HH21	3:C:894:ASP:CB	2.24	0.44
2:A:87:SER:OG	2:A:116:VAL:HG12	2.17	0.44
2:A:209:ALA:HA	2:B:222:ALA:O	2.17	0.44
3:C:1044:THR:OG1	3:C:1046:GLN:HG3	2.18	0.44
8:P:11:DA:H2'	8:P:12:DA:H8	1.82	0.44
2:A:57:ASP:OD1	2:A:58:GLY:N	2.51	0.44
3:C:169:GLN:HG2	3:C:171:VAL:HG13	2.00	0.44
3:C:72:ASN:N	3:C:73:PRO:HD3	2.32	0.44
3:C:952:GLU:O	3:C:953:GLU:CB	2.64	0.44
3:C:29:ARG:CG	3:C:964:ALA:HB2	2.47	0.44
4:D:237:ASP:HB3	4:D:240:LEU:CB	2.44	0.44
4:D:114:LEU:HG	4:D:312:MET:SD	2.57	0.44
4:D:689:LYS:O	4:D:693:ALA:N	2.40	0.44
2:A:47:PRO:HG2	2:B:230:GLU:CB	2.38	0.44
3:C:1082:ILE:O	3:C:1090:ARG:HB3	2.18	0.44
4:D:103:HIS:ND1	4:D:105:TRP:HB2	2.33	0.44
4:D:588:LEU:O	4:D:668:GLY:HA3	2.18	0.44
4:D:646:LEU:HD23	4:D:646:LEU:C	2.38	0.44
7:O:2:DC:H2''	7:O:3:DT:C5'	2.48	0.44
2:A:147:VAL:HG12	2:A:168:TYR:HE2	1.83	0.44
2:A:192:LEU:HD12	2:A:192:LEU:C	2.37	0.44
4:D:1252:ASN:O	4:D:1257:LYS:N	2.50	0.44
4:D:492:ALA:O	5:E:87:LYS:HE2	2.17	0.44
3:C:873:GLY:HA3	3:C:1028:VAL:CG1	2.46	0.44
3:C:984:LEU:N	3:C:984:LEU:HD12	2.33	0.44
4:D:504:LEU:HD23	4:D:1004:GLU:HG2	2.00	0.44
6:F:283:THR:OG1	7:O:29:DA:H8	2.01	0.44
6:F:414:ARG:O	6:F:418:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:ARG:NH1	3:C:962:THR:HB	2.32	0.44
5:E:80:VAL:CG1	5:E:94:ARG:HH21	2.31	0.44
6:F:425:ARG:HB2	6:F:430:ILE:HG12	1.99	0.44
2:B:66:VAL:HG23	2:B:73:VAL:HG22	2.01	0.43
3:C:166:VAL:HG11	3:C:372:VAL:HG23	1.98	0.43
3:C:710:LEU:HD13	3:C:1021:ILE:HG12	2.00	0.43
3:C:797:VAL:CG1	3:C:823:VAL:HG23	2.48	0.43
4:D:113:ARG:NH2	4:D:1232:ARG:HH11	2.16	0.43
4:D:268:PHE:CZ	4:D:273:GLU:HG3	2.53	0.43
4:D:647:GLU:OE1	4:D:648:ALA:N	2.51	0.43
4:D:676:LEU:HD12	4:D:676:LEU:N	2.33	0.43
4:D:770:ASN:O	4:D:774:VAL:HG23	2.18	0.43
4:D:61:TYR:HB3	4:D:78:CYS:HB2	2.00	0.43
2:A:179:GLU:OE1	2:A:191:LYS:NZ	2.35	0.43
2:B:188:ASP:OD2	2:B:188:ASP:N	2.51	0.43
3:C:156:THR:HG22	3:C:165:VAL:HG22	2.00	0.43
3:C:751:ARG:HA	3:C:855:GLY:O	2.18	0.43
3:C:985:PRO:HB3	3:C:990:GLU:O	2.18	0.43
4:D:665:THR:CG2	4:D:684:ASN:HD22	2.31	0.43
3:C:727:ILE:HG22	3:C:888:LYS:HB3	1.99	0.43
4:D:756:GLU:HA	4:D:756:GLU:OE2	2.18	0.43
1:J:53:THR:HA	1:J:62:GLY:O	2.19	0.43
3:C:498:ASN:HB3	3:C:499:PRO:HD2	2.01	0.43
4:D:1140:GLN:HE21	4:D:1155:ILE:CD1	2.31	0.43
4:D:143:MET:HG2	4:D:251:TYR:CD1	2.53	0.43
3:C:1057:GLN:NE2	4:D:427:ARG:HG2	2.32	0.43
4:D:706:ILE:HD11	5:E:36:PRO:HA	2.00	0.43
2:A:38:LEU:HD23	2:A:215:LEU:HD22	2.00	0.43
3:C:710:LEU:CD2	3:C:1021:ILE:HD11	2.34	0.43
3:C:370:ARG:HB2	3:C:375:LEU:HD23	2.01	0.43
3:C:507:TYR:HD1	3:C:522:LEU:HB2	1.82	0.43
4:D:118:LEU:CB	4:D:120:LEU:HD13	2.49	0.43
4:D:653:ASN:OD1	4:D:653:ASN:N	2.52	0.43
2:A:17:ASN:O	2:A:204:PRO:HG3	2.17	0.43
2:B:218:LEU:HD23	2:B:218:LEU:O	2.18	0.43
3:C:1061:GLU:H	4:D:415:GLN:NE2	2.16	0.43
3:C:1108:ILE:N	3:C:1108:ILE:HD12	2.34	0.43
3:C:120:TYR:CB	3:C:158:ILE:HB	2.49	0.43
3:C:477:ILE:O	3:C:477:ILE:HG22	2.18	0.43
2:A:175:THR:OG1	3:C:899:PRO:O	2.30	0.43
4:D:1132:GLN:HG2	4:D:1159:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:237:ASP:O	4:D:239:VAL:HG12	2.19	0.43
4:D:926:THR:HG23	4:D:960:LYS:HD3	2.00	0.43
1:J:102:LEU:HD23	6:F:215:GLN:HE21	1.83	0.43
6:F:246:LYS:HB3	6:F:246:LYS:HE2	1.79	0.43
2:B:97:LEU:HB2	2:B:110:ILE:HB	1.99	0.43
3:C:32:PHE:HE1	3:C:963:VAL:CG1	2.32	0.43
3:C:736:ASP:OD1	3:C:869:LYS:HE2	2.19	0.43
4:D:131:PHE:CZ	4:D:257:GLY:HA3	2.54	0.43
4:D:48:CYS:HB3	4:D:51:ILE:HG13	2.01	0.43
4:D:633:ILE:HD12	4:D:633:ILE:C	2.38	0.43
4:D:576:MET:HG3	4:D:696:ILE:HD12	1.99	0.43
3:C:914:PRO:HG3	4:D:802:VAL:CG2	2.49	0.43
4:D:85:ALA:O	4:D:88:ARG:HB2	2.19	0.43
4:D:365:ILE:HD13	6:F:235:GLU:HG2	1.99	0.43
8:P:3:DC:H2"	8:P:4:DA:H8	1.84	0.43
2:A:199:LYS:O	2:A:200:ASN:HB2	2.17	0.43
2:B:102:PRO:HD3	2:B:131:LYS:H	1.83	0.43
2:B:170:PRO:HA	2:B:199:LYS:CD	2.48	0.43
3:C:144:PHE:CZ	3:C:146:GLY:HA2	2.54	0.43
3:C:894:ASP:HB2	3:C:1005:ARG:HG2	1.99	0.43
4:D:447:MET:O	4:D:451:LEU:HB2	2.19	0.43
4:D:48:CYS:HB3	4:D:51:ILE:CD1	2.48	0.43
4:D:554:GLU:O	4:D:558:LEU:HB2	2.19	0.43
6:F:319:ARG:O	6:F:323:GLU:HG3	2.19	0.43
7:O:4:DT:H2'	7:O:5:DG:C8	2.53	0.43
2:B:147:VAL:O	2:B:147:VAL:HG13	2.19	0.43
2:B:172:LEU:HD12	2:B:172:LEU:O	2.18	0.43
3:C:141:GLN:HB3	3:C:405:PRO:CB	2.49	0.43
3:C:870:ILE:HD11	3:C:886:ILE:CD1	2.49	0.43
4:D:43:LYS:O	4:D:44:ASP:HB2	2.19	0.43
4:D:798:ILE:O	4:D:802:VAL:HG23	2.19	0.43
2:A:68:GLY:CA	2:A:129:ASN:HD21	2.32	0.43
2:A:72:ASP:OD1	2:A:75:ASP:N	2.50	0.43
9:C:1201:SRN:O1	9:C:1201:SRN:C4	2.67	0.43
3:C:435:ASN:HD21	3:C:604:ARG:CA	2.32	0.43
3:C:896:PRO:HD2	3:C:907:ILE:HD11	2.00	0.43
4:D:873:THR:OG1	4:D:1003:GLY:HA3	2.19	0.43
4:D:463:LEU:O	4:D:465:HIS:N	2.48	0.43
2:B:123:MET:HE2	2:B:125:ILE:CD1	2.49	0.42
3:C:48:GLN:O	3:C:151:MET:HE1	2.19	0.42
3:C:844:PHE:HB2	3:C:859:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:239:VAL:HG13	4:D:240:LEU:N	2.34	0.42
4:D:655:TRP:O	4:D:657:PRO:HD3	2.19	0.42
1:J:69:VAL:N	1:J:70:PRO:CD	2.82	0.42
6:F:295:ARG:NH2	7:O:24:DG:O6	2.46	0.42
8:P:12:DA:H2''	8:P:13:DC:C5'	2.48	0.42
3:C:709:ASN:C	3:C:710:LEU:HD12	2.39	0.42
1:J:69:VAL:O	1:J:70:PRO:C	2.56	0.42
2:B:144:ARG:HH11	2:B:144:ARG:HB2	1.84	0.42
3:C:423:GLY:C	3:C:424:THR:HG1	2.13	0.42
3:C:443:LYS:O	3:C:444:ARG:CB	2.67	0.42
3:C:578:VAL:HG12	3:C:579:SER:O	2.19	0.42
4:D:1033:GLN:HE21	4:D:1039:ARG:HH22	1.67	0.42
4:D:1132:GLN:HE21	4:D:1163:LEU:HD12	1.85	0.42
4:D:57:ASP:HB3	4:D:58:TRP:CE3	2.54	0.42
4:D:711:THR:O	4:D:715:LEU:HG	2.18	0.42
2:A:217:GLU:O	2:A:217:GLU:HG3	2.20	0.42
3:C:471:TYR:HB3	3:C:553:ARG:NH1	2.34	0.42
3:C:808:GLU:HG2	6:F:395:GLN:CG	2.48	0.42
4:D:1009:LEU:HD23	4:D:1029:LEU:HA	2.01	0.42
4:D:27:GLU:HB2	4:D:94:HIS:CE1	2.54	0.42
4:D:591:LEU:HD13	4:D:591:LEU:C	2.39	0.42
6:F:427:LEU:HD13	6:F:442:ARG:HB2	2.02	0.42
1:J:89:ARG:HH22	6:F:274:ASP:CG	2.23	0.42
3:C:712:VAL:HG12	3:C:1017:GLY:O	2.20	0.42
3:C:445:ARG:HD2	9:C:1201:SRN:H272	2.01	0.42
4:D:1258:LEU:HA	4:D:1258:LEU:HD12	1.79	0.42
4:D:1273:VAL:HG11	5:E:57:ARG:HB2	2.01	0.42
2:A:129:ASN:N	2:A:129:ASN:HD22	2.13	0.42
2:A:71:GLU:N	2:A:71:GLU:OE1	2.51	0.42
2:B:113:PRO:O	2:B:116:VAL:HG22	2.19	0.42
3:C:1092:LYS:HA	3:C:1092:LYS:HD3	1.90	0.42
6:F:293:ILE:O	6:F:297:MET:HG3	2.19	0.42
2:A:85:VAL:HG22	2:A:86:SER:N	2.35	0.42
3:C:559:VAL:HG12	3:C:559:VAL:O	2.20	0.42
4:D:1231:THR:O	4:D:1235:THR:HG23	2.20	0.42
3:C:471:TYR:HD2	4:D:849:PHE:HD1	1.67	0.42
6:F:319:ARG:HA	6:F:322:ARG:HH22	1.85	0.42
3:C:103:PHE:HE1	3:C:148:PHE:CB	2.32	0.42
3:C:1035:ARG:HD2	3:C:1054:PHE:O	2.20	0.42
3:C:1085:ASP:OD2	4:D:420:LYS:NZ	2.52	0.42
4:D:1266:SER:HA	4:D:1269:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:323:GLU:O	4:D:326:PRO:HD3	2.20	0.42
4:D:451:LEU:HD12	4:D:451:LEU:HA	1.87	0.42
4:D:651:PHE:O	4:D:652:GLU:CB	2.68	0.42
4:D:962:ARG:HB3	4:D:977:CYS:HA	2.01	0.42
6:F:373:LEU:HD23	6:F:373:LEU:C	2.40	0.42
1:J:28:GLN:N	1:J:44:PHE:O	2.34	0.42
2:B:71:GLU:N	2:B:71:GLU:OE1	2.53	0.42
4:D:1054:VAL:HG12	4:D:1104:ASP:O	2.20	0.42
4:D:52:PHE:O	4:D:91:ARG:HD2	2.20	0.42
4:D:49:GLU:HG3	4:D:88:ARG:HH21	1.83	0.42
6:F:409:GLU:HG3	6:F:448:THR:CG2	2.47	0.42
2:A:151:GLN:HA	2:A:163:PRO:HG2	2.02	0.41
2:B:24:GLU:HA	2:B:25:PRO:HA	1.65	0.41
3:C:584:MET:HG2	3:C:621:MET:HB2	2.00	0.41
5:E:30:LEU:H	5:E:33:THR:CG2	2.33	0.41
2:A:174:VAL:O	3:C:901:GLY:HA3	2.19	0.41
4:D:49:GLU:HG2	4:D:88:ARG:HH21	1.85	0.41
3:C:23:VAL:HB	3:C:26:ALA:HB2	2.02	0.41
3:C:992:MET:HA	3:C:992:MET:HE2	2.01	0.41
4:D:474:ARG:NH2	4:D:480:ARG:HD3	2.34	0.41
4:D:846:LEU:O	4:D:850:ILE:HG12	2.20	0.41
5:E:80:VAL:HG12	5:E:81:GLU:N	2.36	0.41
3:C:392:ARG:O	3:C:396:THR:HG23	2.21	0.41
3:C:145:MET:O	3:C:411:ILE:HD12	2.19	0.41
3:C:432:ASP:HB2	9:C:1201:SRN:C18	2.41	0.41
3:C:52:PHE:HB2	3:C:151:MET:CE	2.50	0.41
3:C:834:GLU:O	3:C:835:SER:OG	2.38	0.41
3:C:937:ILE:CD1	3:C:955:TYR:HB3	2.44	0.41
4:D:1278:GLU:CD	4:D:1278:GLU:H	2.24	0.41
4:D:274:ALA:O	4:D:278:ARG:HG2	2.20	0.41
5:E:95:GLU:HB3	5:E:101:LEU:HD21	2.02	0.41
1:J:68:ASP:C	1:J:70:PRO:HD2	2.41	0.41
2:A:24:GLU:CB	2:A:191:LYS:HD3	2.49	0.41
2:B:91:GLU:OE1	2:B:91:GLU:HA	2.19	0.41
3:C:1015:THR:HG1	4:D:731:SER:HG	1.67	0.41
3:C:44:LEU:H	3:C:44:LEU:HG	1.64	0.41
3:C:583:ALA:O	3:C:619:THR:HG21	2.20	0.41
2:A:44:SER:HB3	3:C:893:GLU:OE1	2.21	0.41
4:D:889:ASP:OD2	4:D:962:ARG:NH2	2.53	0.41
2:A:146:TYR:OH	3:C:869:LYS:NZ	2.51	0.41
2:B:88:ASP:N	2:B:88:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:613:GLU:HB3	3:C:708:LYS:CD	2.51	0.41
3:C:748:ILE:HA	3:C:748:ILE:HD12	1.94	0.41
3:C:749:ASP:OD1	3:C:749:ASP:N	2.54	0.41
3:C:748:ILE:HG21	3:C:794:VAL:HG11	2.01	0.41
3:C:900:ASP:OD1	3:C:986:ASN:ND2	2.53	0.41
4:D:886:ARG:HD3	4:D:886:ARG:HA	1.92	0.41
1:J:81:HIS:NE2	6:F:271:GLU:HA	2.35	0.41
2:A:147:VAL:CG1	2:A:166:SER:HB2	2.51	0.41
3:C:45:LEU:HD12	3:C:628:ASP:O	2.21	0.41
1:J:96:GLU:O	1:J:100:GLU:HG3	2.21	0.41
2:A:144:ARG:HA	2:A:168:TYR:HB2	2.03	0.41
2:B:52:THR:O	2:B:164:VAL:HG22	2.21	0.41
3:C:710:LEU:O	3:C:1018:TYR:HA	2.21	0.41
3:C:505:THR:HG23	3:C:506:PRO:HD2	2.01	0.41
3:C:62:ARG:HB2	3:C:62:ARG:CZ	2.51	0.41
3:C:788:ARG:O	3:C:830:VAL:HG21	2.21	0.41
4:D:170:LEU:HD11	4:D:209:ARG:HB2	2.02	0.41
4:D:177:LEU:HD12	4:D:201:GLY:HA3	2.02	0.41
4:D:757:ARG:HD2	4:D:757:ARG:C	2.41	0.41
4:D:788:LEU:C	4:D:788:LEU:HD13	2.41	0.41
3:C:1059:PHE:CZ	3:C:1067:MET:HE3	2.54	0.41
3:C:712:VAL:HG21	3:C:908:LEU:HD12	2.01	0.41
3:C:797:VAL:HG12	3:C:823:VAL:CG2	2.50	0.41
6:F:291:GLN:HG3	6:F:292:ALA:N	2.36	0.41
6:F:424:PRO:O	6:F:425:ARG:HD3	2.21	0.41
1:J:55:LEU:HD13	4:D:50:LYS:NZ	2.36	0.41
2:A:93:VAL:HG22	2:A:113:PRO:HG3	2.03	0.41
4:D:1163:LEU:HD21	4:D:1208:LEU:HG	2.03	0.41
3:C:926:HIS:HD2	4:D:732:MET:HG3	1.85	0.41
5:E:68:LEU:HA	5:E:69:GLY:HA2	1.60	0.41
2:B:104:VAL:O	2:B:104:VAL:HG13	2.21	0.41
2:B:185:GLN:O	4:D:445:LYS:NZ	2.54	0.41
3:C:609:LEU:CD1	3:C:708:LYS:HG2	2.51	0.41
4:D:12:ILE:HD11	4:D:1221:TRP:CE3	2.56	0.41
1:J:108:LYS:C	1:J:108:LYS:HD2	2.41	0.41
2:A:110:ILE:O	2:A:112:PRO:HD3	2.22	0.40
2:B:56:ILE:HD11	2:B:136:VAL:CB	2.46	0.40
3:C:1086:ASP:CG	3:C:1089:GLY:HA3	2.41	0.40
3:C:1138:MET:H	3:C:1138:MET:HG2	1.70	0.40
3:C:766:ASN:O	3:C:767:VAL:HG13	2.20	0.40
3:C:1070:TYR:CG	4:D:559:MET:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:ARG:O	4:D:87:VAL:HG22	2.21	0.40
6:F:350:GLU:OE2	6:F:354:TYR:OH	2.33	0.40
2:B:28:PRO:HG3	2:B:188:ASP:O	2.20	0.40
3:C:166:VAL:CG1	3:C:372:VAL:HG23	2.51	0.40
3:C:29:ARG:CD	3:C:964:ALA:HB2	2.50	0.40
3:C:764:ILE:CG2	3:C:765:PRO:HD2	2.51	0.40
3:C:891:PRO:HB2	3:C:893:GLU:HG2	2.02	0.40
8:P:3:DC:H2''	8:P:4:DA:C8	2.56	0.40
8:P:8:DT:C6	8:P:9:DT:H72	2.56	0.40
4:D:1100:LEU:HD23	4:D:1100:LEU:C	2.42	0.40
4:D:901:ALA:CA	4:D:912:ASP:HB2	2.52	0.40
4:D:982:MET:HE2	4:D:1153:LYS:HD2	2.04	0.40
4:D:989:ASP:OD2	5:E:47:LYS:HG2	2.22	0.40
7:O:10:DA:H2''	7:O:11:DA:O4'	2.21	0.40
2:B:3:ILE:HA	2:B:233:GLU:CB	2.52	0.40
3:C:445:ARG:NE	9:C:1201:SRN:O6	2.54	0.40
3:C:710:LEU:HD22	3:C:1021:ILE:CD1	2.35	0.40
3:C:590:HIS:HB3	3:C:919:ILE:HG23	2.02	0.40
3:C:921:GLN:HG3	3:C:1019:MET:HE1	2.03	0.40
4:D:1165:ARG:HA	4:D:1182:THR:O	2.20	0.40
4:D:119:ASP:C	4:D:120:LEU:HD12	2.42	0.40
4:D:581:MET:CE	4:D:716:LYS:HA	2.50	0.40
4:D:624:ARG:HG2	4:D:625:GLY:N	2.37	0.40
4:D:683:VAL:HG11	4:D:695:ILE:HD11	2.01	0.40
6:F:254:ALA:HA	12:F:501:SO4:S	2.61	0.40
3:C:32:PHE:O	3:C:34:LYS:HD2	2.21	0.40
3:C:512:ASN:ND2	3:C:512:ASN:O	2.55	0.40
3:C:939:VAL:HG23	3:C:939:VAL:O	2.20	0.40
4:D:449:LEU:CD2	4:D:476:VAL:HG13	2.52	0.40
4:D:573:PRO:HG2	4:D:576:MET:CE	2.52	0.40
4:D:82:VAL:HG13	4:D:82:VAL:O	2.22	0.40
6:F:409:GLU:CD	6:F:448:THR:HG22	2.42	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)
3:C:777:GLU:OE1	4:D:209:ARG:NH1[2_356]	2.13	0.07

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	82/114 (72%)	77 (94%)	3 (4%)	2 (2%)	6	22
2	A	220/350 (63%)	197 (90%)	22 (10%)	1 (0%)	29	61
2	B	221/350 (63%)	203 (92%)	15 (7%)	3 (1%)	11	36
3	C	869/1169 (74%)	796 (92%)	64 (7%)	9 (1%)	15	45
4	D	1186/1317 (90%)	1133 (96%)	41 (4%)	12 (1%)	15	45
5	E	80/107 (75%)	71 (89%)	8 (10%)	1 (1%)	12	37
6	F	301/466 (65%)	299 (99%)	2 (1%)	0	100	100
All	All	2959/3873 (76%)	2776 (94%)	155 (5%)	28 (1%)	17	48

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	70	PRO
3	C	967	VAL
3	C	1053	GLN
4	D	281	ILE
2	A	49	ALA
2	B	183	VAL
3	C	953	GLU
4	D	279	GLU
4	D	736	LEU
4	D	1229	GLU
5	E	72	ILE
2	B	231	HIS
3	C	43	GLY
3	C	765	PRO
4	D	900	LEU
4	D	1227	PHE
2	B	226	ASN
3	C	917	MET

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Mol	Chain	Res	Type
4	D	238	GLU
4	D	464	ASN
4	D	762	GLY
4	D	902	GLU
1	J	68	ASP
3	C	988	ASP
4	D	937	ILE
3	C	369	LEU
4	D	657	PRO
3	C	24	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	70/98 (71%)	63 (90%)	7 (10%)	7	23
2	A	180/297 (61%)	168 (93%)	12 (7%)	16	43
2	B	167/297 (56%)	150 (90%)	17 (10%)	7	22
3	C	656/984 (67%)	605 (92%)	51 (8%)	12	34
4	D	915/1095 (84%)	866 (95%)	49 (5%)	22	54
5	E	61/86 (71%)	53 (87%)	8 (13%)	4	12
6	F	250/379 (66%)	239 (96%)	11 (4%)	28	61
All	All	2299/3236 (71%)	2144 (93%)	155 (7%)	16	43

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	ASP
1	J	55	LEU
1	J	68	ASP
1	J	76	LYS
1	J	97	LEU
1	J	105	ILE
1	J	108	LYS

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Mol	Chain	Res	Type
2	A	2	LEU
2	A	30	PHE
2	A	40	ARG
2	A	74	THR
2	A	88	ASP
2	A	117	THR
2	A	127	THR
2	A	129	ASN
2	A	141	GLU
2	A	190	ASP
2	A	215	LEU
2	A	221	LEU
2	B	24	GLU
2	B	43	LEU
2	B	56	ILE
2	B	71	GLU
2	B	84	VAL
2	B	87	SER
2	B	138	LEU
2	B	144	ARG
2	B	161	ARG
2	B	172	LEU
2	B	176	TYR
2	B	177	LYS
2	B	178	VAL
2	B	182	ARG
2	B	186	ARG
2	B	188	ASP
2	B	224	GLU
3	C	30	VAL
3	C	44	LEU
3	C	45	LEU
3	C	46	ASP
3	C	53	GLU
3	C	60	ARG
3	C	62	ARG
3	C	77	LEU
3	C	81	LEU
3	C	84	LEU
3	C	147	ASP
3	C	153	GLU
3	C	375	LEU

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Mol	Chain	Res	Type
3	C	418	ILE
3	C	420	GLU
3	C	434	ASN
3	C	443	LYS
3	C	446	LEU
3	C	447	LEU
3	C	511	GLU
3	C	512	ASN
3	C	531	VAL
3	C	597	LEU
3	C	636	ASP
3	C	678	ARG
3	C	688	GLU
3	C	715	MET
3	C	721	ASN
3	C	727	ILE
3	C	737	VAL
3	C	749	ASP
3	C	777	GLU
3	C	822	GLU
3	C	826	THR
3	C	848	ASP
3	C	849	ASP
3	C	852	LEU
3	C	890	LEU
3	C	919	ILE
3	C	927	LEU
3	C	936	ASN
3	C	937	ILE
3	C	945	ASP
3	C	952	GLU
3	C	965	THR
3	C	1008	GLU
3	C	1053	GLN
3	C	1116	LEU
3	C	1122	LEU
3	C	1126	VAL
3	C	1138	MET
4	D	7	PHE
4	D	12	ILE
4	D	28	VAL
4	D	51	ILE

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Mol	Chain	Res	Type
4	D	56	ARG
4	D	70	PHE
4	D	88	ARG
4	D	89	ARG
4	D	144	ARG
4	D	148	LEU
4	D	181	LEU
4	D	211	ARG
4	D	244	LEU
4	D	267	ASN
4	D	277	LEU
4	D	280	VAL
4	D	330	LEU
4	D	365	ILE
4	D	396	ASN
4	D	404	ASP
4	D	449	LEU
4	D	456	VAL
4	D	474	ARG
4	D	490	VAL
4	D	588	LEU
4	D	609	GLN
4	D	627	LEU
4	D	641	ARG
4	D	667	LEU
4	D	675	LEU
4	D	713	ASP
4	D	736	LEU
4	D	769	ARG
4	D	849	PHE
4	D	851	ASN
4	D	853	HIS
4	D	862	THR
4	D	864	LEU
4	D	939	ARG
4	D	1042	ARG
4	D	1058	GLU
4	D	1063	PHE
4	D	1104	ASP
4	D	1112	LEU
4	D	1184	ARG
4	D	1208	LEU

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Mol	Chain	Res	Type
4	D	1249	LEU
4	D	1250	LYS
4	D	1258	LEU
5	E	37	ILE
5	E	50	LEU
5	E	53	TYR
5	E	57	ARG
5	E	85	GLN
5	E	101	LEU
5	E	102	GLU
5	E	103	HIS
6	F	182	GLU
6	F	216	ARG
6	F	253	MET
6	F	291	GLN
6	F	317	LEU
6	F	325	LEU
6	F	348	VAL
6	F	349	LEU
6	F	402	LEU
6	F	460	VAL
6	F	463	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	ASN
2	A	129	ASN
2	B	17	ASN
2	B	79	ASN
3	C	48	GLN
3	C	426	GLN
3	C	434	ASN
3	C	467	HIS
3	C	512	ASN
3	C	700	GLN
3	C	721	ASN
3	C	866	GLN
3	C	926	HIS
3	C	936	ASN
3	C	1025	HIS
3	C	1053	GLN

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Mol	Chain	Res	Type
4	D	165	GLN
4	D	175	GLN
4	D	213	GLN
4	D	329	GLN
4	D	368	ASN
4	D	465	HIS
4	D	468	ASN
4	D	494	HIS
4	D	564	ASN
4	D	609	GLN
4	D	684	ASN
4	D	692	GLN
4	D	796	ASN
4	D	851	ASN
4	D	1140	GLN
4	D	1146	GLN
5	E	62	ASN
5	E	85	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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z > 2$
12	SO4	F	503	-	4,4,4	0.14	0	6,6,6	0.06	0
12	SO4	D	2007	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	D	2005	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SRN	C	1201	-	57,62,62	5.23	31 (54%)	58,84,84	1.60	10 (17%)
12	SO4	D	2006	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	D	2003	-	4,4,4	0.13	0	6,6,6	0.09	0
12	SO4	F	501	-	4,4,4	0.13	0	6,6,6	0.09	0
10	EDO	C	1202	-	3,3,3	0.45	0	2,2,2	0.31	0
12	SO4	D	2004	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	F	504	-	4,4,4	0.13	0	6,6,6	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SRN	C	1201	-	-	6/50/105/105	0/2/5/5
10	EDO	C	1202	-	-	0/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	SRN	O3-C8	19.93	1.80	1.44
9	C	1201	SRN	O3-C9	16.27	1.81	1.45
9	C	1201	SRN	C34-C9	-11.11	1.28	1.52
9	C	1201	SRN	C3-C2	9.61	1.59	1.34
9	C	1201	SRN	C34-C35	-8.87	1.33	1.52
9	C	1201	SRN	C4-C5	8.26	1.57	1.36
9	C	1201	SRN	C13-C14	6.77	1.60	1.31
9	C	1201	SRN	C24-C25	6.22	1.58	1.31
9	C	1201	SRN	C6-C7	6.04	1.57	1.33
9	C	1201	SRN	C8-C7	-5.91	1.30	1.50
9	C	1201	SRN	C12-C13	-5.58	1.31	1.50
9	C	1201	SRN	O7-C32	5.56	1.52	1.43
9	C	1201	SRN	C10-C9	-5.23	1.43	1.53
9	C	1201	SRN	C28-C29	5.16	1.61	1.31
9	C	1201	SRN	C3-C4	4.86	1.58	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	SRN	C5-C6	4.75	1.57	1.44
9	C	1201	SRN	O8-C12	4.31	1.51	1.43
9	C	1201	SRN	C35-C8	-4.17	1.46	1.53
9	C	1201	SRN	C11-C10	-4.17	1.44	1.53
9	C	1201	SRN	O1-C1	3.93	1.42	1.34
9	C	1201	SRN	O1-C33	3.81	1.52	1.46
9	C	1201	SRN	C46-C47	3.79	1.44	1.33
9	C	1201	SRN	C30-C29	3.70	1.61	1.50
9	C	1201	SRN	C2-C1	3.51	1.56	1.48
9	C	1201	SRN	O7-C31	3.44	1.53	1.44
9	C	1201	SRN	C33-C47	-3.40	1.44	1.49
9	C	1201	SRN	C23-C24	3.26	1.55	1.50
9	C	1201	SRN	C15-C14	2.73	1.58	1.50
9	C	1201	SRN	C31-C46	2.48	1.54	1.50
9	C	1201	SRN	C22-C21	2.39	1.56	1.52
9	C	1201	SRN	O8-C35	2.07	1.49	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1201	SRN	O9-C21-C20	4.37	114.47	109.94
9	C	1201	SRN	C8-C7-C6	-4.01	117.75	125.61
9	C	1201	SRN	C6-C5-C4	-3.30	117.46	124.81
9	C	1201	SRN	C9-C34-C35	3.17	112.89	103.73
9	C	1201	SRN	C37-C36-C32	2.84	120.58	115.68
9	C	1201	SRN	C32-C33-C47	2.79	113.48	110.64
9	C	1201	SRN	C15-C16-C17	-2.59	107.65	113.67
9	C	1201	SRN	C30-C29-C28	-2.04	118.81	126.40
9	C	1201	SRN	C12-C13-C14	-2.01	118.79	124.60
9	C	1201	SRN	C11-C10-C9	-2.00	108.26	111.96

There are no chirality outliers.

All (6) torsion outliers are listed below:

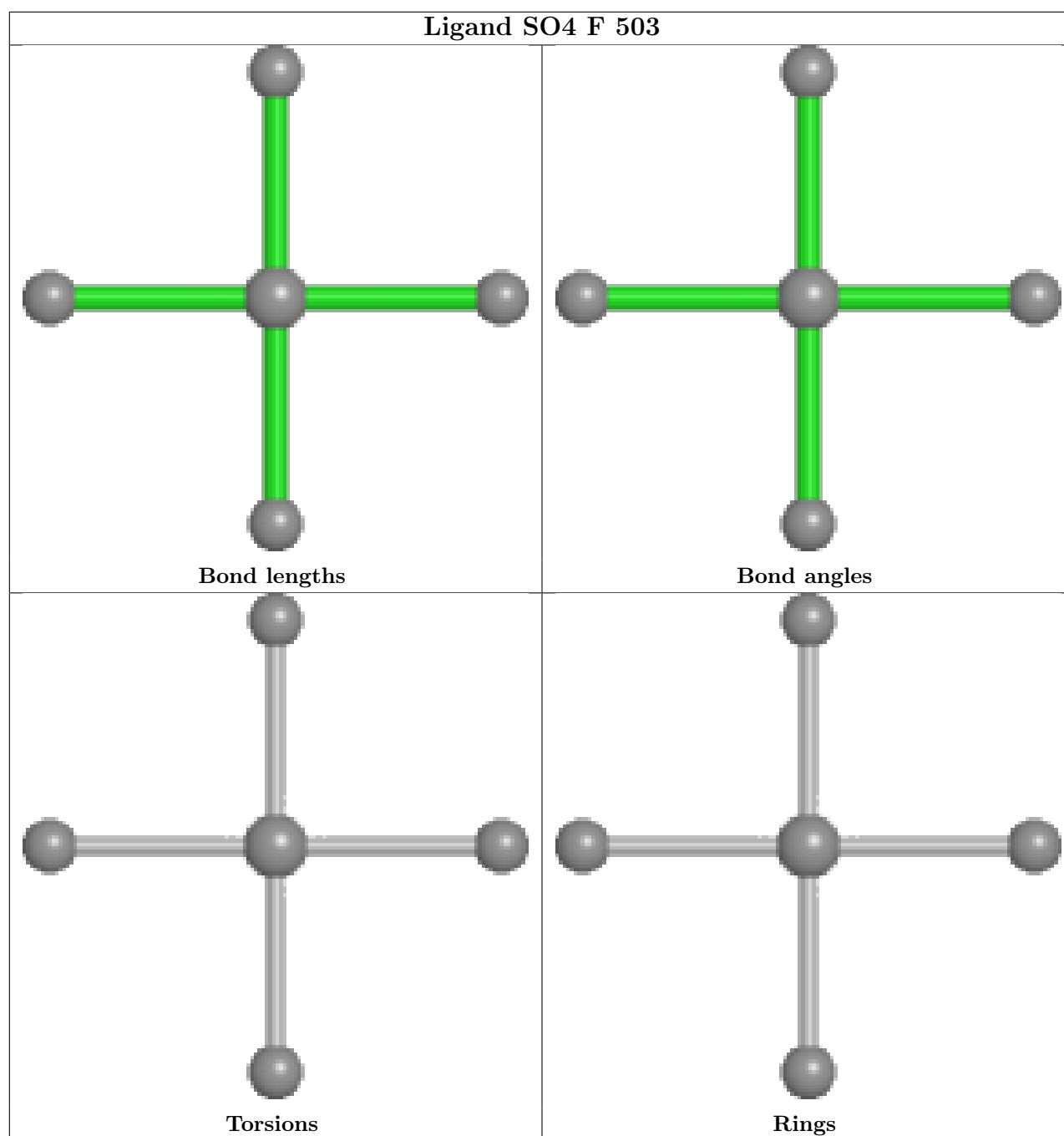
Mol	Chain	Res	Type	Atoms
9	C	1201	SRN	C42-C43-C44-C45
9	C	1201	SRN	C25-C26-C27-C28
9	C	1201	SRN	C14-C15-C16-O9
9	C	1201	SRN	C39-C41-C42-C43
9	C	1201	SRN	C14-C15-C16-C17
9	C	1201	SRN	O2-C1-O1-C33

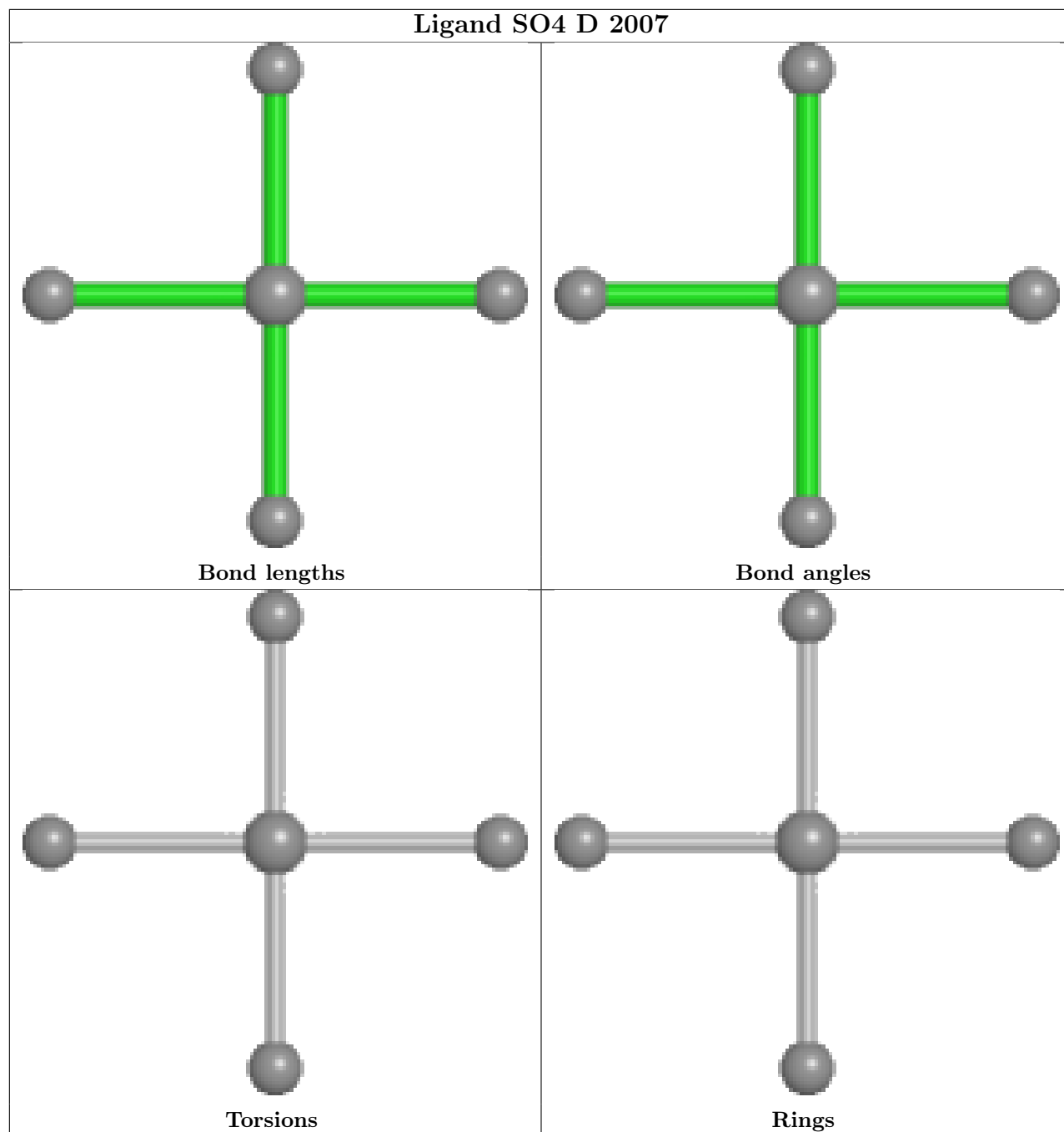
There are no ring outliers.

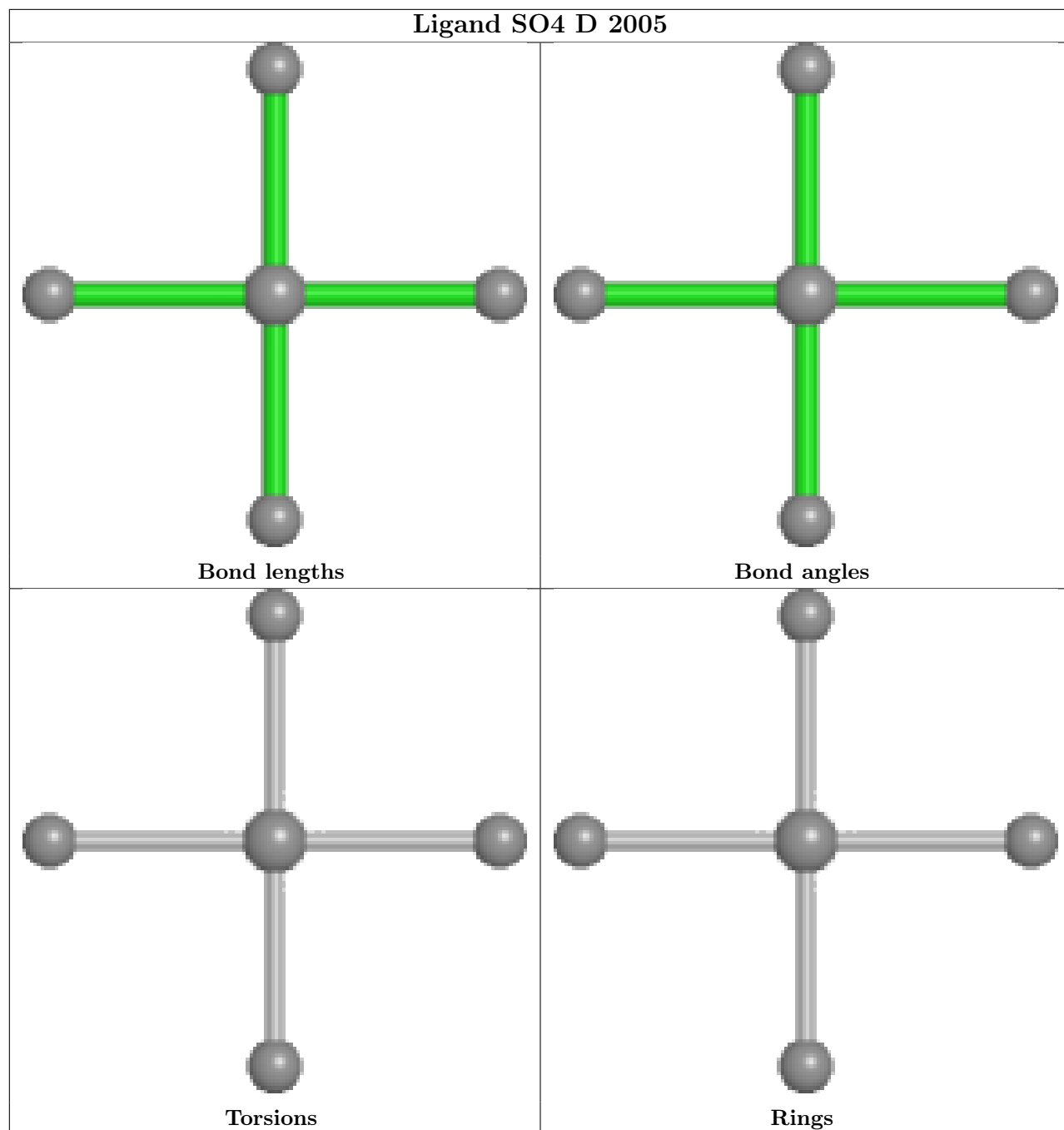
4 monomers are involved in 19 short contacts:

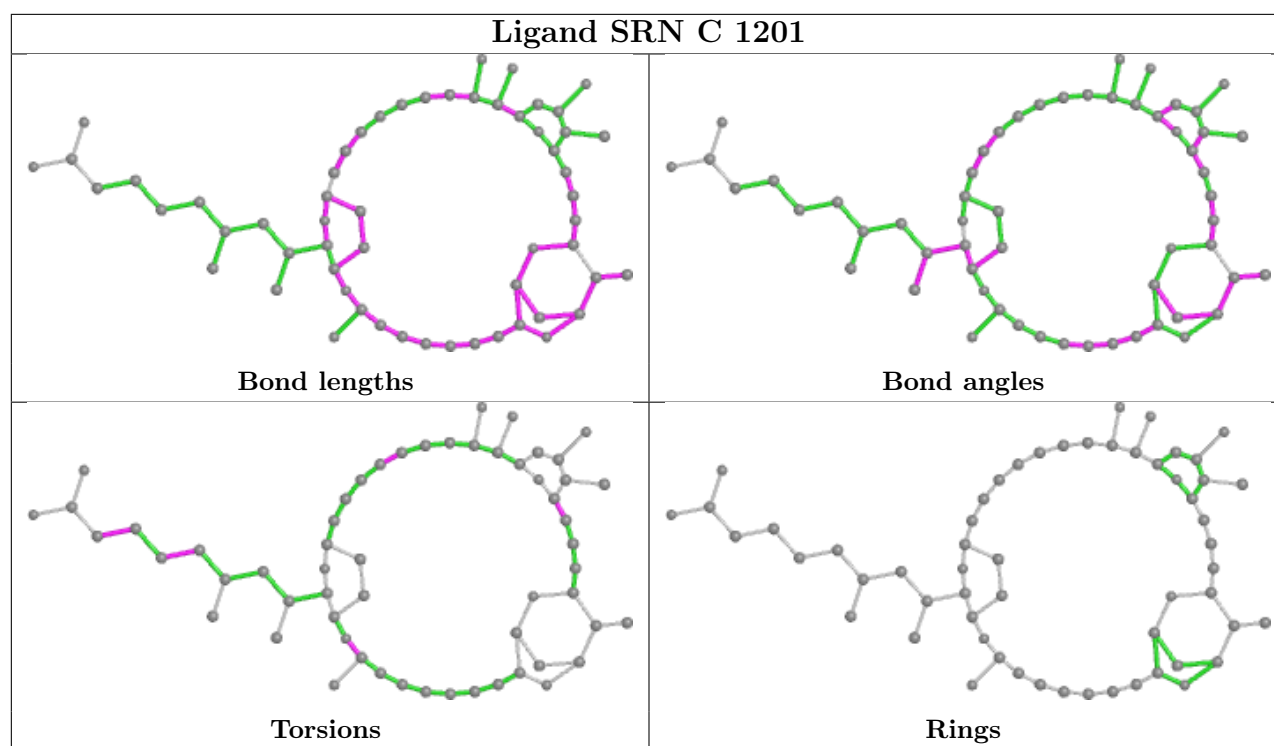
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1201	SRN	16	0
12	D	2006	SO4	1	0
12	F	501	SO4	1	0
12	F	504	SO4	1	0

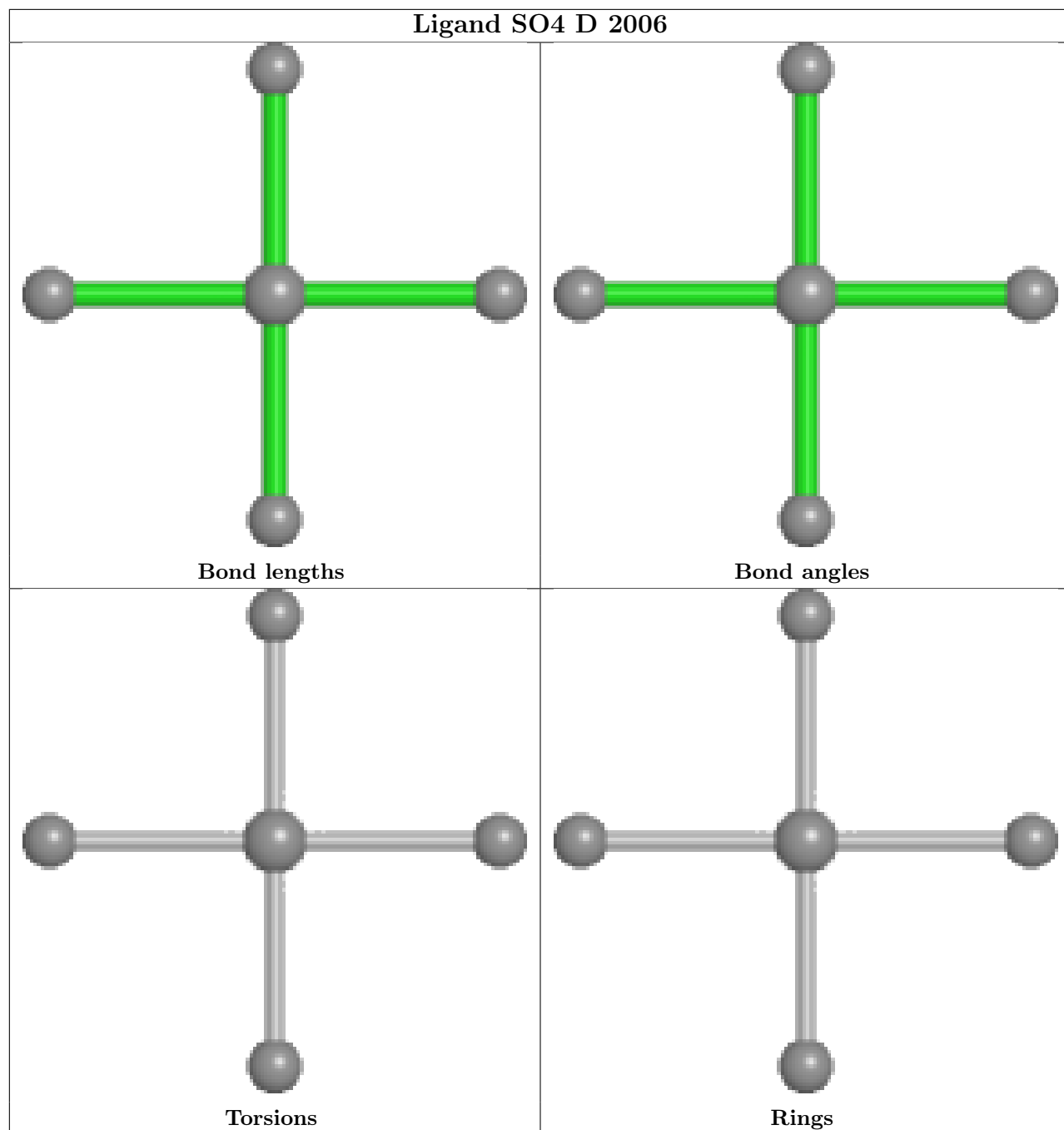
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

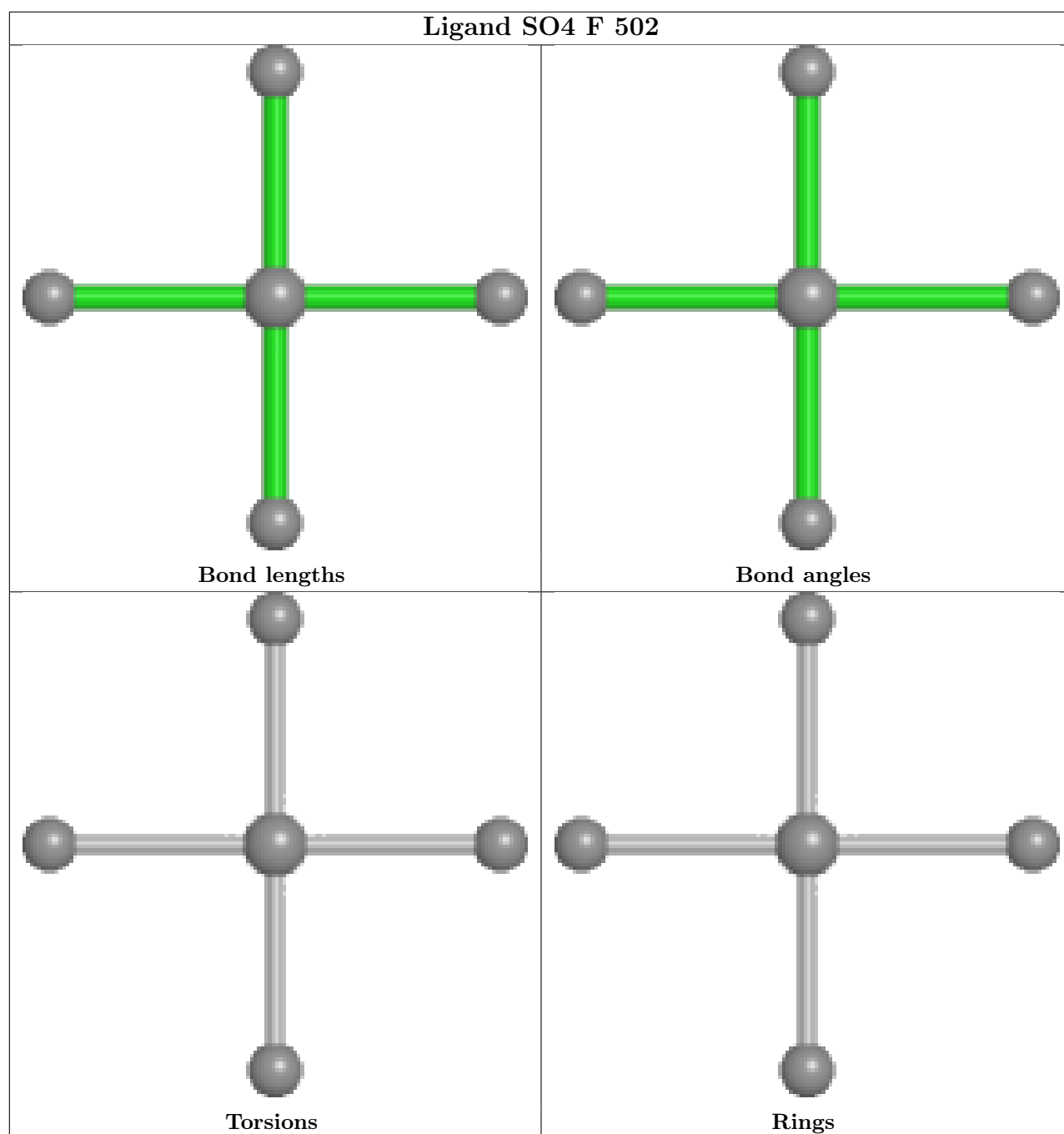


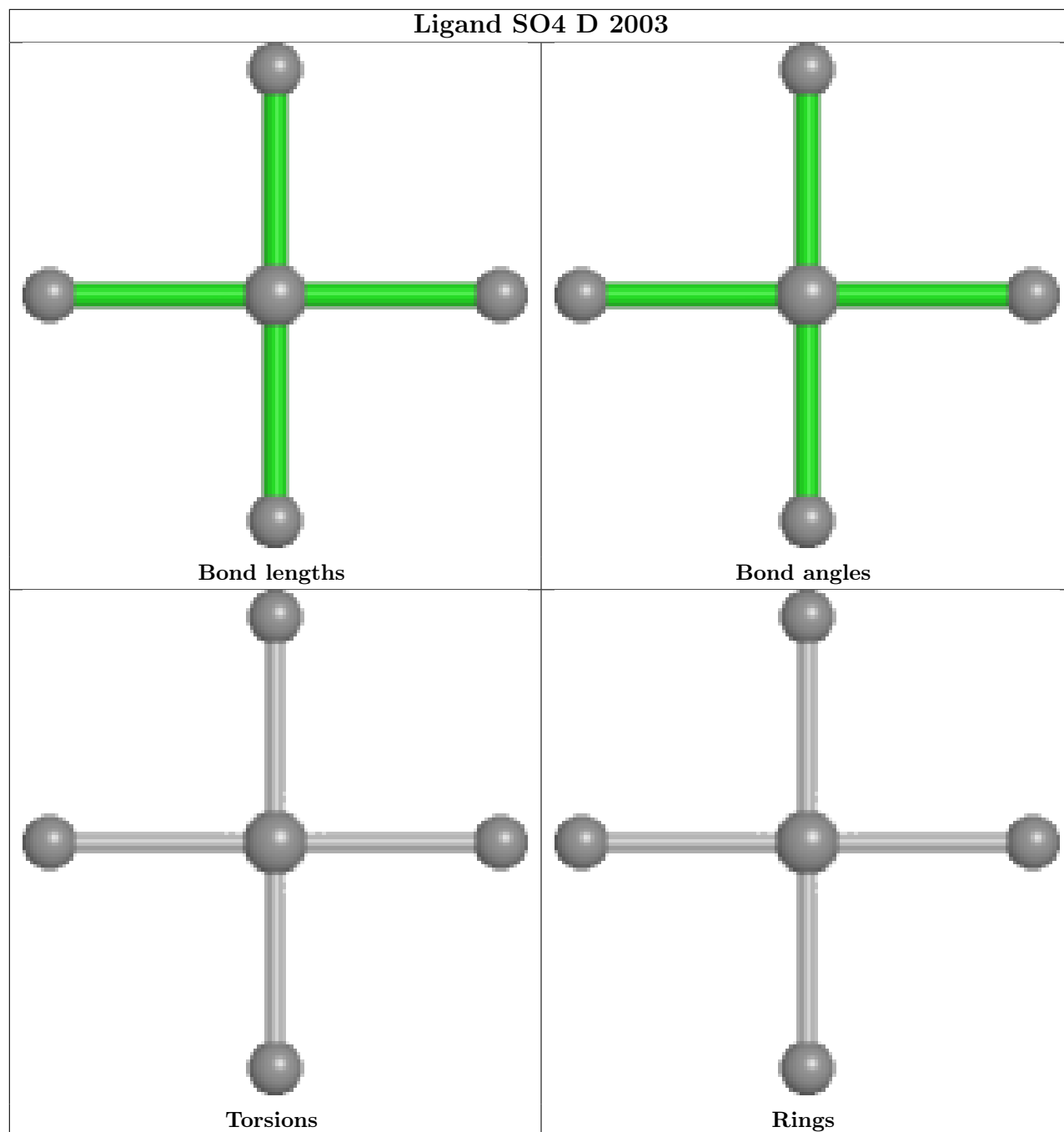


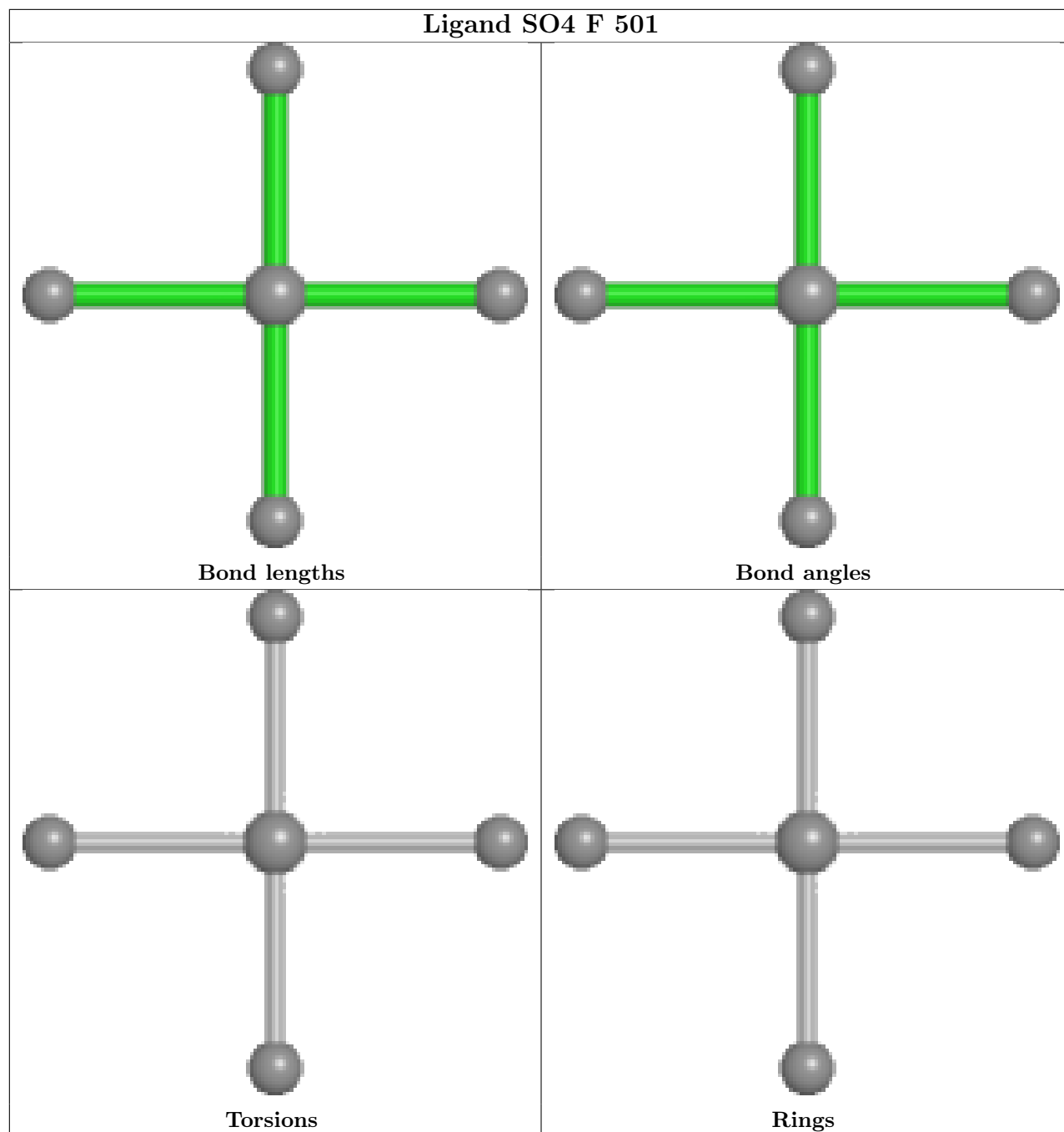


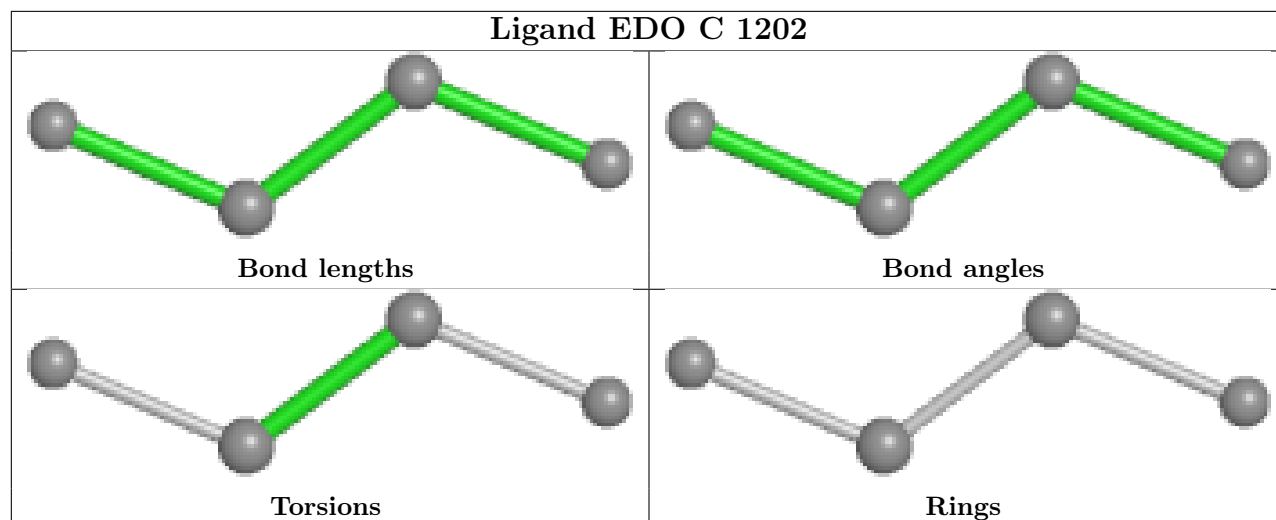


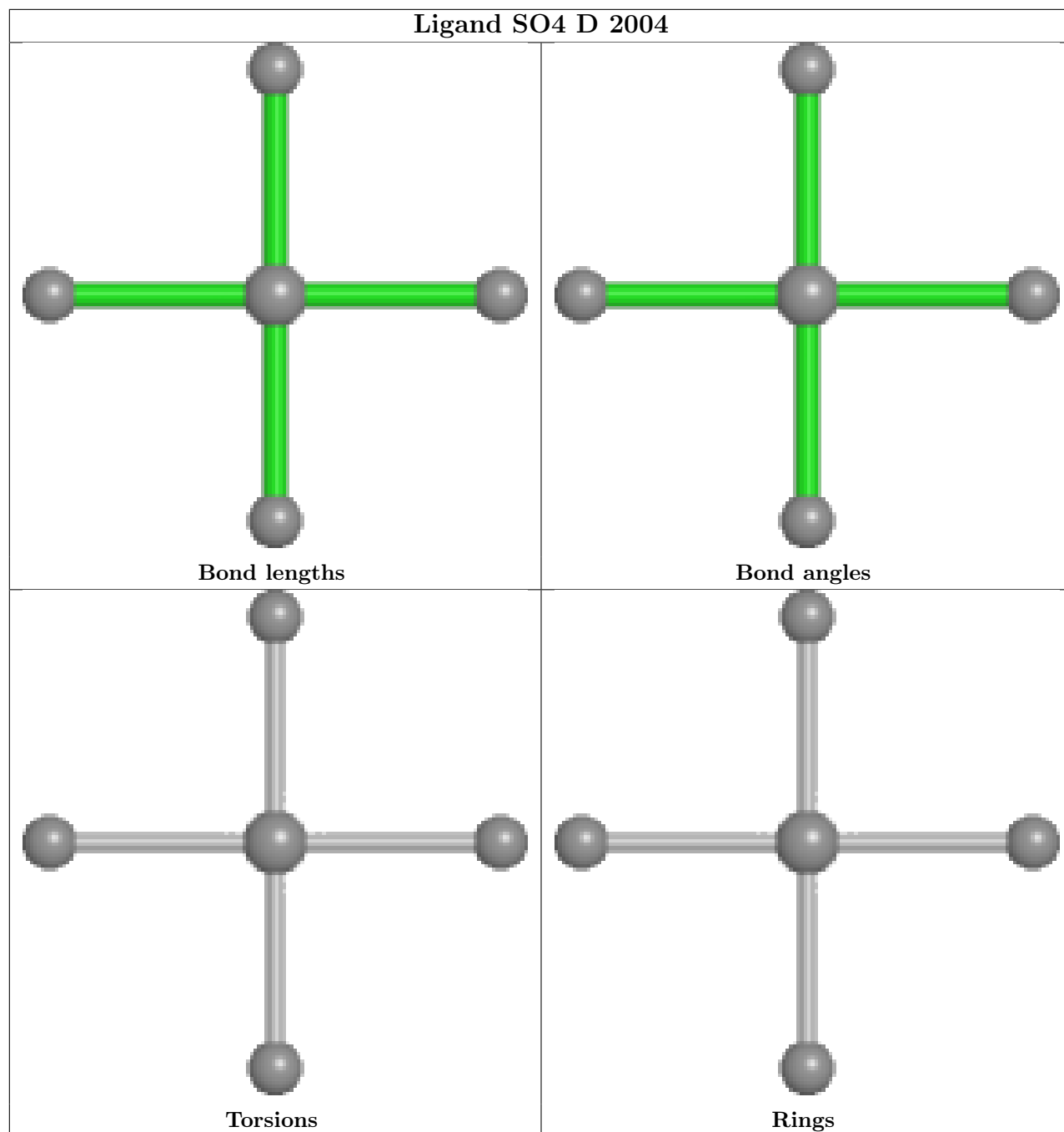


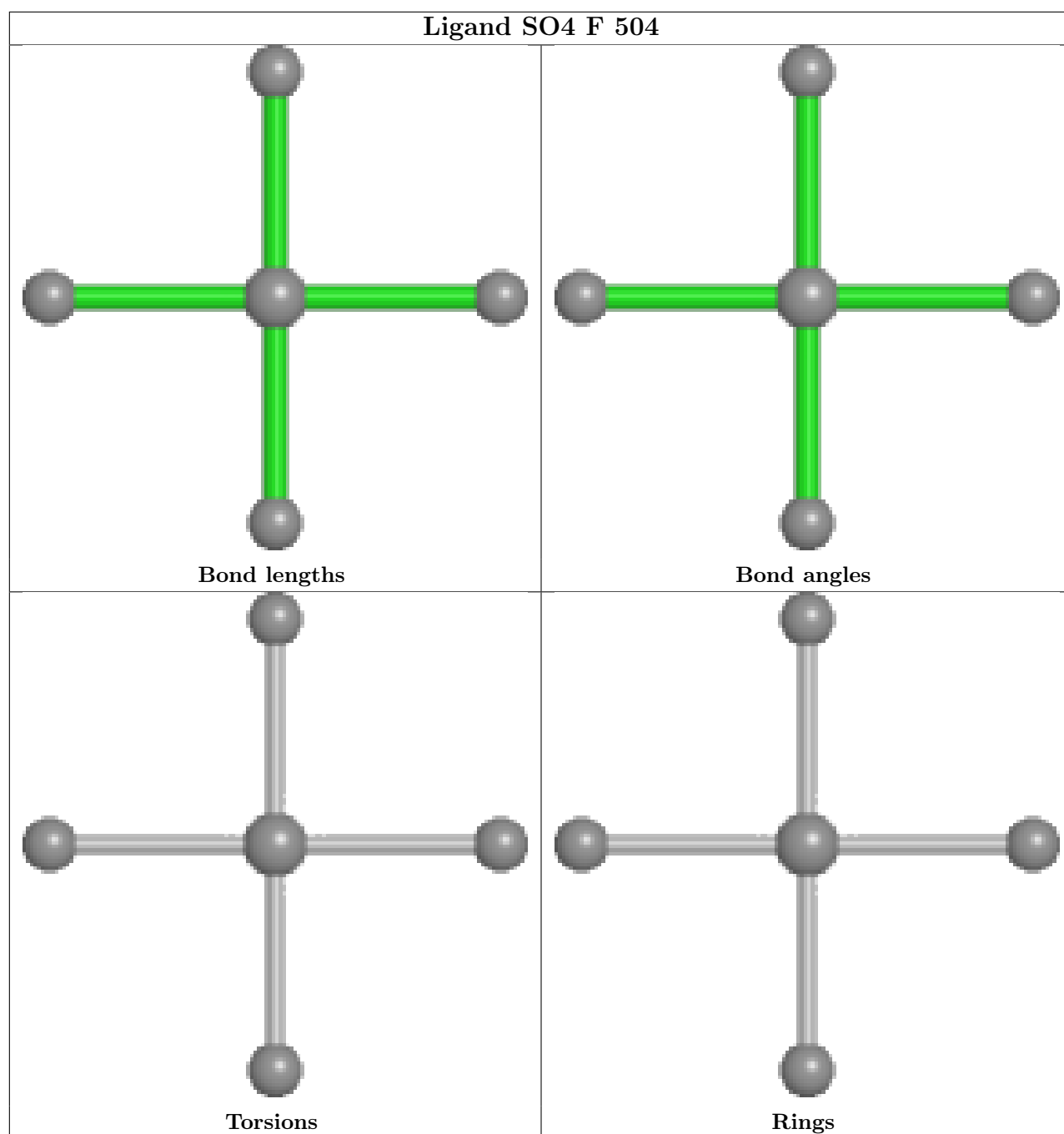












5.7 Other polymers [i](#)

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	84/114 (73%)	0.20	2 (2%) 59 56	69, 105, 148, 164	0
2	A	222/350 (63%)	0.33	13 (5%) 22 18	69, 93, 127, 154	0
2	B	225/350 (64%)	0.32	14 (6%) 20 16	71, 111, 135, 153	0
3	C	883/1169 (75%)	0.53	70 (7%) 12 10	53, 98, 144, 184	0
4	D	1200/1317 (91%)	0.44	78 (6%) 18 14	49, 90, 140, 171	0
5	E	82/107 (76%)	0.80	11 (13%) 3 2	68, 97, 152, 182	0
6	F	303/466 (65%)	0.21	9 (2%) 50 45	47, 88, 121, 155	0
7	O	31/31 (100%)	-0.67	0 100 100	70, 87, 118, 128	0
8	P	26/26 (100%)	-0.63	0 100 100	77, 92, 124, 130	0
All	All	3056/3930 (77%)	0.41	197 (6%) 19 15	47, 95, 141, 184	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	71	GLY	9.5
5	E	72	ILE	8.8
1	J	75	VAL	6.8
3	C	477	ILE	6.6
4	D	773	LEU	5.9
3	C	145	MET	5.2
5	E	106	GLY	5.1
3	C	77	LEU	5.1
4	D	1113	MET	4.9
4	D	738	PRO	4.9
5	E	104	THR	4.9
3	C	81	LEU	4.7
5	E	70	ASP	4.6
3	C	1132	ASP	4.5
3	C	170	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
3	C	384	LEU	4.2
4	D	784	VAL	4.2
3	C	515	VAL	4.1
4	D	751	GLU	4.0
3	C	168	SER	4.0
4	D	1112	LEU	3.9
3	C	503	ILE	3.9
2	B	21	PHE	3.9
4	D	412	ARG	3.9
3	C	385	SER	3.8
3	C	146	GLY	3.8
4	D	1283	ALA	3.8
3	C	497	VAL	3.7
3	C	514	VAL	3.7
3	C	98	PHE	3.7
3	C	83	GLU	3.7
4	D	754	ALA	3.6
3	C	402	ALA	3.6
2	A	140	VAL	3.6
3	C	380	ILE	3.6
4	D	776	ILE	3.6
4	D	788	LEU	3.5
3	C	532	VAL	3.5
4	D	413	PHE	3.5
4	D	1111	GLN	3.5
3	C	70	GLU	3.5
3	C	143	VAL	3.5
4	D	186	ALA	3.5
2	B	104	VAL	3.5
2	B	95	MET	3.4
4	D	265	ILE	3.4
4	D	1279	ALA	3.4
4	D	1087	LEU	3.4
4	D	1063	PHE	3.4
4	D	417	LEU	3.4
3	C	500	PHE	3.4
4	D	1167	THR	3.4
3	C	422	PHE	3.3
4	D	807	THR	3.3
4	D	753	ASP	3.3
3	C	71	GLU	3.2
4	D	755	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	411	GLY	3.2
3	C	56	VAL	3.1
3	C	464	ARG	3.1
2	A	2	LEU	3.1
3	C	941	ALA	3.1
2	A	192	LEU	3.1
2	B	127	THR	3.1
3	C	55	LEU	3.1
4	D	848	TYR	3.1
2	B	14	VAL	3.1
4	D	1282	ALA	3.1
2	A	21	PHE	3.1
5	E	69	GLY	3.1
4	D	1100	LEU	3.1
2	B	162	ILE	3.1
3	C	1133	GLY	3.1
4	D	1046	PRO	3.1
4	D	928	ALA	3.0
6	F	369	GLY	3.0
4	D	760	GLN	3.0
4	D	759	TYR	3.0
3	C	448	ALA	3.0
4	D	847	GLU	3.0
3	C	101	PRO	3.0
5	E	53	TYR	2.9
4	D	1009	LEU	2.9
4	D	64	LYS	2.9
6	F	461	LEU	2.9
4	D	758	LYS	2.9
3	C	383	GLY	2.8
4	D	770	ASN	2.8
5	E	79	LEU	2.8
3	C	551	MET	2.8
3	C	854	ALA	2.8
6	F	445	GLU	2.7
4	D	1170	ASP	2.7
2	A	1	MET	2.7
4	D	1042	ARG	2.7
4	D	846	LEU	2.7
3	C	512	ASN	2.7
3	C	400	VAL	2.7
2	B	114	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	362	ASP	2.7
3	C	954	LEU	2.7
3	C	513	GLY	2.7
3	C	801	GLY	2.7
2	A	38	LEU	2.6
1	J	69	VAL	2.6
3	C	72	ASN	2.6
2	B	112	PRO	2.6
2	B	201	SER	2.6
6	F	452	LEU	2.6
3	C	372	VAL	2.6
6	F	270	VAL	2.6
3	C	538	PRO	2.6
4	D	781	THR	2.6
4	D	1027	GLY	2.6
3	C	816	PHE	2.6
2	A	194	ILE	2.6
3	C	577	MET	2.6
3	C	501	GLY	2.5
2	B	111	VAL	2.5
6	F	365	ILE	2.5
2	B	138	LEU	2.5
4	D	1067	ILE	2.5
2	A	23	ILE	2.5
3	C	410	ASN	2.5
4	D	1182	THR	2.5
3	C	521	TYR	2.5
4	D	1080	LYS	2.5
4	D	1169	ILE	2.5
3	C	476	PRO	2.4
4	D	739	PRO	2.4
4	D	787	ALA	2.4
4	D	774	VAL	2.4
3	C	80	VAL	2.4
4	D	762	GLY	2.4
4	D	650	LEU	2.4
3	C	76	GLY	2.4
3	C	142	THR	2.4
4	D	1060	ASP	2.4
3	C	786	GLU	2.3
3	C	408	LEU	2.3
3	C	1006	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	815	ILE	2.3
2	B	146	TYR	2.3
3	C	1003	ASP	2.3
2	A	4	SER	2.3
4	D	14	LEU	2.3
3	C	169	GLN	2.3
4	D	785	GLY	2.3
3	C	648	TYR	2.3
3	C	121	ALA	2.3
3	C	516	THR	2.3
4	D	1085	GLN	2.3
4	D	925	ALA	2.3
5	E	26	TYR	2.3
3	C	32	PHE	2.3
2	B	13	THR	2.3
4	D	936	ILE	2.3
3	C	811	LEU	2.2
2	A	118	VAL	2.2
4	D	772	SER	2.2
4	D	1143	TYR	2.2
6	F	419	LEU	2.2
3	C	144	PHE	2.2
2	A	34	LEU	2.2
4	D	405	LEU	2.2
4	D	1168	ILE	2.2
4	D	264	LEU	2.2
3	C	366	ASN	2.2
4	D	1189	ALA	2.2
2	A	22	VAL	2.2
6	F	434	TYR	2.2
4	D	270	ILE	2.1
4	D	898	VAL	2.1
4	D	1056	LEU	2.1
3	C	927	LEU	2.1
2	B	102	PRO	2.1
4	D	1273	VAL	2.1
4	D	943	LEU	2.1
5	E	50	LEU	2.1
3	C	450	GLY	2.1
4	D	856	ARG	2.1
4	D	1084	ARG	2.1
6	F	433	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	173	SER	2.1
4	D	646	LEU	2.1
3	C	399	ASP	2.1
2	A	17	ASN	2.1
4	D	1208	LEU	2.0
4	D	745	LEU	2.0
4	D	900	LEU	2.0
4	D	1079	ASP	2.0
4	D	783	GLU	2.0
5	E	76	VAL	2.0
4	D	798	ILE	2.0
3	C	167	VAL	2.0
4	D	234	LEU	2.0
4	D	951	LEU	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
12	SO4	F	501	5/5	0.81	0.19	75,106,114,121	0
12	SO4	D	2007	5/5	0.84	0.14	119,123,149,152	0
12	SO4	D	2006	5/5	0.85	0.21	128,128,144,151	0
9	SRN	C	1201	58/58	0.86	0.46	75,100,123,127	0
12	SO4	F	504	5/5	0.86	0.31	111,120,134,141	0
10	EDO	C	1202	4/4	0.89	0.25	98,117,127,134	0
12	SO4	D	2003	5/5	0.90	0.14	99,102,122,134	0
12	SO4	D	2004	5/5	0.93	0.29	108,118,134,141	0
12	SO4	D	2005	5/5	0.97	0.09	88,92,106,120	0

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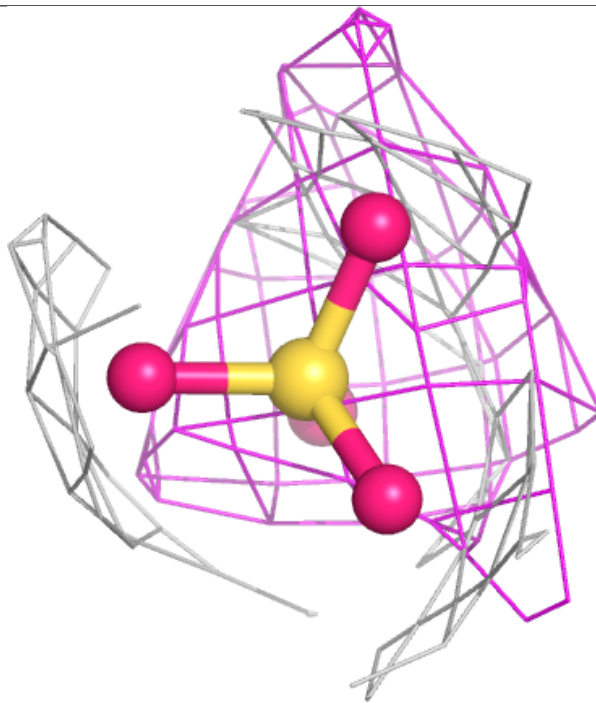
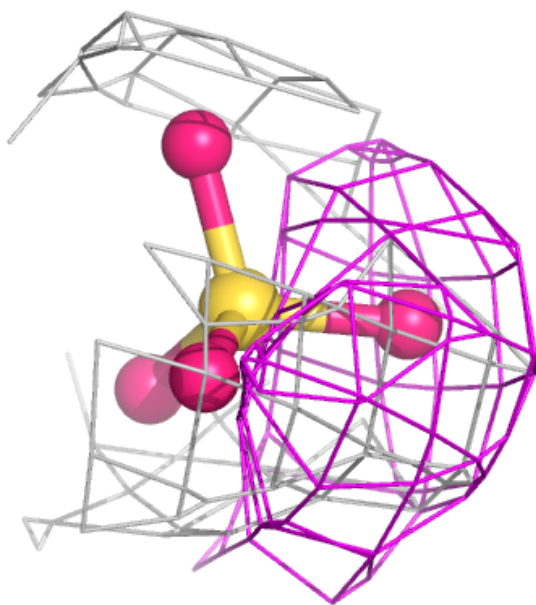
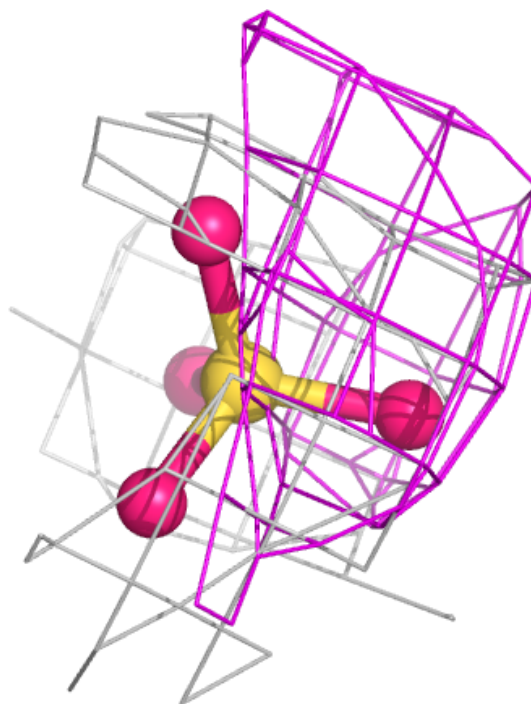
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	SO4	F	503	5/5	0.97	0.15	76,93,104,112	0
12	SO4	F	502	5/5	0.98	0.08	88,88,97,106	0
11	ZN	D	2002	1/1	0.98	0.27	139,139,139,139	0
11	ZN	D	2001	1/1	0.99	0.23	85,85,85,85	0

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.

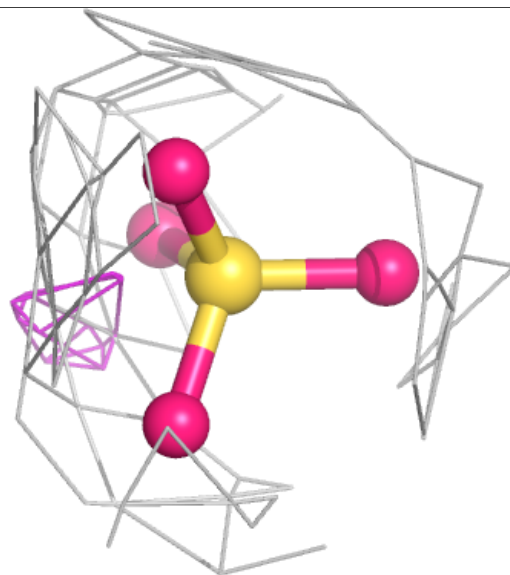
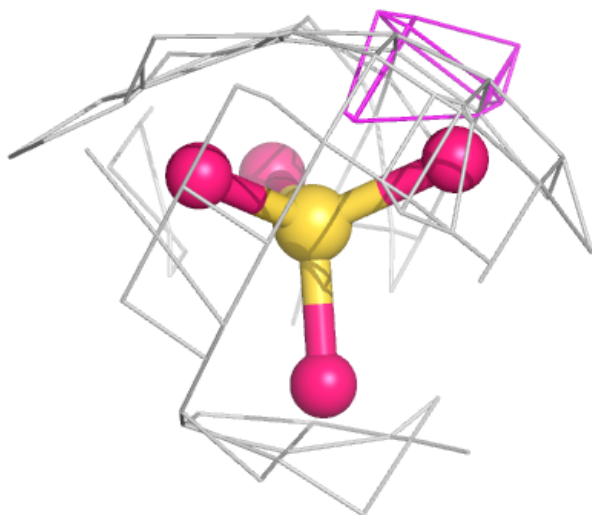
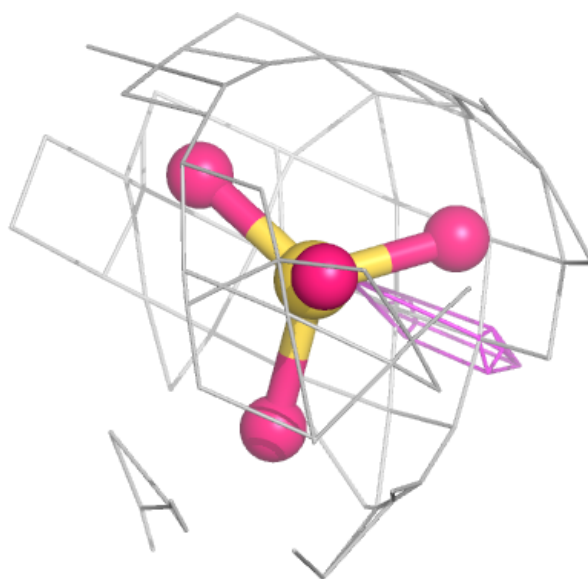
Electron density around SO4 F 501:

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



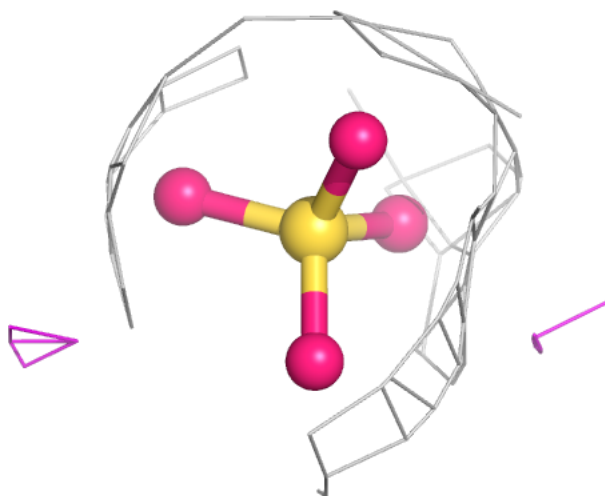
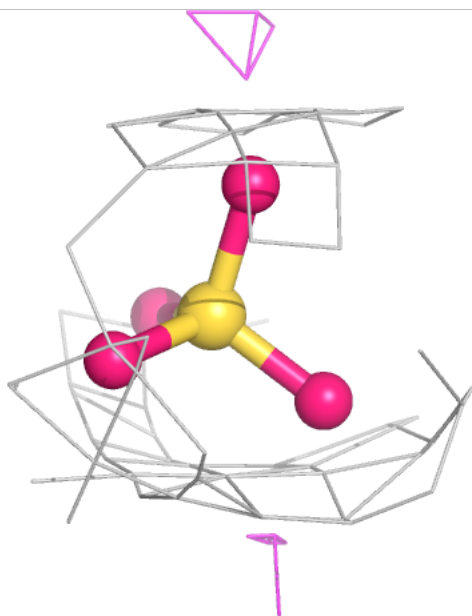
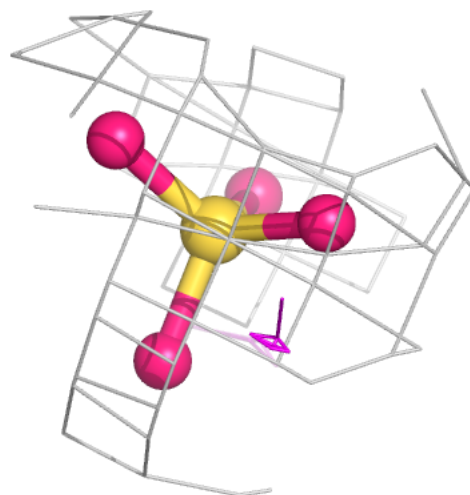
Electron density around SO4 D 2007:

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



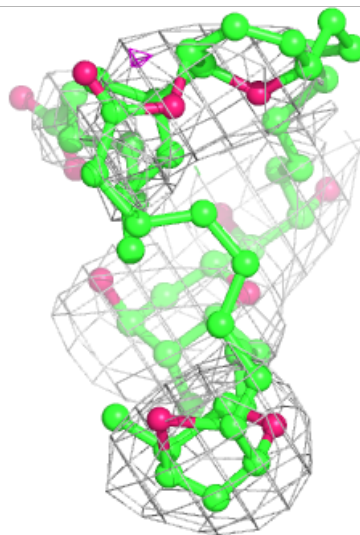
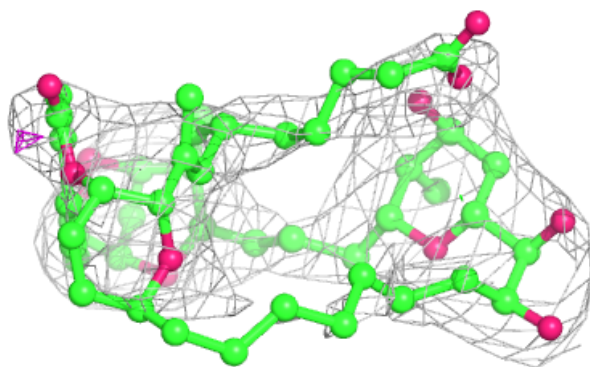
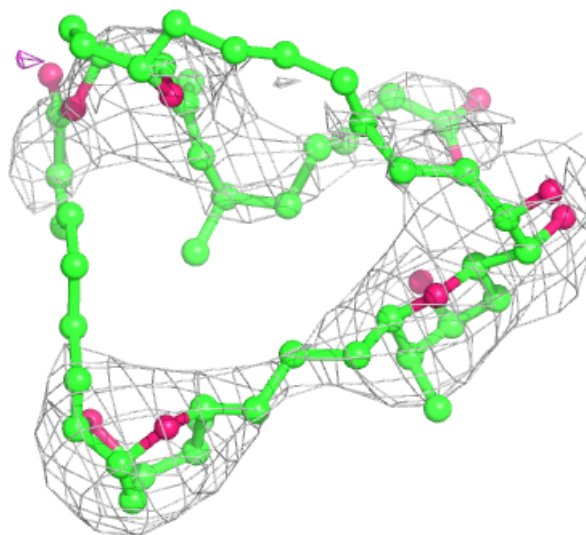
Electron density around SO4 D 2006:

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



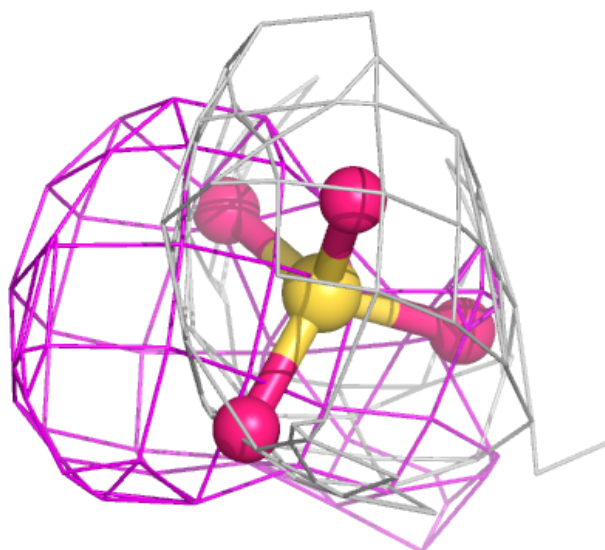
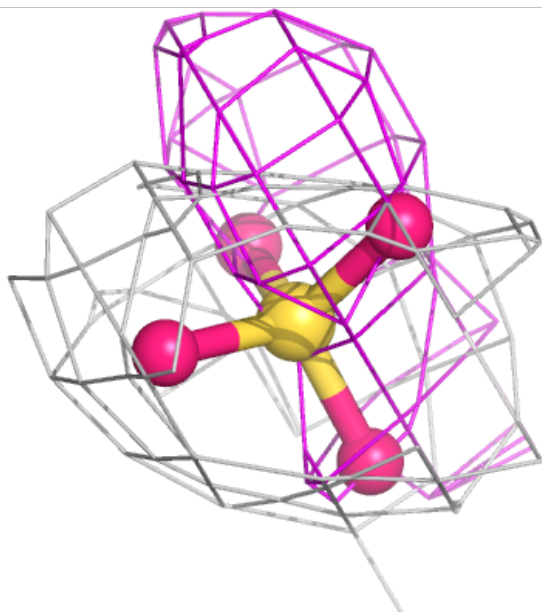
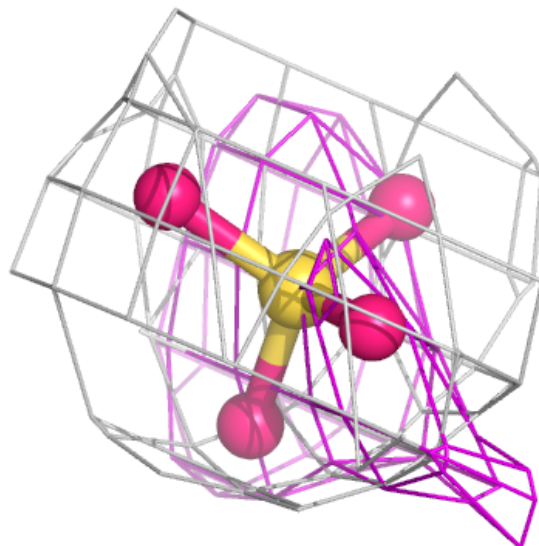
Electron density around SRN C 1201:

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



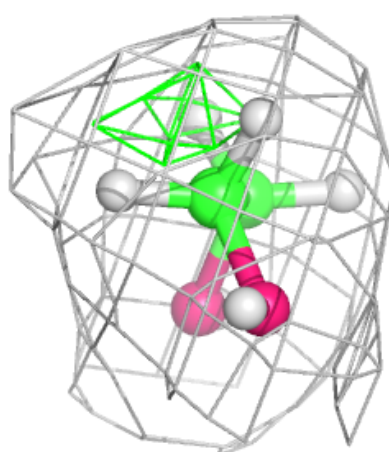
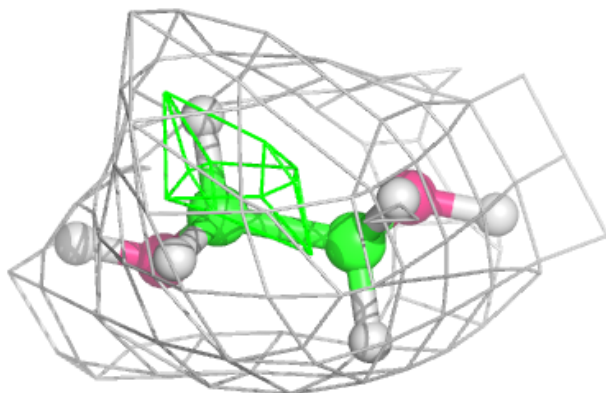
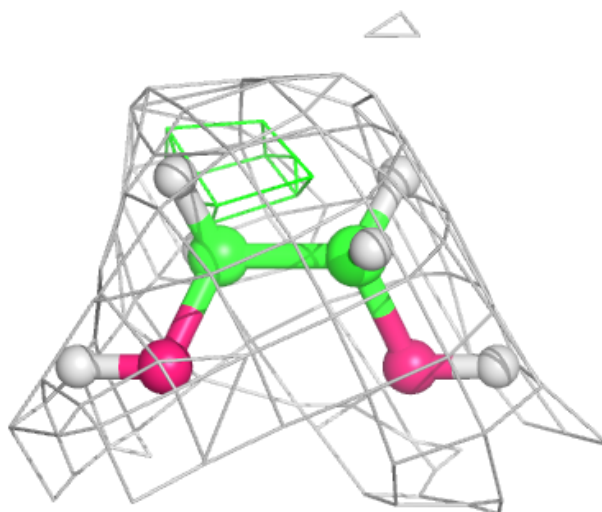
Electron density around SO4 F 504:

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



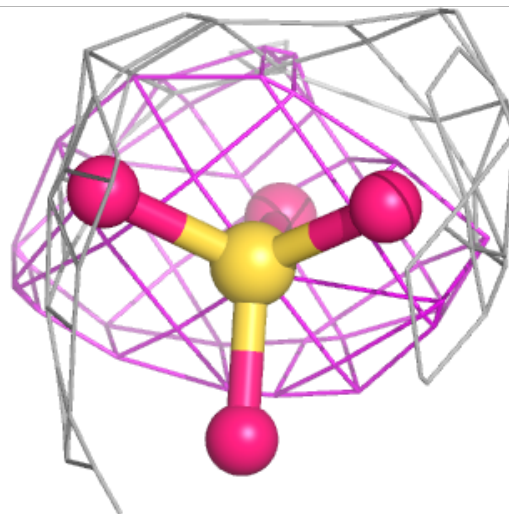
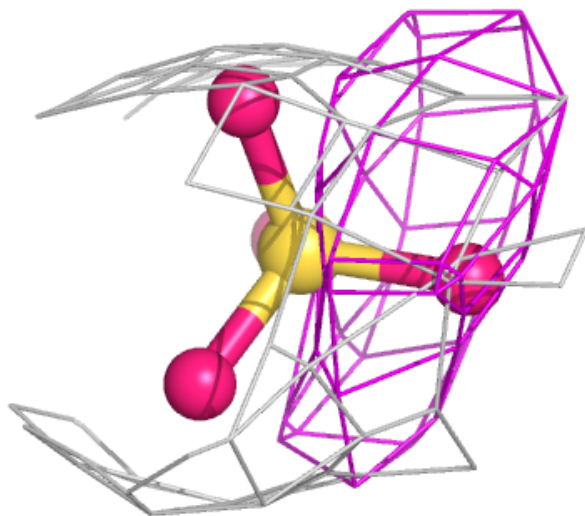
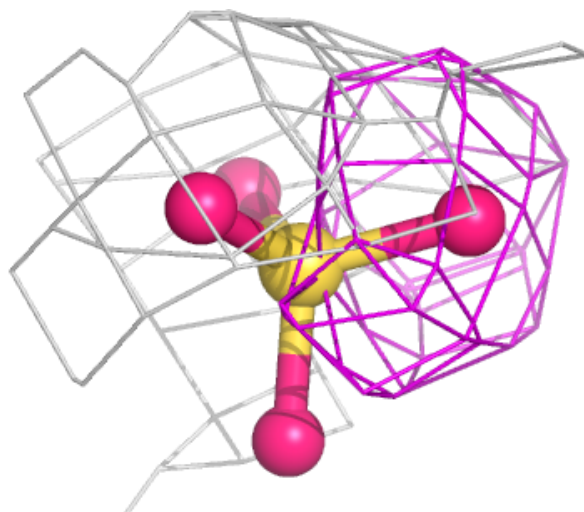
Electron density around EDO C 1202:

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



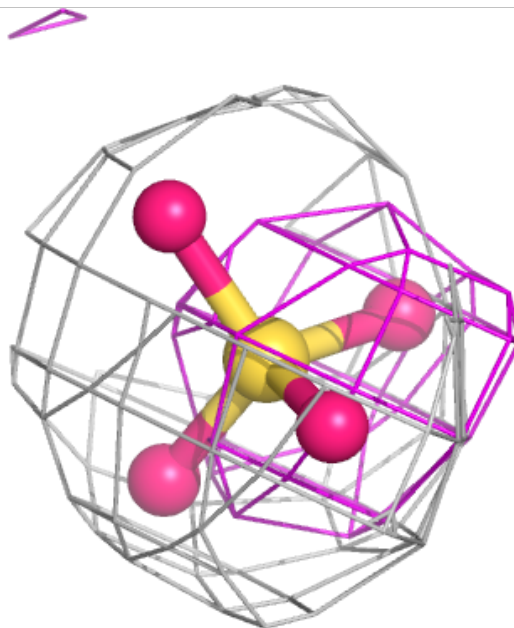
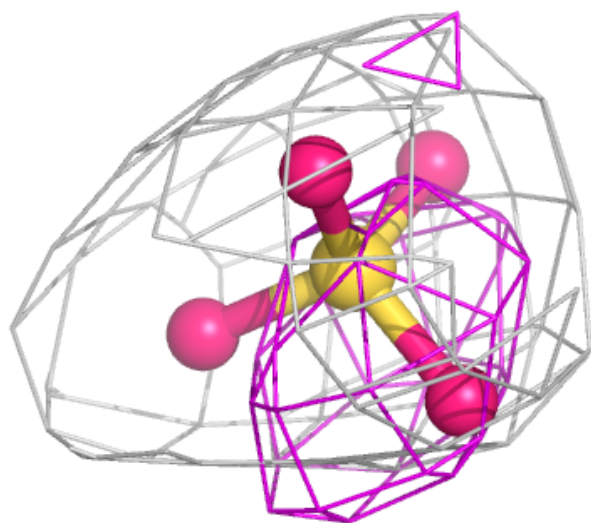
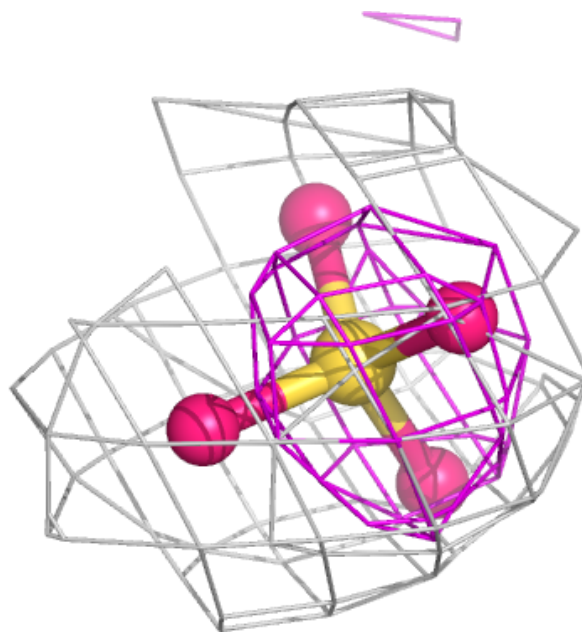
Electron density around SO4 D 2003:

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



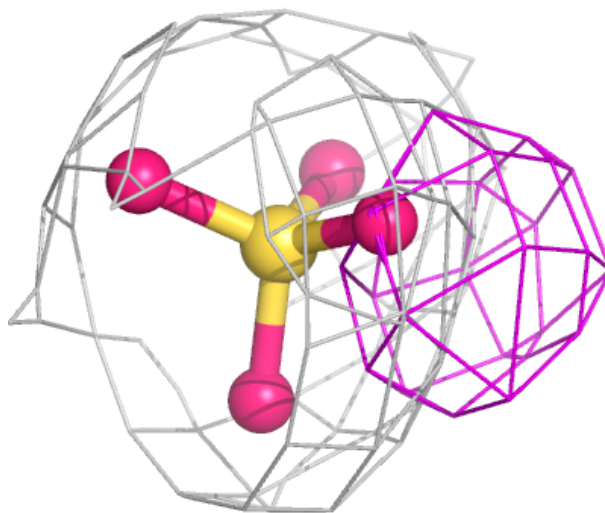
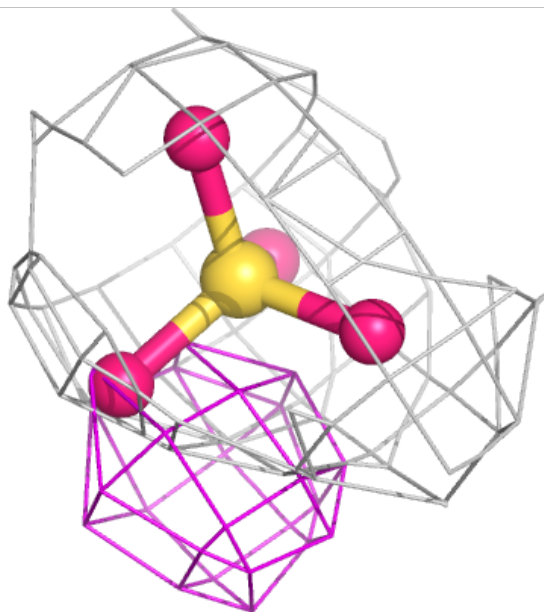
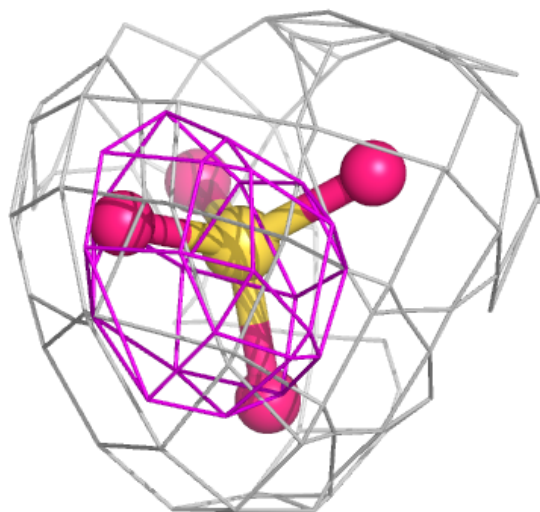
Electron density around SO4 D 2004:

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



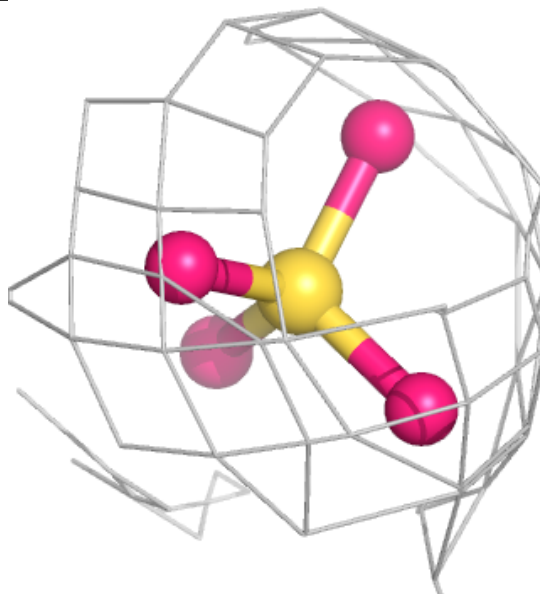
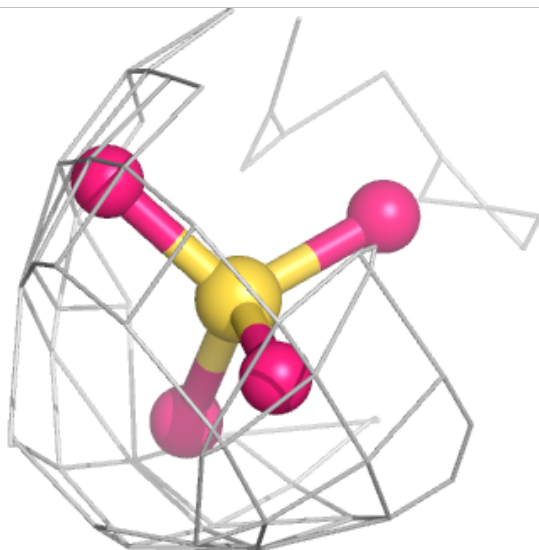
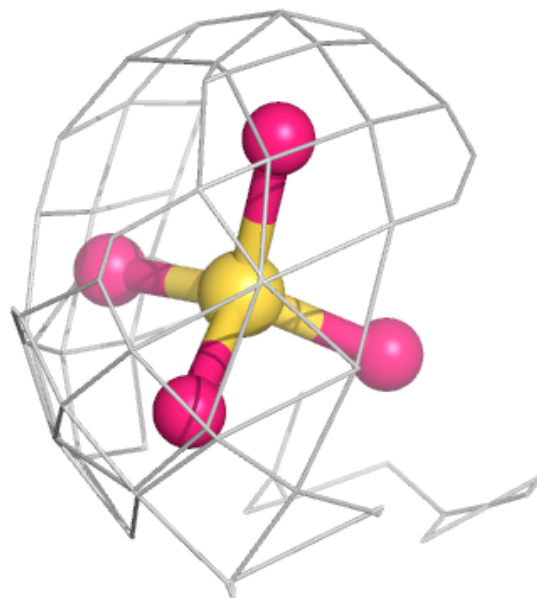
Electron density around SO4 D 2005:

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



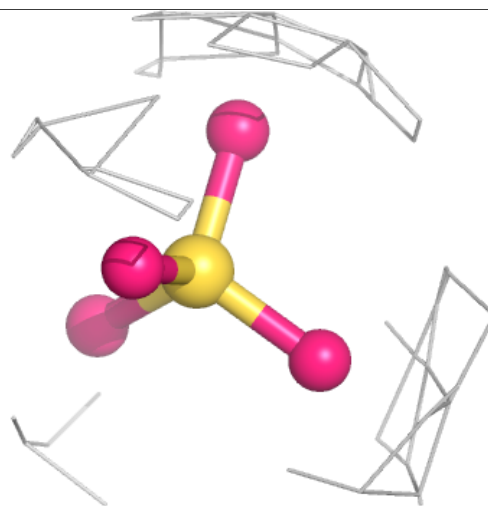
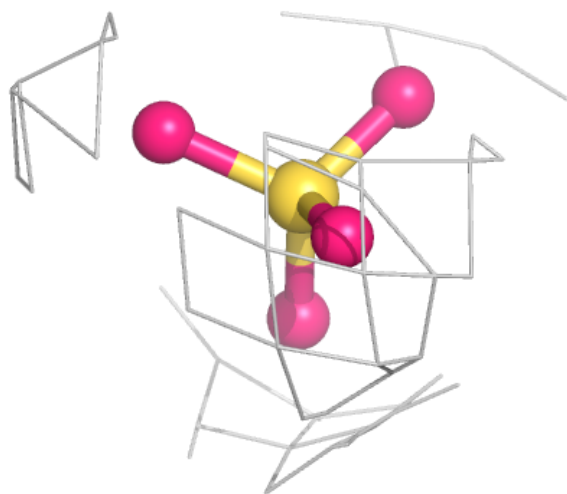
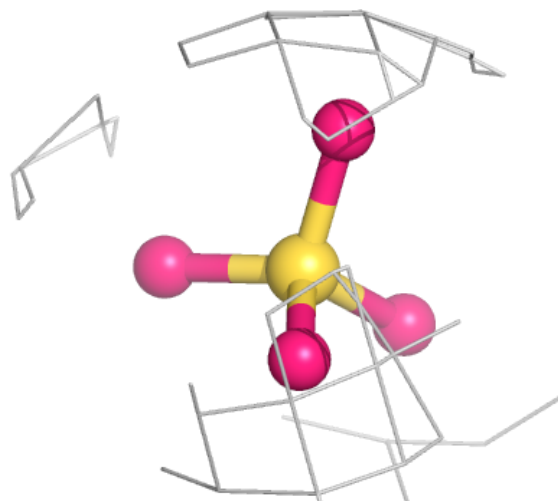
Electron density around SO4 F 503:

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



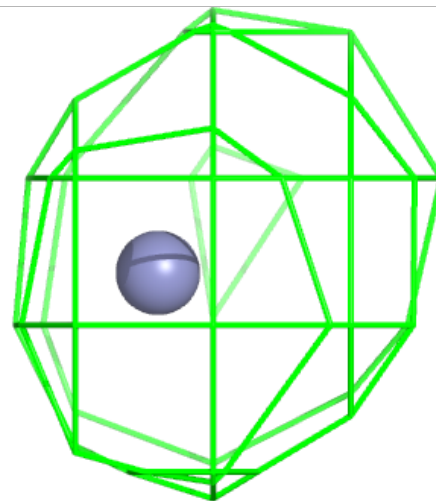
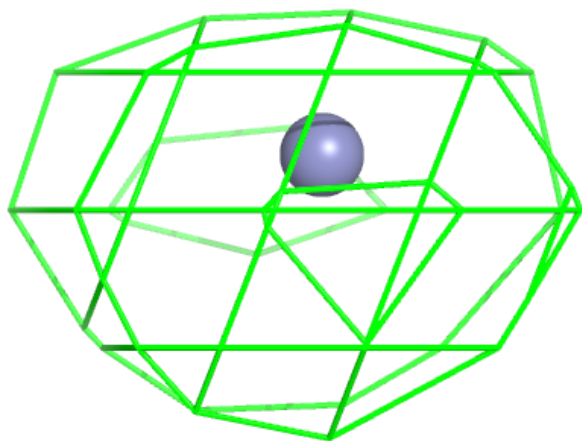
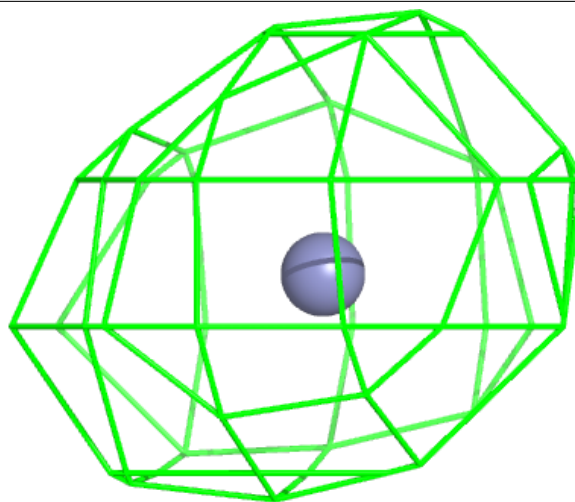
Electron density around SO4 F 502:

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



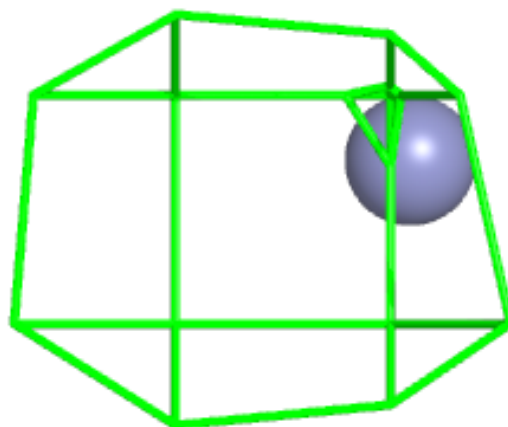
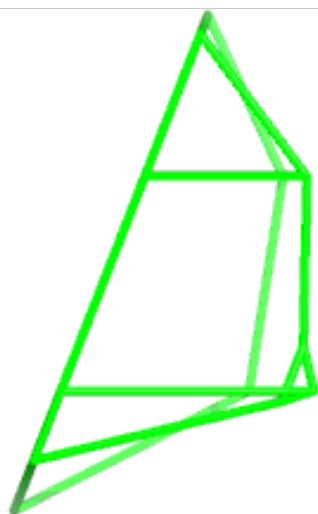
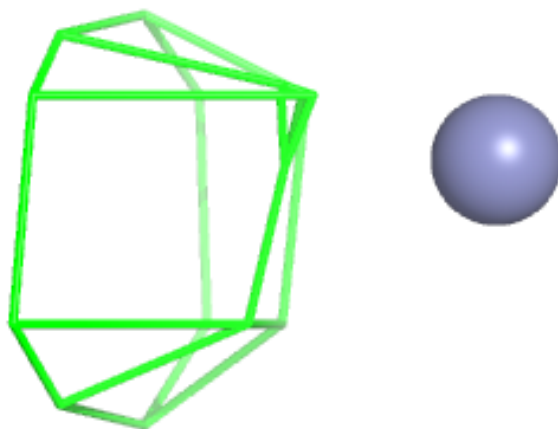
Electron density around ZN D 2002:

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



Electron density around ZN D 2001:

$2mF_o - DF_c$ (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.