



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2020 – 12:30 PM EDT

PDB ID : 6VVS
Title : Crystal structure of a Mycobacterium smegmatis RNA polymerase transcription initiation complex with antibiotic Sorangicin
Authors : Lilic, M.; Braffman, N.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 3.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

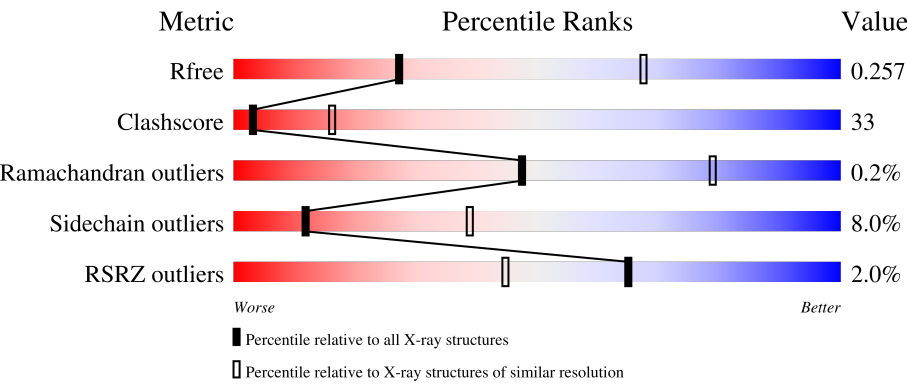
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



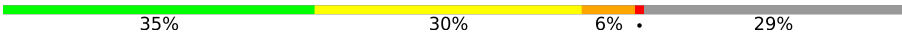
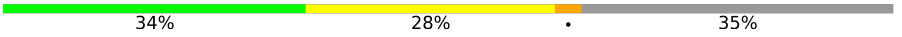
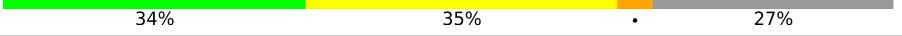

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	A	350	<div><div>%</div><div>31%29%38%</div></div>
1	B	350	<div><div>2%</div><div>26%35%5%33%</div></div>
1	T	350	<div><div>3%</div><div>12%85%</div></div>
2	C	1169	<div><div>3%</div><div>43%47%6%</div></div>
3	D	1317	<div><div>%</div><div>50%41%5%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	107	
5	F	466	
6	G	17	
7	J	114	
8	O	31	
9	P	26	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	D	2004	-	-	X	-
11	EDO	D	2007	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26620 atoms, of which 56 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1605	1015	276	311	3			
1	B	233	Total	C	N	O	S	0	0	0
			1672	1056	289	325	2			
1	T	53	Total	C	N	O	S	0	0	0
			342	208	65	68	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1099	Total	C	N	O	S	0	0	0
			8275	5181	1453	1606	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1246	Total	C	N	O	S	0	0	0
			9555	5995	1720	1800	40			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	76	Total	C	N	O	0	0	0
			592	378	100	114			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	305	Total	C	N	O	S	0	0	0
			2407	1509	436	455	7			

- Molecule 6 is a protein called unknown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 7 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	83	Total	C	N	O	S	0	0	0
			671	422	119	128	2			

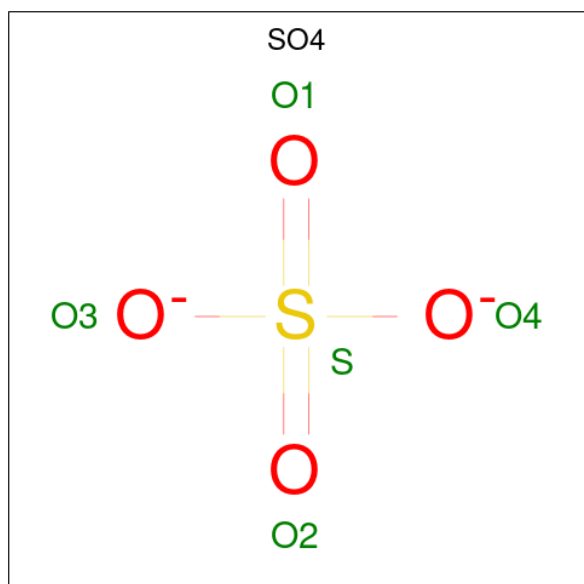
- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	O	31	Total	C	N	O	P	0	0	0
			633	305	114	184	30			

- Molecule 9 is a DNA chain called DNA (26-MER).

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

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

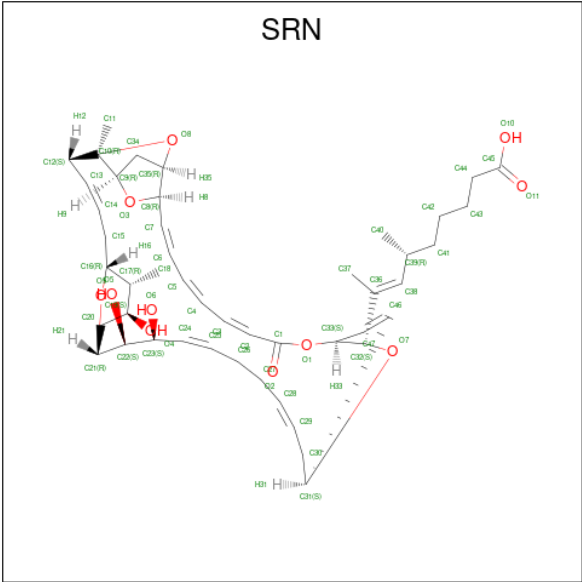
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10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

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by author).



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

- Molecule 12 is SORANGICIN A (three-letter code: SRN) (formula: C₄₇H₆₆O₁₁) (labeled as "Ligand of Interest" by author).



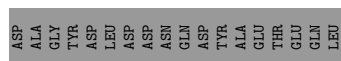
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			58	47	11		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

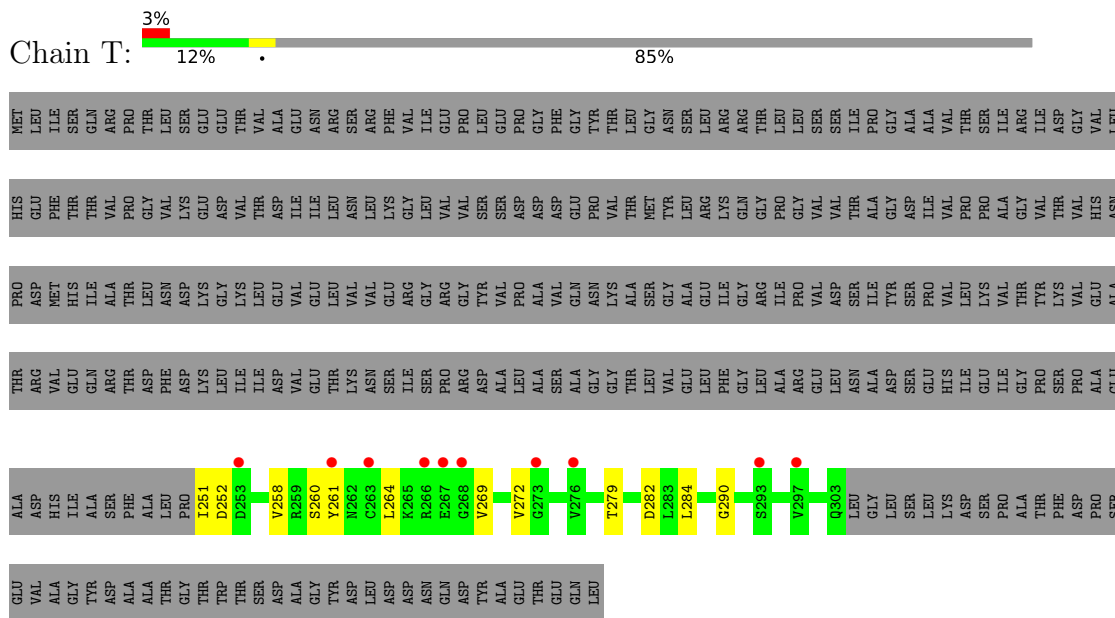
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	2	Total	Zn	0	0
			2	2		

- Molecule 14 is water.

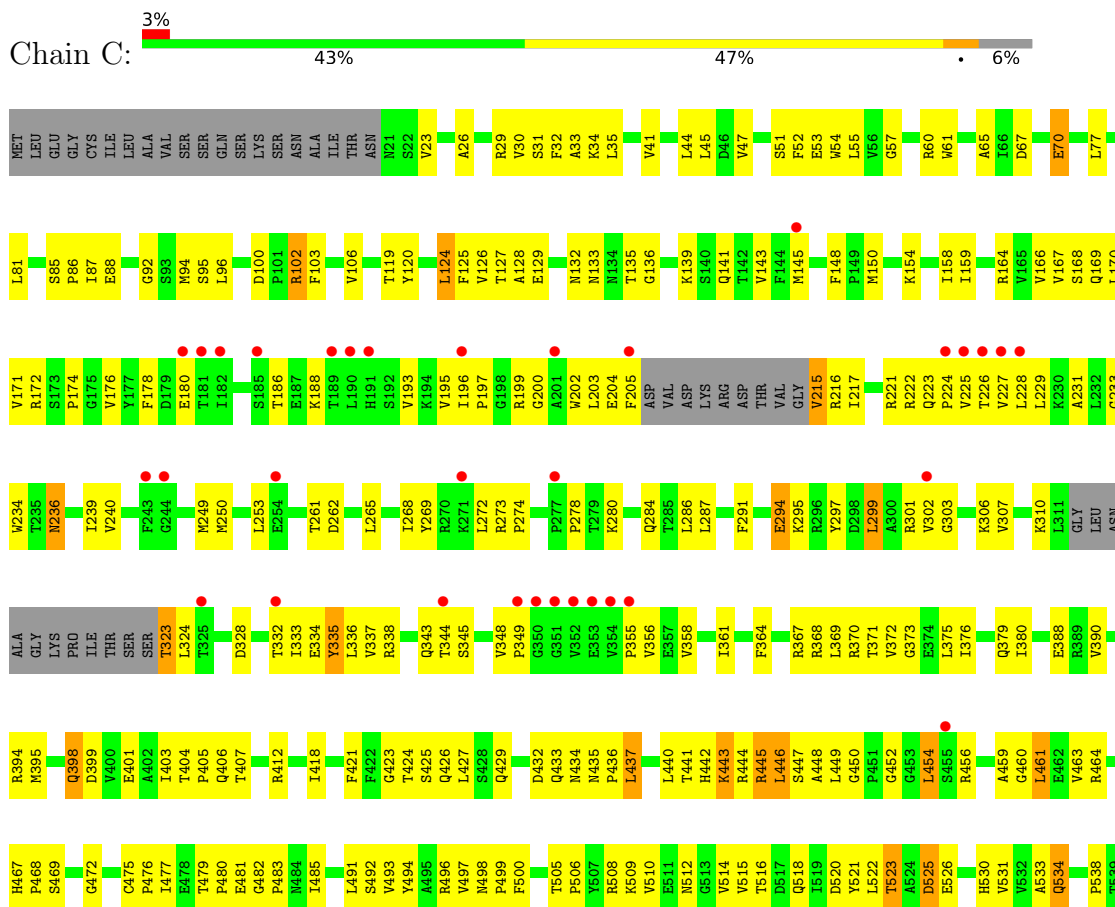
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	7	Total	H	O	0	0
			11	4	7		
14	D	21	Total	H	O	0	0
			29	8	21		
14	E	1	Total	O		0	0
			1	1			
14	F	8	Total	H	O	0	0
			10	2	8		
14	J	1	Total	O		0	0
			1	1			
14	O	3	Total	O		0	0
			3	3			
14	P	2	Total	O		0	0
			2	2			

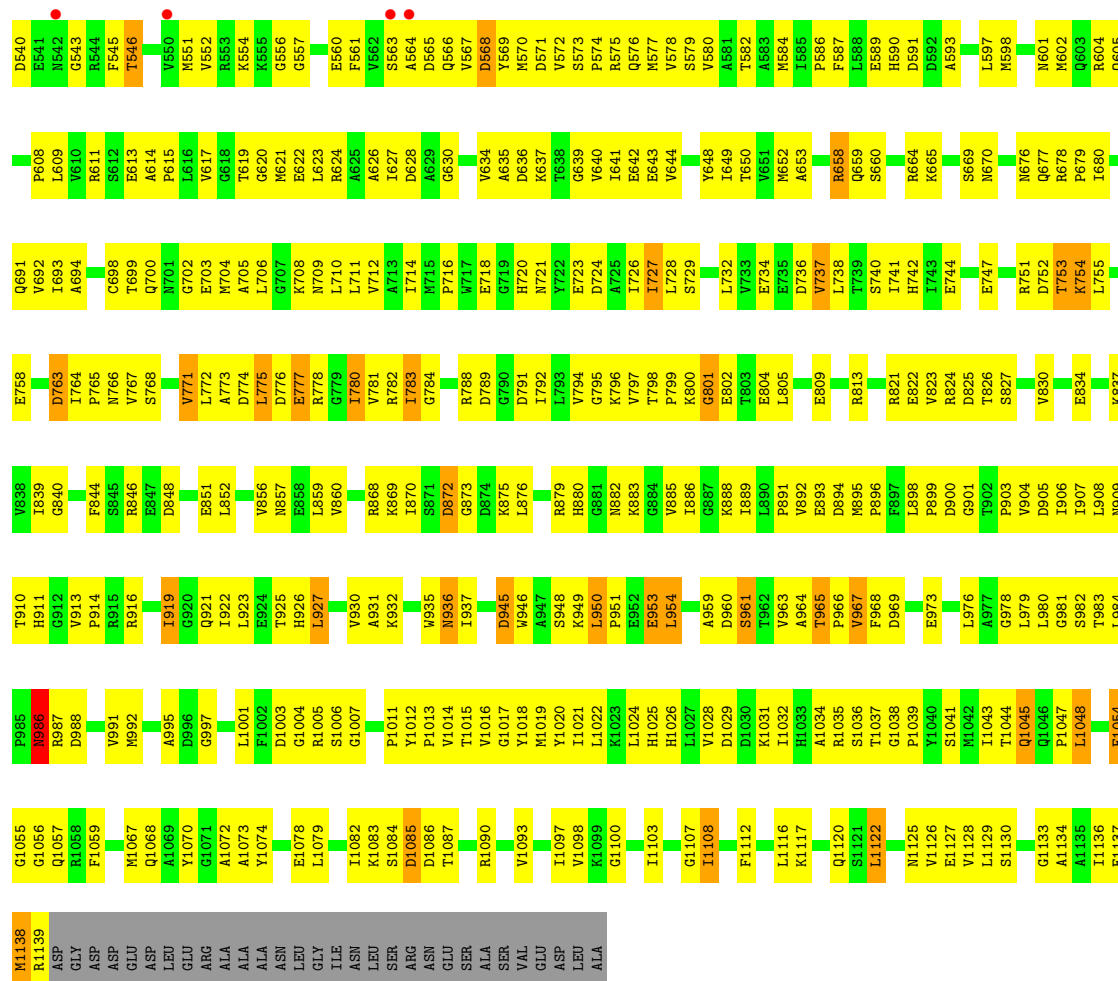


- Molecule 1: DNA-directed RNA polymerase subunit alpha

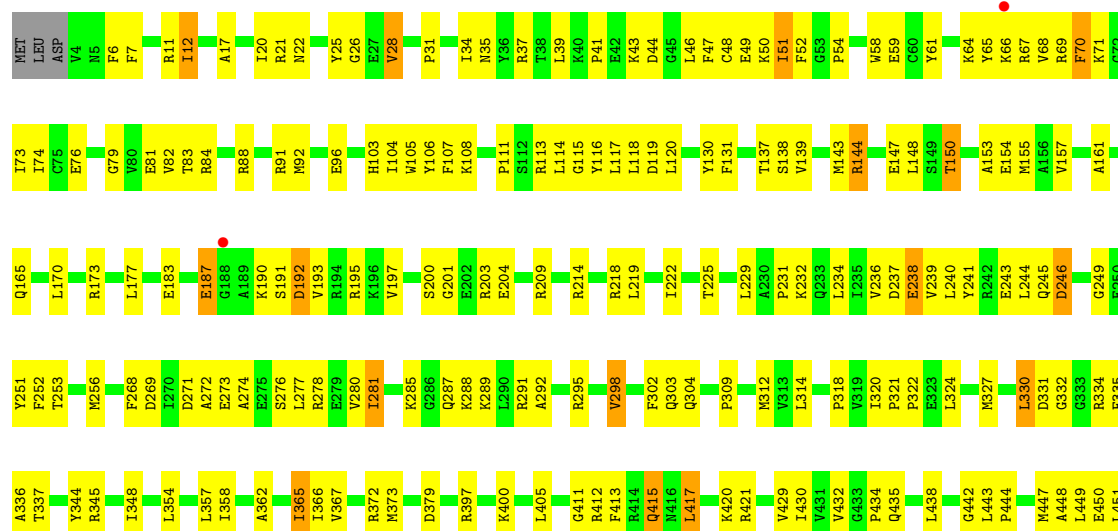


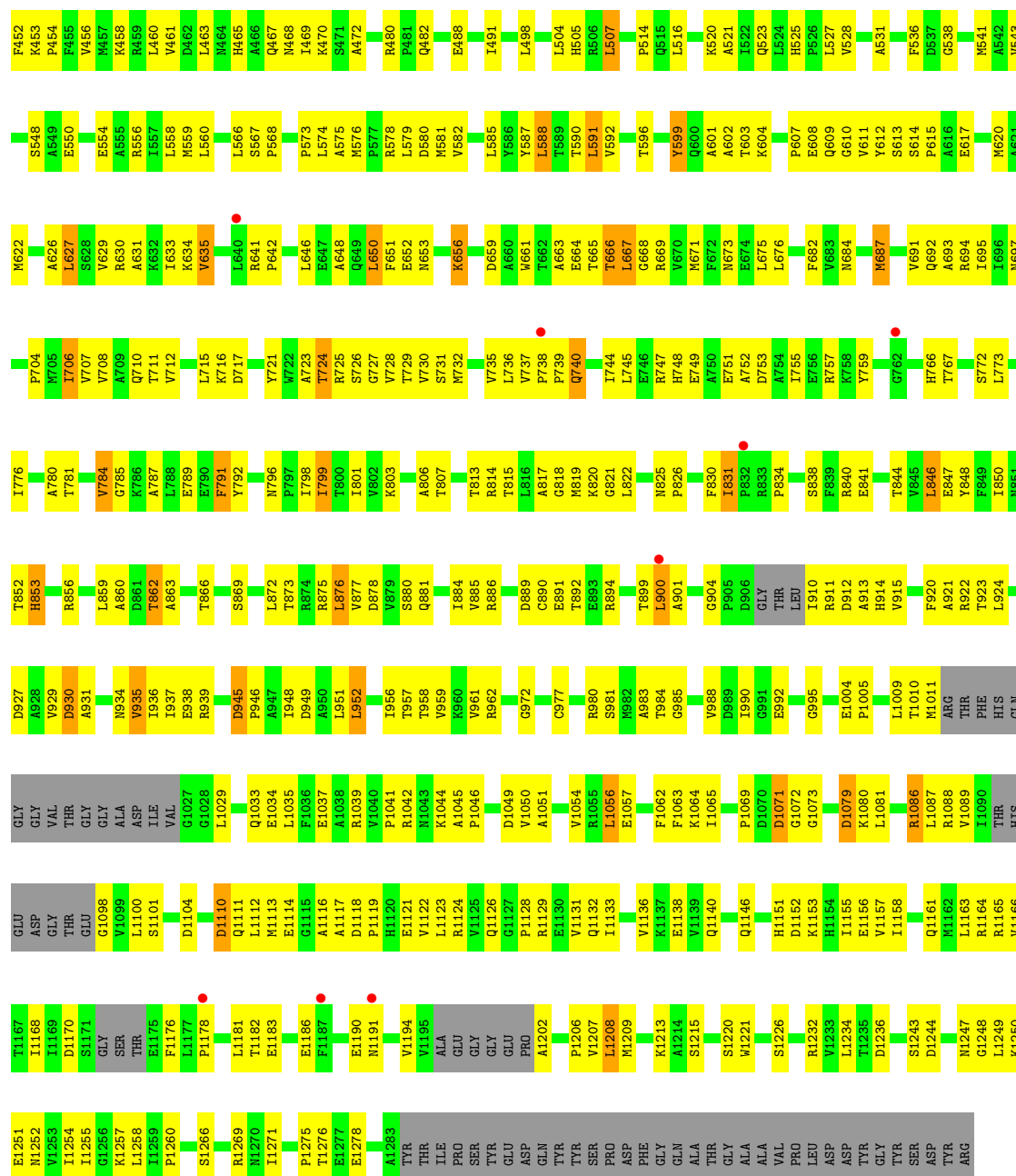
- Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 3: DNA-directed RNA polymerase subunit beta'





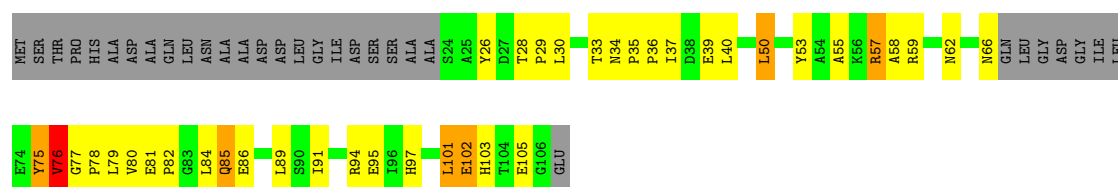
Chain E:

35%

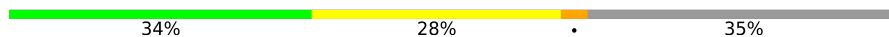
30%

6%

29%



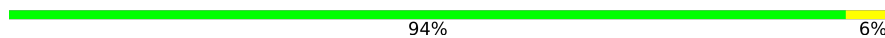
Chain F:



E429	P345	F273	E182	LYS	PRO	MET
L430		D274	E183	ALA	GLU	ALA
V433	V348	T275	E184	ALA	ASP	ALA
	L349	T276	V185	ASP	GLY	THR
R438	E350	K277	E186	ASP	VAL	LYS
S439	I351	G278	L187	ASP	THR	ALA
R440	Q352	Y279		ILE	ASP	SER
		K280	I191		ASP	PRO
	R356			GLU	LEU	ALA
Q443	E357	T283	G194	PRO	GLU	THR
I444	P358		L195	GLY	VAL	GLU
	I359	W288	Y196	LEU	THR	GLU
T448	S360	I289		LYS	ASP	PRO
M449		K290	Q199	ASP	VAL	
	Q363	Q291	K200	LYS	LEU	LYS
L452	T364	A292	L201	ALA	GLU	ARG
R453	I365	I293		SER	ALA	THR
H454	G366	T294	L204	GLY	GLU	ALA
P455	D367	R295		ASP	PRO	ALA
S456	E368	A296	G208	PHE	GLY	THR
R457	G369	M297		THR	GLU	THR
	D370		L211	TRP	ASP	PRO
R462	S371	Q300		ASP	LEU	ALA
D463	Q372		Q214	GLU	ASP	LYS
Y464	L373	I304	Q215	GLU	VAL	LYS
		R305	R216	GLU	GLU	ALA
L465	F376	I306		SER	ASP	PRO
D466		P307	M219	GLU	THR	ALA
	A385	V308		ALA	ASP	LYS
		H309	I222	LEU	LEU	ARG
	V389	M310		ARG	GLU	ALA
	L394	V313	K230	GLN	LEU	ALA
		I314	N231	ALA	ASP	LYS
	Q397		L234	ARG	SER	ALA
	L398	L317	E235	LYS	LEU	ALA
	Q399			ASP	ALA	ALA
	V400	I320	L238	GLU	SER	ALA
	F401	Q321	R239	LEU	ASP	LYS
	L402	R322	L240	THR	ASP	ALA
	F403	E323	V241	ALA	THR	GLY
	T404	L324		THR	ASP	GLY
		L325	L244	S162	ALA	LYS
	E407	Q326	A245	D164	VAL	ALA
	E409	L328	K246	S165	GLU	PRO
		G329	R251	V166	ASP	ALA
	V413	R330	G352	R167	GLU	LYS
	R414	E331	M253		GLU	ALA
	R416	P332	A254		GLU	PRO
			F255	Q172	ALA	ALA
		E335	L256	I173	ALA	ARG
	D421	L337	D257	G174	ALA	ALA
	G422	I337	L258	K175	THR	ALA
	Q423	A338		V176	PRO	ALA
	P424	K339	R268	A177	ALA	LYS
	R425	E340	A269	L178	VAL	GLY
	T426		V270	L179	THR	ALA
	L427	I343	E271	N180	ALA	ALA
	S428	T344	K272	A181	THR	LYS

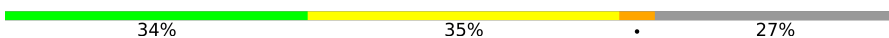
- Molecule 6: unknown

Chain G:



- Molecule 7: RNA polymerase-binding protein RbpA

Chain J:



P77	P78	P79	T80	R81	W82	E83	M84		R88	R89	S90	V91	E92	E93	L94	E95	E96	L97	L98	K99	E100	R101	L102	T103	L104	I105	K106	A107	K108	ARG	ARG	GLY	THR	GLY	SER																									
P77	P78	P79	T80	R81	W82	E83	M84		R88	R89	S90	V91	E92	E93	L94	E95	E96	L97	L98	K99	E100	R101	L102	T103	L104	I105	K106	A107	K108	ARG	ARG	GLY	THR	GLY	SER																									
NET	ALA	ASP	ARG	VAL	LEU	ARG	GLY	SER	ARG	ARG	LEU	GLY	ALA	VAL	SER	TYR	GLU	THR	ASP	ARG	ASN	HIS	ASP	LEU	ALA	P26	R27	Q28		R31		E39	F40	F41	V42	F43	F44	A45	D46	D47		I50		W54	L55	G56	R57	M58	G59	L60		L64	I65		D68	V69		K74	W75	V76

- Molecule 8: DNA (31-MER)

Chain 0:



G1	C2	T3	T4	G5	A6	C7	A11	G12	T13	G14	T15	T16	A19	T20	T23	G24	C25	T28	A29	C30	T31
----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 9: DNA (26-MER)

Chain P:



A1	G2		A11		G20	C26
C3	A4		A12			
C5	A6		C13			
			A14			
			C15			
			T16			
			T17			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.46Å 162.91Å 139.32Å 90.00° 107.32° 90.00°	Depositor
Resolution (Å)	54.66 – 3.11 54.66 – 3.11	Depositor EDS
% Data completeness (in resolution range)	96.7 (54.66-3.11) 96.7 (54.66-3.11)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.13Å)	Xtriage
Refinement program	PHENIX v0	Depositor
R, R_{free}	0.216 , 0.258 0.216 , 0.257	Depositor DCC
R_{free} test set	1997 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26620	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	0.24	0/1629	0.46	0/2220
1	B	0.24	0/1698	0.45	0/2322
1	T	0.23	0/343	0.37	0/468
2	C	0.26	0/8421	0.45	0/11444
3	D	0.26	0/9706	0.44	0/13140
4	E	0.25	0/604	0.42	0/822
5	F	0.25	0/2438	0.43	0/3291
7	J	0.25	0/685	0.43	0/927
8	O	0.56	0/710	0.93	0/1095
9	P	0.62	0/589	0.95	0/906
All	All	0.28	0/26823	0.49	0/36635

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
5	F	0	1
6	G	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	801	GLY	Peptide
2	C	950	LEU	Peptide
2	C	986	ASN	Peptide
5	F	368	GLU	Peptide
6	G	155	UNK	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1605	0	1623	141	0
1	B	1672	0	1643	177	0
1	T	342	0	275	14	0
2	C	8275	0	8025	681	1
3	D	9555	0	9509	574	1
4	E	592	0	583	41	0
5	F	2407	0	2428	155	0
6	G	85	0	19	0	0
7	J	671	0	660	48	0
8	O	633	0	350	38	0
9	P	526	0	296	14	0
10	C	20	0	0	3	0
10	D	25	0	0	2	0
10	F	25	0	0	2	0
11	C	8	12	12	1	0
11	D	16	24	24	3	0
11	F	4	6	6	1	0
12	C	58	0	64	14	0
13	D	2	0	0	0	0
14	C	7	4	0	1	0
14	D	21	8	0	2	0
14	E	1	0	0	0	0
14	F	8	2	0	1	0
14	J	1	0	0	0	0
14	O	3	0	0	0	0
14	P	2	0	0	0	0
All	All	26564	56	25517	1737	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 33.

All (1737) 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)
12:C:1205:SRN:C10	12:C:1205:SRN:C12	1.77	1.57
12:C:1205:SRN:O3	12:C:1205:SRN:C8	1.80	1.28
12:C:1205:SRN:O3	12:C:1205:SRN:C9	1.80	1.28
3:D:922:ARG:HB3	3:D:961:VAL:HG21	1.31	1.13
2:C:203:LEU:HG	2:C:217:ILE:HG22	1.35	1.08
2:C:951:PRO:HB2	2:C:954:LEU:HB2	1.36	1.06
1:A:197:GLU:OE1	2:C:987:ARG:NH1	1.90	1.05
2:C:771:VAL:HG22	2:C:772:LEU:HD12	1.39	1.04
1:A:177:LYS:HE2	1:A:193:ILE:HD11	1.40	1.03
2:C:53:GLU:OE2	2:C:60:ARG:NH1	1.92	1.03
7:J:106:LYS:HA	7:J:106:LYS:HE2	1.37	1.02
2:C:348:VAL:HB	2:C:349:PRO:HD2	1.42	1.02
3:D:755:ILE:HD12	3:D:776:ILE:HD11	1.41	1.01
2:C:540:ASP:HB2	2:C:546:THR:HG22	1.42	1.01
2:C:176:VAL:HG12	2:C:195:VAL:HG22	1.43	1.00
1:A:152:ASN:HB2	1:A:157:ALA:HB3	1.43	1.00
3:D:951:LEU:HB3	3:D:956:ILE:HD11	1.39	1.00
3:D:288:LYS:HD2	3:D:291:ARG:HH21	1.27	0.99
5:F:253:MET:HE3	5:F:297:MET:HA	1.44	0.99
5:F:253:MET:HE2	5:F:300:GLN:HB2	1.45	0.99
3:D:59:GLU:OE2	3:D:66:LYS:NZ	1.95	0.98
2:C:758:GLU:HG2	2:C:798:THR:HG22	1.46	0.97
2:C:711:LEU:HD23	2:C:904:VAL:HA	1.47	0.95
2:C:224:PRO:HB2	2:C:227:VAL:HG13	1.46	0.95
2:C:215:VAL:HG22	2:C:225:VAL:HA	1.44	0.95
3:D:47:PHE:O	3:D:88:ARG:NH2	2.00	0.95
3:D:656:LYS:HE3	3:D:656:LYS:H	1.29	0.94
2:C:799:PRO:HA	2:C:823:VAL:HG12	1.51	0.93
1:A:31:GLY:HA2	1:A:192:LEU:HD23	1.48	0.92
2:C:464:ARG:NH2	2:C:483:PRO:O	2.01	0.92
3:D:432:VAL:HG22	3:D:434:PRO:HD3	1.49	0.92
1:B:24:GLU:OE2	1:B:191:LYS:HD3	1.70	0.91
1:A:1:MET:N	1:B:142:ARG:O	2.03	0.91
2:C:710:LEU:HD22	2:C:1021:ILE:HD11	1.51	0.91
2:C:204:GLU:OE1	2:C:216:ARG:NH1	2.02	0.91
2:C:984:LEU:HD13	2:C:991:VAL:HG23	1.52	0.91
5:F:324:LEU:HD22	5:F:332:PRO:HB3	1.52	0.90
2:C:88:GLU:HG2	2:C:92:GLY:HA2	1.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1009:LEU:HD12	3:D:1146:GLN:HG3	1.54	0.90
3:D:892:THR:OG1	3:D:894:ARG:NH1	2.04	0.90
2:C:584:MET:HA	2:C:619:THR:HG21	1.51	0.90
2:C:649:ILE:HD11	2:C:679:PRO:HB3	1.51	0.89
3:D:581:MET:HE2	3:D:716:LYS:HA	1.53	0.89
2:C:41:VAL:O	2:C:624:ARG:NH2	2.05	0.88
1:B:9:LEU:HD21	1:B:208:LEU:HD21	1.55	0.88
2:C:602:MET:HE1	2:C:883:LYS:HB3	1.53	0.88
3:D:590:THR:HG21	3:D:630:ARG:HH21	1.37	0.88
2:C:1048:LEU:HD23	2:C:1048:LEU:H	1.37	0.87
2:C:531:VAL:HG13	2:C:552:VAL:HG13	1.55	0.87
2:C:891:PRO:HB2	2:C:893:GLU:HG2	1.57	0.87
2:C:1126:VAL:HG12	3:D:12:ILE:HG23	1.55	0.87
2:C:578:VAL:HG13	2:C:582:THR:HB	1.55	0.87
12:C:1205:SRN:C10	12:C:1205:SRN:C13	2.52	0.87
1:A:40:ARG:NH1	1:B:33:THR:HG22	1.90	0.86
2:C:574:PRO:O	2:C:575:ARG:HG2	1.76	0.86
3:D:603:THR:HG22	3:D:604:LYS:HG3	1.55	0.86
5:F:399:GLN:NE2	5:F:403:GLU:OE2	2.09	0.86
1:T:252:ASP:OD2	1:T:261:TYR:OH	1.92	0.85
2:C:92:GLY:O	2:C:133:ASN:ND2	2.09	0.85
1:T:251:ILE:HA	1:T:272:VAL:HG22	1.57	0.85
3:D:922:ARG:HB3	3:D:961:VAL:CG2	2.06	0.85
2:C:132:ASN:HB3	2:C:135:THR:HG22	1.57	0.85
7:J:31:ARG:NH2	7:J:39:GLU:OE1	2.10	0.85
2:C:394:ARG:HG3	2:C:398:GLN:HG3	1.56	0.84
2:C:763:ASP:HB3	2:C:821:ARG:HH22	1.41	0.84
5:F:438:ARG:NH1	9:P:20:DG:N7	2.25	0.84
3:D:400:LYS:HE2	3:D:405:LEU:HD23	1.60	0.84
3:D:796:ASN:HD21	3:D:798:ILE:HB	1.43	0.84
2:C:804:GLU:HG3	3:D:66:LYS:HE3	1.60	0.83
3:D:622:MET:HE3	3:D:667:LEU:HD13	1.61	0.83
5:F:324:LEU:HD23	5:F:328:LEU:HD13	1.59	0.83
5:F:320:ILE:HG23	5:F:340:GLU:HG2	1.61	0.83
3:D:344:TYR:O	3:D:348:ILE:HG22	1.79	0.83
5:F:280:LYS:HG2	8:O:30:DC:OP2	1.79	0.82
7:J:68:ASP:HA	7:J:69:VAL:HB	1.60	0.82
4:E:84:LEU:HB2	4:E:85:GLN:HE21	1.45	0.82
5:F:308:VAL:HG21	8:O:23:DT:H71	1.60	0.82
2:C:754:LYS:HE2	2:C:754:LYS:H	1.45	0.81
3:D:1164:ARG:NH1	10:D:2004:SO4:O1	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:510:VAL:N	2:C:568:ASP:O	2.11	0.81
2:C:1100:GLY:HA3	3:D:458:LYS:HE3	1.61	0.81
2:C:265:LEU:HD21	2:C:284:GLN:HA	1.63	0.81
3:D:1248:GLY:O	3:D:1252:ASN:ND2	2.14	0.81
3:D:327:MET:HG3	3:D:337:THR:HB	1.60	0.80
3:D:84:ARG:NH1	14:D:2101:HOH:O	2.14	0.80
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.14	0.80
3:D:642:PRO:HD3	3:D:656:LYS:HD2	1.63	0.80
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.63	0.80
3:D:269:ASP:HB3	3:D:272:ALA:HB3	1.64	0.80
1:A:40:ARG:HD3	1:B:33:THR:HG22	1.62	0.80
1:A:98:ARG:HG2	1:A:135:GLU:HG2	1.63	0.79
2:C:764:ILE:HB	2:C:767:VAL:HG21	1.63	0.79
3:D:417:LEU:HG	3:D:1254:ILE:HG23	1.61	0.79
8:O:19:DA:H2''	8:O:20:DT:O5'	1.81	0.79
2:C:444:ARG:HH21	2:C:491:LEU:HD23	1.48	0.79
4:E:84:LEU:H	4:E:84:LEU:HD12	1.48	0.79
2:C:51:SER:OG	2:C:373:GLY:N	2.15	0.79
1:A:14:VAL:HG13	1:A:18:ARG:HG3	1.65	0.78
2:C:773:ALA:O	2:C:782:ARG:NH2	2.16	0.78
3:D:365:ILE:HD12	3:D:365:ILE:H	1.46	0.78
3:D:1088:ARG:HG2	3:D:1089:VAL:H	1.49	0.78
3:D:1232:ARG:NH1	3:D:1236:ASP:OD2	2.16	0.78
3:D:641:ARG:HA	3:D:656:LYS:NZ	1.98	0.78
1:B:100:GLN:HA	1:B:133:LYS:HA	1.64	0.78
3:D:327:MET:HE2	5:F:304:ILE:HD11	1.65	0.78
2:C:1072:ALA:HB1	3:D:554:GLU:OE2	1.84	0.78
2:C:494:TYR:HB3	2:C:506:PRO:HG3	1.65	0.78
1:A:66:VAL:O	1:A:69:VAL:HG22	1.85	0.77
2:C:650:THR:HG22	2:C:660:SER:OG	1.84	0.77
3:D:1168:ILE:HD13	3:D:1176:PHE:HB3	1.65	0.77
1:A:113:PRO:HD2	1:A:116:VAL:HG21	1.67	0.77
1:B:84:VAL:HB	1:B:199:LYS:HD3	1.64	0.77
3:D:444:PRO:HG3	3:D:521:ALA:O	1.85	0.77
2:C:228:LEU:HD21	2:C:268:ILE:HG12	1.66	0.76
2:C:508:ARG:HD3	2:C:515:VAL:HG11	1.68	0.76
3:D:588:LEU:HD22	3:D:668:GLY:HA3	1.67	0.76
8:O:12:DG:H2''	8:O:13:DT:H5'	1.67	0.76
2:C:624:ARG:NH1	2:C:628:ASP:OD2	2.18	0.76
2:C:176:VAL:HG22	2:C:307:VAL:HG12	1.67	0.76
2:C:299:LEU:HB3	2:C:323:THR:HB	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:895:MET:SD	14:C:1303:HOH:O	2.42	0.76
3:D:622:MET:HE1	3:D:629:VAL:HG13	1.68	0.76
8:O:6:DA:H2''	8:O:7:DC:H5'	1.65	0.76
3:D:937:ILE:HD12	3:D:951:LEU:HG	1.66	0.76
3:D:607:PRO:O	3:D:609:GLN:HG2	1.86	0.75
2:C:635:ALA:HB2	2:C:693:ILE:HD11	1.67	0.75
2:C:899:PRO:HD2	2:C:992:MET:HE1	1.67	0.75
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.66	0.75
2:C:215:VAL:HG22	2:C:225:VAL:CA	2.16	0.75
5:F:402:LEU:HD23	5:F:414:ARG:HE	1.51	0.75
1:A:152:ASN:CB	1:A:157:ALA:HB3	2.16	0.75
2:C:729:SER:OG	2:C:905:ASP:HA	1.87	0.75
1:A:40:ARG:HH11	1:B:33:THR:HG22	1.50	0.75
2:C:1045:GLN:HG2	2:C:1087:THR:HG22	1.66	0.75
2:C:590:HIS:HB3	2:C:919:ILE:CD1	2.17	0.74
2:C:482:GLY:O	2:C:485:ILE:HG13	1.87	0.74
2:C:224:PRO:O	2:C:227:VAL:HG22	1.88	0.74
12:C:1205:SRN:C12	12:C:1205:SRN:C11	2.65	0.74
2:C:768:SER:O	2:C:771:VAL:HG13	1.87	0.74
2:C:467:HIS:CG	2:C:468:PRO:HD2	2.23	0.74
3:D:781:THR:HG22	3:D:814:ARG:HD2	1.69	0.74
3:D:962:ARG:NH1	3:D:977:CYS:SG	2.61	0.74
2:C:159:ILE:HB	2:C:164:ARG:HD2	1.69	0.74
3:D:735:VAL:HG12	3:D:840:ARG:HD2	1.69	0.74
2:C:404:THR:HG22	2:C:407:THR:HG23	1.69	0.73
3:D:951:LEU:HB3	3:D:956:ILE:CD1	2.16	0.73
5:F:201:LEU:HD11	5:F:219:MET:HB3	1.71	0.73
8:O:14:DG:H2''	8:O:15:DT:OP2	1.89	0.73
2:C:203:LEU:HG	2:C:217:ILE:CG2	2.18	0.73
3:D:930:ASP:OD2	3:D:931:ALA:N	2.22	0.73
2:C:1108:ILE:H	2:C:1108:ILE:HD12	1.53	0.73
2:C:984:LEU:CD1	2:C:991:VAL:HG23	2.19	0.72
3:D:922:ARG:CB	3:D:961:VAL:HG21	2.15	0.72
3:D:1079:ASP:N	3:D:1079:ASP:OD1	2.22	0.72
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.70	0.72
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.70	0.72
1:B:69:VAL:HG12	1:B:128:LEU:HA	1.71	0.72
3:D:846:LEU:H	3:D:846:LEU:HD12	1.53	0.72
5:F:454:HIS:ND1	5:F:455:PRO:HD2	2.03	0.72
2:C:150:MET:HE2	2:C:150:MET:HA	1.71	0.72
2:C:590:HIS:HB3	2:C:919:ILE:HD13	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:LEU:HD11	3:D:295:ARG:HG2	1.71	0.72
1:B:63:PHE:CE2	3:D:603:THR:HG23	2.25	0.72
2:C:771:VAL:HG23	2:C:792:ILE:HD13	1.72	0.72
8:O:15:DT:OP1	1:T:258:VAL:HG21	1.90	0.72
1:A:177:LYS:HE2	1:A:193:ILE:CD1	2.18	0.72
3:D:822:LEU:HD23	3:D:834:PRO:HA	1.70	0.72
1:B:47:PRO:HA	1:B:144:ARG:HG3	1.72	0.71
2:C:533:ALA:HB2	2:C:567:VAL:HG11	1.71	0.71
2:C:575:ARG:HE	2:C:967:VAL:HG22	1.52	0.71
2:C:1116:LEU:O	2:C:1120:GLN:HG3	1.90	0.71
3:D:1071:ASP:HB2	3:D:1072:GLY:C	2.11	0.71
5:F:291:GLN:NE2	10:F:505:SO4:O4	2.23	0.71
2:C:361:ILE:H	2:C:361:ILE:HD12	1.55	0.71
2:C:797:VAL:HG12	2:C:823:VAL:HB	1.72	0.71
2:C:899:PRO:HD2	2:C:992:MET:CE	2.21	0.71
3:D:587:TYR:O	3:D:590:THR:HG22	1.90	0.71
1:A:12:GLU:HG2	1:A:13:THR:H	1.55	0.71
1:B:64:THR:O	1:B:65:THR:OG1	2.06	0.71
2:C:265:LEU:HD11	2:C:287:LEU:HG	1.72	0.71
2:C:460:GLY:O	2:C:463:VAL:HG22	1.90	0.71
2:C:742:HIS:CD2	2:C:868:ARG:HG3	2.25	0.71
3:D:106:TYR:HB3	3:D:312:MET:HE3	1.71	0.71
5:F:253:MET:CE	5:F:300:GLN:HB2	2.19	0.71
3:D:622:MET:CE	3:D:667:LEU:HD13	2.20	0.71
2:C:228:LEU:CD2	2:C:268:ILE:HG12	2.20	0.71
3:D:1041:PRO:HB3	3:D:1116:ALA:HB3	1.72	0.70
5:F:176:VAL:HG12	5:F:177:ALA:H	1.56	0.70
2:C:710:LEU:HD13	2:C:1021:ILE:HG12	1.73	0.70
2:C:338:ARG:HH11	2:C:343:GLN:HE22	1.38	0.70
5:F:462:ARG:NH1	5:F:465:LEU:HB2	2.07	0.70
2:C:613:GLU:O	2:C:705:ALA:HB1	1.92	0.70
1:B:74:THR:HG21	3:D:611:VAL:HG11	1.72	0.70
2:C:894:ASP:HA	2:C:1004:GLY:HA3	1.73	0.70
1:A:207:ALA:O	1:A:210:SER:OG	2.08	0.70
1:B:97:LEU:HB3	1:B:136:VAL:HG13	1.74	0.70
2:C:1086:ASP:O	2:C:1090:ARG:HG2	1.91	0.70
1:A:11:GLU:OE2	1:A:205:ARG:HD3	1.92	0.69
3:D:28:VAL:HG21	3:D:46:LEU:HD23	1.72	0.69
3:D:1276:THR:HG22	4:E:102:GLU:HG3	1.73	0.69
1:B:41:THR:O	1:B:45:SER:HB3	1.91	0.69
3:D:596:THR:HG22	3:D:626:ALA:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:732:LEU:HD22	2:C:737:VAL:HG11	1.75	0.69
3:D:139:VAL:CG1	3:D:231:PRO:HD3	2.23	0.69
3:D:818:GLY:O	3:D:838:SER:HB3	1.91	0.69
3:D:641:ARG:HA	3:D:656:LYS:HZ3	1.56	0.69
3:D:815:THR:HG22	3:D:820:LYS:HA	1.74	0.69
1:A:36:ASN:HB2	1:A:176:TYR:OH	1.93	0.69
1:A:38:LEU:HD13	1:A:208:LEU:HD11	1.73	0.69
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.58	0.69
1:B:74:THR:CG2	3:D:611:VAL:HG11	2.22	0.69
2:C:302:VAL:O	2:C:306:LYS:HG2	1.92	0.69
2:C:333:ILE:O	2:C:337:VAL:HG23	1.92	0.69
2:C:568:ASP:OD1	2:C:568:ASP:N	2.23	0.69
5:F:462:ARG:HH12	5:F:465:LEU:HD12	1.57	0.69
1:A:158:GLU:H	1:A:161:ARG:HH11	1.40	0.69
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.75	0.69
3:D:930:ASP:HB3	3:D:934:ASN:HB2	1.75	0.69
2:C:509:LYS:O	2:C:516:THR:HG22	1.93	0.68
2:C:872:ASP:N	2:C:872:ASP:OD1	2.20	0.68
2:C:344:THR:O	2:C:355:PRO:HA	1.92	0.68
3:D:721:TYR:O	3:D:725:ARG:HG2	1.92	0.68
1:B:107:ALA:O	1:B:110:ILE:HG22	1.93	0.68
1:B:88:ASP:N	1:B:88:ASP:OD2	2.26	0.68
3:D:111:PRO:O	3:D:113:ARG:NH1	2.27	0.68
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.75	0.68
2:C:139:LYS:NZ	2:C:401:GLU:O	2.27	0.68
2:C:545:PHE:CD2	2:C:564:ALA:HB1	2.27	0.68
2:C:102:ARG:HG2	2:C:125:PHE:HB2	1.76	0.68
2:C:764:ILE:HB	2:C:767:VAL:CG2	2.23	0.68
1:A:56:ILE:HG12	1:A:136:VAL:HB	1.76	0.68
2:C:953:GLU:N	2:C:953:GLU:OE1	2.27	0.68
3:D:430:ILE:HD13	3:D:541:MET:HG3	1.76	0.68
3:D:656:LYS:CE	3:D:656:LYS:H	2.03	0.68
3:D:614:SER:HB2	3:D:615:PRO:HD2	1.76	0.68
2:C:1059:PHE:HZ	2:C:1067:MET:HE3	1.58	0.68
2:C:215:VAL:O	2:C:223:GLN:HB2	1.94	0.68
3:D:981:SER:HB3	3:D:984:THR:OG1	1.93	0.68
1:A:31:GLY:CA	1:A:192:LEU:HD23	2.22	0.67
3:D:772:SER:O	3:D:776:ILE:HG13	1.94	0.67
2:C:87:ILE:O	2:C:95:SER:HA	1.94	0.67
3:D:929:VAL:HG12	3:D:935:VAL:HG22	1.76	0.67
1:A:34:LEU:HD11	1:B:218:LEU:HD13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:96:LEU:HA	2:C:129:GLU:O	1.95	0.67
3:D:330:LEU:H	3:D:330:LEU:HD22	1.58	0.67
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.75	0.67
2:C:348:VAL:HB	2:C:349:PRO:CD	2.23	0.67
2:C:742:HIS:HD2	2:C:868:ARG:HG3	1.59	0.67
3:D:1168:ILE:O	3:D:1178:PRO:HA	1.95	0.67
3:D:642:PRO:CD	3:D:656:LYS:HD2	2.24	0.67
5:F:338:ALA:HB2	5:F:348:VAL:HG11	1.75	0.67
5:F:360:SER:HB3	5:F:363:GLN:HG3	1.76	0.67
2:C:169:GLN:OE1	2:C:370:ARG:NH2	2.27	0.67
2:C:637:LYS:HD2	2:C:659:GLN:NE2	2.08	0.67
1:B:56:ILE:HG22	1:B:136:VAL:HB	1.75	0.67
2:C:910:THR:HG23	3:D:730:VAL:HG23	1.77	0.67
3:D:1275:PRO:HG3	4:E:76:VAL:HG11	1.75	0.67
2:C:434:ASN:OD1	2:C:1025:HIS:ND1	2.28	0.67
3:D:1071:ASP:HB2	3:D:1073:GLY:N	2.09	0.67
2:C:753:THR:HG21	2:C:799:PRO:HD2	1.78	0.66
2:C:1079:LEU:HD23	2:C:1083:LYS:HD2	1.77	0.66
1:B:56:ILE:CD1	1:B:59:VAL:HB	2.25	0.66
2:C:728:LEU:CD2	2:C:906:ILE:HG22	2.26	0.66
7:J:74:LYS:O	7:J:74:LYS:NZ	2.17	0.66
8:O:6:DA:C2'	8:O:7:DC:H5'	2.26	0.66
9:P:11:DA:H2''	9:P:12:DA:O5'	1.96	0.66
1:A:11:GLU:CD	1:A:205:ARG:HD3	2.16	0.66
1:B:76:ILE:HA	1:B:79:ASN:HB2	1.77	0.66
3:D:755:ILE:CD1	3:D:776:ILE:HD11	2.23	0.66
1:A:70:LYS:HB3	1:A:127:THR:HG23	1.77	0.66
3:D:1247:ASN:O	3:D:1260:PRO:HG3	1.96	0.66
3:D:527:LEU:HD22	3:D:575:ALA:O	1.96	0.66
5:F:204:LEU:O	5:F:208:GLY:N	2.29	0.66
3:D:599:TYR:HB2	3:D:610:GLY:HA3	1.78	0.66
3:D:76:GLU:HA	7:J:44:PHE:HE2	1.59	0.66
4:E:85:GLN:HE21	4:E:85:GLN:H	1.44	0.66
1:A:99:LYS:HE3	1:A:109:ASP:OD1	1.96	0.65
2:C:899:PRO:CD	2:C:992:MET:HE1	2.26	0.65
3:D:190:LYS:NZ	3:D:192:ASP:HB3	2.10	0.65
3:D:218:ARG:O	3:D:222:ILE:HG13	1.96	0.65
5:F:180:ASN:OD1	5:F:183:GLU:HG3	1.96	0.65
2:C:623:LEU:HA	2:C:703:GLU:HA	1.78	0.65
3:D:1081:LEU:CB	3:D:1113:MET:HE3	2.26	0.65
3:D:1275:PRO:HB3	4:E:79:LEU:HD11	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:1205:SRN:H4	12:C:1205:SRN:O1	1.97	0.65
2:C:215:VAL:HG23	2:C:223:GLN:HB3	1.77	0.65
2:C:910:THR:CG2	3:D:730:VAL:HG23	2.27	0.65
3:D:622:MET:CE	3:D:629:VAL:HG22	2.27	0.65
1:A:211:ALA:O	1:A:215:LEU:N	2.27	0.65
3:D:65:TYR:HB3	3:D:70:PHE:CE2	2.31	0.65
3:D:785:GLY:O	3:D:789:GLU:HG3	1.96	0.65
2:C:128:ALA:HB1	2:C:405:PRO:HB3	1.78	0.65
3:D:980:ARG:HD3	3:D:985:GLY:O	1.97	0.65
5:F:421:ASP:OD2	5:F:425:ARG:NH2	2.30	0.65
8:O:14:DG:H3'	1:T:258:VAL:HG11	1.79	0.65
1:B:95:MET:HG2	1:B:113:PRO:CD	2.25	0.65
1:B:90:ASP:O	1:B:91:GLU:HG3	1.97	0.65
3:D:1249:LEU:HD12	3:D:1250:LYS:N	2.12	0.65
1:B:144:ARG:HB2	1:B:144:ARG:NH1	2.12	0.65
1:B:24:GLU:OE2	1:B:181:THR:HG21	1.97	0.65
2:C:932:LYS:HG2	2:C:1018:TYR:CE2	2.31	0.65
3:D:1123:LEU:HA	3:D:1131:VAL:CG2	2.27	0.65
2:C:573:SER:HB2	2:C:574:PRO:HD2	1.78	0.64
2:C:584:MET:HA	2:C:619:THR:CG2	2.26	0.64
2:C:732:LEU:HA	2:C:737:VAL:CG1	2.26	0.64
3:D:573:PRO:HG2	3:D:576:MET:CE	2.27	0.64
7:J:47:ASP:N	7:J:47:ASP:OD1	2.22	0.64
9:P:11:DA:H4'	9:P:12:DA:OP1	1.97	0.64
2:C:765:PRO:HD2	2:C:825:ASP:HB2	1.78	0.64
1:B:162:ILE:HG23	3:D:607:PRO:HG2	1.79	0.64
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.29	0.64
5:F:191:ILE:O	5:F:195:LEU:HD13	1.98	0.64
1:A:14:VAL:HG12	1:A:19:SER:HA	1.79	0.64
3:D:848:TYR:O	3:D:852:THR:HG23	1.98	0.64
4:E:57:ARG:NE	4:E:95:GLU:OE1	2.26	0.64
2:C:338:ARG:HB3	2:C:343:GLN:HG2	1.78	0.64
3:D:278:ARG:O	3:D:281:ILE:HD12	1.96	0.64
3:D:668:GLY:HA2	3:D:671:MET:CE	2.27	0.64
3:D:585:LEU:HD12	3:D:692:GLN:NE2	2.12	0.64
2:C:1014:VAL:HG13	3:D:729:THR:HG21	1.80	0.64
1:A:66:VAL:HB	1:A:69:VAL:HG21	1.77	0.64
2:C:45:LEU:HD22	2:C:443:LYS:HD2	1.80	0.64
2:C:900:ASP:OD2	2:C:992:MET:HG3	1.97	0.64
3:D:17:ALA:O	3:D:21:ARG:HG3	1.98	0.64
4:E:30:LEU:O	4:E:33:THR:HG22	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LEU:HB3	1:B:136:VAL:CG1	2.27	0.64
1:B:183:VAL:HG22	3:D:488:GLU:OE2	1.97	0.64
2:C:338:ARG:HH11	2:C:343:GLN:NE2	1.95	0.64
3:D:1266:SER:HA	3:D:1269:ARG:NH1	2.13	0.64
3:D:177:LEU:HD23	3:D:177:LEU:O	1.96	0.64
3:D:31:PRO:HB2	3:D:345:ARG:HG2	1.79	0.64
7:J:28:GLN:HG2	7:J:46:ASP:HA	1.80	0.64
1:A:82:GLY:HA3	1:A:123:MET:HE1	1.78	0.64
1:B:93:VAL:HG11	1:B:116:VAL:HG11	1.80	0.64
2:C:1003:ASP:OD1	2:C:1006:SER:N	2.27	0.64
2:C:578:VAL:HG13	2:C:582:THR:CB	2.27	0.64
3:D:173:ARG:NH2	3:D:201:GLY:HA2	2.11	0.64
3:D:755:ILE:HD12	3:D:776:ILE:CD1	2.23	0.64
1:B:20:ARG:HG2	1:B:195:ASP:OD1	1.98	0.64
3:D:320:ILE:HG12	3:D:321:PRO:HD2	1.80	0.64
3:D:144:ARG:NH2	3:D:229:LEU:O	2.31	0.64
3:D:52:PHE:O	3:D:91:ARG:HD2	1.97	0.64
3:D:585:LEU:HD12	3:D:692:GLN:HE21	1.63	0.64
5:F:444:ILE:O	5:F:448:THR:HG23	1.97	0.64
2:C:379:GLN:HG2	2:C:421:PHE:HB2	1.78	0.64
3:D:12:ILE:HD11	3:D:1221:TRP:CD2	2.33	0.64
1:A:94:THR:HG22	1:A:139:VAL:HG22	1.80	0.63
1:B:147:VAL:CG1	1:B:166:SER:HB2	2.28	0.63
2:C:132:ASN:HB3	2:C:135:THR:CG2	2.28	0.63
2:C:215:VAL:HG23	2:C:223:GLN:CB	2.28	0.63
3:D:73:ILE:HD12	7:J:45:ALA:HB2	1.79	0.63
4:E:80:VAL:HG12	4:E:81:GLU:H	1.63	0.63
5:F:254:ALA:HA	10:F:502:SO4:O3	1.98	0.63
2:C:751:ARG:NH1	3:D:332:GLY:O	2.31	0.63
2:C:776:ASP:HB2	2:C:777:GLU:OE1	1.97	0.63
2:C:789:ASP:HA	2:C:830:VAL:HG13	1.80	0.63
3:D:1122:VAL:HG23	3:D:1126:GLN:HE21	1.64	0.63
3:D:288:LYS:HD2	3:D:291:ARG:NH2	2.08	0.63
2:C:249:MET:O	2:C:253:LEU:HD23	1.99	0.63
3:D:137:THR:HG22	3:D:253:THR:O	1.98	0.63
3:D:631:ALA:O	3:D:666:THR:HA	1.99	0.63
2:C:250:MET:HA	2:C:253:LEU:HD21	1.80	0.63
2:C:533:ALA:HB3	2:C:570:MET:HG3	1.81	0.63
3:D:665:THR:HG22	3:D:684:ASN:ND2	2.14	0.63
1:A:119:HIS:CD2	1:A:201:SER:HA	2.33	0.63
2:C:754:LYS:H	2:C:754:LYS:CE	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:956:ILE:HD12	3:D:956:ILE:O	1.97	0.63
1:B:144:ARG:HH11	1:B:144:ARG:HB2	1.61	0.63
2:C:132:ASN:CB	2:C:135:THR:HG22	2.27	0.63
3:D:1081:LEU:HB3	3:D:1113:MET:HE3	1.80	0.63
8:O:11:DA:H2"	8:O:12:DG:H5"	1.81	0.63
2:C:421:PHE:O	2:C:425:SER:HB3	1.99	0.63
2:C:876:LEU:HD11	2:C:886:ILE:HD11	1.81	0.63
5:F:462:ARG:HH12	5:F:465:LEU:CD1	2.12	0.63
2:C:540:ASP:CB	2:C:546:THR:HG22	2.25	0.63
2:C:538:PRO:O	2:C:546:THR:HG23	1.99	0.63
2:C:589:GLU:OE1	2:C:589:GLU:N	2.22	0.63
8:O:5:DG:H2"	8:O:6:DA:OP2	1.99	0.63
1:B:22:VAL:HG12	1:B:193:ILE:HD12	1.81	0.63
2:C:224:PRO:HD2	2:C:227:VAL:HG21	1.78	0.63
2:C:229:LEU:HD11	2:C:234:TRP:CE3	2.33	0.63
5:F:308:VAL:HG21	8:O:23:DT:C7	2.28	0.63
7:J:106:LYS:O	7:J:108:LYS:HG3	1.99	0.63
1:A:33:THR:HG21	1:B:37:SER:HA	1.81	0.62
1:A:86:SER:HG	1:A:119:HIS:CE1	2.12	0.62
1:A:42:LEU:O	1:A:171:VAL:HG11	1.98	0.62
3:D:706:ILE:O	3:D:710:GLN:HG3	1.99	0.62
1:A:63:PHE:HE1	2:C:741:ILE:HD13	1.64	0.62
2:C:87:ILE:HD12	2:C:388:GLU:HG3	1.81	0.62
2:C:52:PHE:HZ	2:C:150:MET:HE2	1.63	0.62
5:F:219:MET:HE2	5:F:219:MET:HA	1.82	0.62
7:J:79:ARG:NH2	8:O:25:DC:OP1	2.32	0.62
2:C:193:VAL:CG1	2:C:205:PHE:HB2	2.29	0.62
2:C:980:LEU:HB3	2:C:995:ALA:HA	1.82	0.62
3:D:656:LYS:N	3:D:656:LYS:HE3	2.08	0.62
2:C:984:LEU:HB3	2:C:991:VAL:HG22	1.81	0.62
1:B:72:ASP:OD1	1:B:73:VAL:N	2.26	0.62
12:C:1205:SRN:H401	12:C:1205:SRN:C3	2.29	0.62
2:C:328:ASP:O	2:C:332:THR:HG23	2.00	0.62
2:C:33:ALA:HB2	2:C:966:PRO:HG3	1.80	0.62
3:D:648:ALA:O	3:D:652:GLU:HB2	1.99	0.62
1:B:105:VAL:HG23	1:B:128:LEU:HD13	1.82	0.62
2:C:375:LEU:HD13	2:C:427:LEU:HD22	1.81	0.62
3:D:460:LEU:HD11	3:D:472:ALA:CB	2.29	0.62
3:D:781:THR:CG2	3:D:814:ARG:HD2	2.29	0.62
3:D:859:LEU:O	3:D:862:THR:HG22	2.00	0.62
1:A:33:THR:CG2	1:B:37:SER:HA	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:1205:SRN:C12	12:C:1205:SRN:C9	2.61	0.62
2:C:1098:VAL:HG11	3:D:469:ILE:HD12	1.81	0.62
2:C:789:ASP:HA	2:C:830:VAL:CG1	2.30	0.62
2:C:795:GLY:HA2	2:C:827:SER:OG	1.99	0.62
5:F:204:LEU:HD11	5:F:211:LEU:HD21	1.81	0.62
2:C:1128:VAL:HG13	2:C:1136:ILE:HB	1.81	0.61
2:C:967:VAL:HG23	2:C:968:PHE:H	1.64	0.61
2:C:231:ALA:HB1	2:C:265:LEU:HD13	1.82	0.61
2:C:429:GLN:OE1	2:C:442:HIS:NE2	2.31	0.61
2:C:523:THR:HG23	2:C:526:GLU:OE2	2.00	0.61
2:C:783:ILE:HD13	2:C:784:GLY:N	2.15	0.61
4:E:62:ASN:O	4:E:66:ASN:ND2	2.34	0.61
2:C:176:VAL:HG12	2:C:195:VAL:CG2	2.26	0.61
2:C:891:PRO:HB2	2:C:893:GLU:CG	2.31	0.61
1:A:98:ARG:O	1:A:99:LYS:HD2	2.01	0.61
1:B:76:ILE:HG23	1:B:125:ILE:HD11	1.83	0.61
2:C:935:TRP:HB2	2:C:982:SER:HB3	1.82	0.61
1:A:14:VAL:HG13	1:A:15:ALA:H	1.64	0.61
2:C:291:PHE:HB3	2:C:324:LEU:CD2	2.31	0.61
2:C:433:GLN:HG3	2:C:669:SER:OG	2.00	0.61
2:C:680:ILE:HD11	2:C:692:VAL:O	2.00	0.61
3:D:1063:PHE:HB2	3:D:1081:LEU:HB2	1.83	0.61
2:C:792:ILE:HD12	2:C:792:ILE:H	1.65	0.61
3:D:137:THR:HG22	3:D:253:THR:C	2.21	0.61
7:J:50:ILE:HG22	7:J:64:LEU:HD11	1.81	0.61
1:B:151:GLN:HB2	1:B:155:SER:OG	2.01	0.61
2:C:1059:PHE:CZ	2:C:1067:MET:HE3	2.35	0.61
3:D:1132:GLN:NE2	3:D:1163:LEU:HD12	2.16	0.61
3:D:245:GLN:O	3:D:249:GLY:HA3	2.00	0.61
1:B:212:GLY:O	1:B:216:VAL:HG12	2.01	0.60
3:D:737:VAL:HG22	3:D:817:ALA:HB1	1.84	0.60
2:C:291:PHE:HB3	2:C:324:LEU:HD22	1.82	0.60
2:C:979:LEU:O	2:C:982:SER:OG	2.16	0.60
7:J:76:LYS:HG3	7:J:76:LYS:O	2.00	0.60
1:T:264:LEU:HB3	1:T:269:VAL:CG2	2.31	0.60
2:C:1128:VAL:HG11	2:C:1138:MET:CE	2.30	0.60
3:D:443:LEU:HD22	3:D:514:PRO:HB3	1.83	0.60
2:C:404:THR:OG1	2:C:405:PRO:HD2	2.01	0.60
3:D:1220:SER:OG	3:D:1244:ASP:OD2	2.15	0.60
3:D:642:PRO:HG3	3:D:661:TRP:CE2	2.37	0.60
3:D:889:ASP:OD2	3:D:891:GLU:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:CA	1:A:121:PRO:HB3	2.32	0.60
2:C:176:VAL:HG13	2:C:307:VAL:HG11	1.82	0.60
2:C:636:ASP:N	2:C:636:ASP:OD1	2.32	0.60
3:D:1168:ILE:HD13	3:D:1176:PHE:CB	2.31	0.60
2:C:1028:VAL:HG12	3:D:429:VAL:CG1	2.31	0.60
3:D:920:PHE:CE2	3:D:948:ILE:HG13	2.36	0.60
1:B:76:ILE:HG23	1:B:125:ILE:CD1	2.32	0.60
5:F:293:ILE:O	5:F:297:MET:HG3	2.01	0.60
2:C:935:TRP:HA	2:C:983:THR:HG23	1.84	0.60
7:J:50:ILE:CG2	7:J:64:LEU:HD11	2.32	0.60
2:C:444:ARG:NH2	2:C:492:SER:O	2.34	0.60
3:D:948:ILE:O	3:D:952:LEU:HD22	2.02	0.60
4:E:29:PRO:HG2	4:E:34:ASN:HB2	1.83	0.60
5:F:330:ARG:NH2	5:F:336:GLU:OE2	2.34	0.60
1:A:14:VAL:CG1	1:A:18:ARG:HG3	2.32	0.60
5:F:201:LEU:HD11	5:F:219:MET:CB	2.32	0.60
2:C:560:GLU:HG3	2:C:561:PHE:H	1.67	0.59
2:C:65:ALA:HB1	2:C:70:GLU:OE1	2.02	0.59
3:D:67:ARG:HG3	3:D:69:ARG:H	1.67	0.59
2:C:965:THR:O	2:C:965:THR:OG1	2.19	0.59
2:C:590:HIS:O	2:C:919:ILE:HD11	2.02	0.59
2:C:1043:ILE:HG23	2:C:1044:THR:H	1.68	0.59
2:C:873:GLY:HA3	2:C:1028:VAL:HG11	1.84	0.59
3:D:73:ILE:O	3:D:82:VAL:HG12	2.03	0.59
1:B:112:PRO:HB2	1:B:116:VAL:HG23	1.82	0.59
3:D:740:GLN:H	3:D:740:GLN:HE21	1.48	0.59
3:D:781:THR:O	3:D:784:VAL:HG23	2.02	0.59
2:C:338:ARG:NH1	2:C:343:GLN:HE22	2.00	0.59
2:C:380:ILE:HG12	2:C:418:ILE:HD11	1.85	0.59
3:D:673:ASN:HA	3:D:676:LEU:HD13	1.84	0.59
1:A:40:ARG:HD3	1:B:33:THR:CG2	2.30	0.59
2:C:538:PRO:HB2	2:C:546:THR:OG1	2.01	0.59
2:C:710:LEU:HD13	2:C:1021:ILE:CG1	2.32	0.59
3:D:881:GLN:HE22	3:D:1250:LYS:HE2	1.67	0.59
5:F:404:THR:OG1	5:F:457:ARG:NE	2.36	0.59
3:D:924:LEU:HD21	3:D:959:VAL:CG1	2.33	0.59
4:E:85:GLN:NE2	4:E:85:GLN:H	2.01	0.59
4:E:86:GLU:OE2	4:E:94:ARG:NH1	2.35	0.59
1:A:70:LYS:HB3	1:A:71:GLU:OE1	2.03	0.59
2:C:94:MET:CE	2:C:395:MET:HB3	2.32	0.59
3:D:666:THR:OG1	3:D:669:ARG:HG3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1011:PRO:HB2	2:C:1012:TYR:HD2	1.68	0.59
2:C:262:ASP:OD2	2:C:280:LYS:HE2	2.03	0.59
2:C:494:TYR:HD2	2:C:572:VAL:HG21	1.67	0.59
3:D:334:ARG:HD3	5:F:356:ARG:HH21	1.67	0.59
1:B:202:ILE:CG1	1:B:206:ASP:HB2	2.33	0.58
2:C:1039:PRO:HB2	2:C:1048:LEU:HD21	1.84	0.58
2:C:436:PRO:HD2	2:C:698:CYS:HB2	1.84	0.58
2:C:29:ARG:CD	2:C:964:ALA:HB2	2.33	0.58
3:D:1100:LEU:HD23	3:D:1101:SER:N	2.18	0.58
3:D:957:THR:O	3:D:958:THR:HG23	2.03	0.58
4:E:80:VAL:HG12	4:E:81:GLU:N	2.18	0.58
1:A:111:VAL:O	1:A:111:VAL:HG23	2.02	0.58
1:B:4:SER:HB2	1:B:27:GLU:OE2	2.02	0.58
2:C:1130:SER:HB3	2:C:1133:GLY:HA3	1.84	0.58
2:C:479:THR:HG22	2:C:597:LEU:HD11	1.85	0.58
3:D:634:LYS:HA	3:D:664:GLU:HA	1.86	0.58
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.38	0.58
1:B:143:GLY:HA3	1:B:168:TYR:CD1	2.38	0.58
2:C:727:ILE:HG22	2:C:888:LYS:HB3	1.84	0.58
2:C:950:LEU:CB	2:C:951:PRO:CD	2.81	0.58
2:C:766:ASN:HB3	5:F:465:LEU:HD21	1.85	0.58
2:C:935:TRP:CB	2:C:982:SER:HB3	2.34	0.58
8:O:19:DA:H4'	8:O:20:DT:OP1	2.03	0.58
1:A:42:LEU:O	1:A:46:ILE:HG12	2.02	0.58
1:B:24:GLU:HG3	1:B:191:LYS:HG3	1.84	0.58
2:C:52:PHE:CZ	2:C:150:MET:HE2	2.39	0.58
2:C:556:GLY:N	2:C:557:GLY:HA2	2.18	0.58
2:C:602:MET:HE2	2:C:1024:LEU:HD21	1.83	0.58
2:C:614:ALA:HA	2:C:705:ALA:HB2	1.85	0.58
2:C:892:VAL:CG2	2:C:903:PRO:HG2	2.33	0.58
2:C:984:LEU:HG	2:C:984:LEU:O	2.03	0.58
1:B:172:LEU:HD12	3:D:620:MET:SD	2.43	0.58
3:D:706:ILE:HD12	4:E:36:PRO:HB3	1.85	0.58
3:D:846:LEU:O	3:D:850:ILE:HG12	2.04	0.58
1:A:157:ALA:HB1	1:A:161:ARG:HD2	1.86	0.58
2:C:338:ARG:HB3	2:C:343:GLN:CG	2.32	0.58
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.86	0.58
4:E:35:PRO:HG2	4:E:40:LEU:HD11	1.86	0.58
1:A:2:LEU:HD12	1:B:143:GLY:HA2	1.84	0.58
3:D:1191:ASN:OD1	3:D:1202:ALA:HB3	2.03	0.58
2:C:1130:SER:HB3	2:C:1133:GLY:CA	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:LEU:CD2	2:C:443:LYS:HD2	2.34	0.58
3:D:1086:ARG:O	3:D:1087:LEU:HD23	2.03	0.58
3:D:880:SER:O	3:D:995:GLY:HA3	2.03	0.58
1:A:9:LEU:HD13	1:A:23:ILE:CG1	2.34	0.58
2:C:1028:VAL:O	2:C:1032:ILE:HG22	2.04	0.58
3:D:642:PRO:HD3	3:D:656:LYS:CD	2.34	0.58
5:F:276:THR:HG23	7:J:89:ARG:NH2	2.19	0.58
2:C:1011:PRO:HB2	2:C:1012:TYR:CD2	2.39	0.58
2:C:498:ASN:OD1	2:C:499:PRO:HD2	2.03	0.58
2:C:523:THR:HG23	2:C:526:GLU:CD	2.23	0.58
2:C:622:GLU:N	2:C:622:GLU:OE1	2.37	0.58
2:C:809:GLU:O	2:C:813:ARG:HG2	2.04	0.58
1:A:68:GLY:HA3	1:A:129:ASN:HD21	1.69	0.57
1:A:24:GLU:OE1	1:A:191:LYS:HD3	2.03	0.57
2:C:481:GLU:O	2:C:485:ILE:HD11	2.04	0.57
2:C:534:GLN:HE21	2:C:534:GLN:HA	1.68	0.57
1:B:95:MET:HB2	1:B:110:ILE:HD11	1.85	0.57
1:B:50:ALA:HB3	1:B:168:TYR:HD2	1.68	0.57
2:C:178:PHE:HD1	2:C:193:VAL:HB	1.70	0.57
3:D:708:VAL:O	3:D:712:VAL:HG23	2.04	0.57
2:C:496:ARG:HH21	2:C:521:TYR:HB2	1.70	0.57
5:F:423:GLN:HG3	5:F:425:ARG:HE	1.68	0.57
2:C:578:VAL:HG12	2:C:579:SER:O	2.03	0.57
5:F:399:GLN:O	5:F:403:GLU:HG2	2.04	0.57
8:O:12:DG:H2''	8:O:13:DT:C5'	2.34	0.57
2:C:480:PRO:O	2:C:485:ILE:HG12	2.04	0.57
3:D:1069:PRO:HB2	3:D:1073:GLY:H	1.69	0.57
3:D:740:GLN:O	3:D:744:ILE:HG13	2.05	0.57
1:A:82:GLY:HA3	1:A:123:MET:CE	2.34	0.57
1:A:83:LEU:HD23	1:A:123:MET:SD	2.44	0.57
2:C:534:GLN:HB2	2:C:551:MET:HB2	1.85	0.57
2:C:732:LEU:CD2	2:C:737:VAL:HG11	2.35	0.57
3:D:1276:THR:CG2	4:E:102:GLU:HG3	2.34	0.57
2:C:1100:GLY:CA	3:D:458:LYS:HE3	2.32	0.57
3:D:438:LEU:HA	3:D:525:HIS:CD2	2.39	0.57
3:D:579:LEU:HD23	3:D:807:THR:HB	1.87	0.57
2:C:432:ASP:HB2	12:C:1205:SRN:H182	1.85	0.57
3:D:1088:ARG:HD2	3:D:1111:GLN:HB3	1.86	0.57
3:D:951:LEU:CB	3:D:956:ILE:HD11	2.24	0.57
2:C:1026:HIS:HB3	2:C:1031:LYS:HE3	1.87	0.57
2:C:51:SER:HB2	2:C:371:THR:OG1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:190:LYS:HZ2	3:D:192:ASP:HB3	1.69	0.57
3:D:193:VAL:O	3:D:197:VAL:HG23	2.04	0.57
3:D:237:ASP:HB3	3:D:240:LEU:HB3	1.86	0.57
2:C:1029:ASP:OD1	3:D:520:LYS:HD2	2.04	0.57
3:D:661:TRP:CZ3	3:D:663:ALA:HB2	2.39	0.57
3:D:627:LEU:HD13	3:D:667:LEU:HD12	1.87	0.57
3:D:850:ILE:O	3:D:853:HIS:HB2	2.04	0.57
5:F:409:GLU:HG3	11:F:506:EDO:O2	2.05	0.57
7:J:88:ARG:HG3	7:J:89:ARG:H	1.70	0.57
1:A:152:ASN:HB2	1:A:157:ALA:CB	2.28	0.57
1:B:3:ILE:HG23	1:B:232:ILE:CB	2.34	0.57
2:C:224:PRO:O	2:C:227:VAL:N	2.31	0.57
2:C:766:ASN:O	2:C:767:VAL:HG13	2.05	0.57
3:D:153:ALA:O	3:D:157:VAL:HG23	2.05	0.57
3:D:924:LEU:HD21	3:D:959:VAL:HG13	1.85	0.57
5:F:335:GLU:OE1	5:F:335:GLU:N	2.36	0.57
1:A:177:LYS:CE	1:A:193:ILE:HD11	2.26	0.56
2:C:509:LYS:HA	2:C:569:TYR:HA	1.86	0.56
2:C:641:ILE:HG21	2:C:644:VAL:HG13	1.85	0.56
2:C:637:LYS:HD2	2:C:659:GLN:HE22	1.70	0.56
3:D:1071:ASP:N	3:D:1071:ASP:OD2	2.38	0.56
3:D:106:TYR:HB3	3:D:312:MET:CE	2.34	0.56
3:D:588:LEU:HD22	3:D:668:GLY:CA	2.33	0.56
3:D:872:LEU:HG	3:D:876:LEU:CD2	2.35	0.56
8:O:15:DT:H2"	8:O:16:DT:OP2	2.04	0.56
1:A:152:ASN:HD21	2:C:837:LYS:NZ	2.02	0.56
2:C:269:TYR:CE2	2:C:278:PRO:HB3	2.39	0.56
3:D:668:GLY:HA2	3:D:671:MET:HE3	1.87	0.56
3:D:706:ILE:HD11	4:E:36:PRO:HA	1.87	0.56
5:F:320:ILE:O	5:F:324:LEU:HB2	2.05	0.56
9:P:17:DT:H5"	1:T:290:GLY:N	2.21	0.56
1:B:56:ILE:CG2	1:B:136:VAL:HB	2.35	0.56
1:B:85:VAL:HG23	1:B:117:THR:O	2.05	0.56
3:D:108:LYS:HG3	3:D:108:LYS:O	2.06	0.56
3:D:327:MET:CE	5:F:304:ILE:HD11	2.34	0.56
1:A:210:SER:CB	1:B:229:SER:HB2	2.35	0.56
1:B:26:LEU:HD12	1:B:31:GLY:HA2	1.87	0.56
1:A:30:PHE:CE1	1:B:40:ARG:HG3	2.40	0.56
2:C:1041:SER:HB3	2:C:1044:THR:O	2.05	0.56
3:D:488:GLU:HG3	3:D:516:LEU:HD12	1.87	0.56
2:C:437:LEU:HB2	2:C:704:MET:CE	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1166:VAL:HA	3:D:1207:VAL:HG23	1.87	0.56
2:C:1073:ALA:HB1	3:D:1258:LEU:HG	1.87	0.56
3:D:362:ALA:HB3	3:D:367:VAL:HG23	1.86	0.56
3:D:726:SER:OG	3:D:728:VAL:HG23	2.04	0.56
3:D:899:THR:O	3:D:900:LEU:HB3	2.05	0.56
1:A:9:LEU:HD13	1:A:23:ILE:HG13	1.87	0.56
2:C:217:ILE:HD11	2:C:272:LEU:HD11	1.88	0.56
2:C:609:LEU:HD13	2:C:737:VAL:O	2.06	0.56
2:C:927:LEU:HD23	2:C:930:VAL:HB	1.87	0.56
3:D:143:MET:HG2	3:D:251:TYR:CE1	2.41	0.56
5:F:397:GLN:O	5:F:401:VAL:HG23	2.06	0.56
1:A:40:ARG:NH1	1:B:33:THR:CG2	2.66	0.56
2:C:736:ASP:OD1	2:C:869:LYS:HE2	2.05	0.56
5:F:219:MET:HA	5:F:219:MET:CE	2.36	0.56
7:J:68:ASP:HA	7:J:69:VAL:CB	2.31	0.56
3:D:435:GLN:OE1	3:D:435:GLN:N	2.34	0.56
3:D:656:LYS:HG2	3:D:656:LYS:O	2.05	0.56
3:D:676:LEU:HD12	3:D:676:LEU:N	2.21	0.56
5:F:462:ARG:HD3	5:F:462:ARG:O	2.05	0.56
1:A:21:PHE:HB2	1:A:194:ILE:HG12	1.86	0.56
1:B:102:PRO:HG3	1:B:131:LYS:H	1.70	0.56
1:B:32:TYR:CE2	1:B:178:VAL:HG21	2.41	0.56
2:C:1048:LEU:CD2	2:C:1048:LEU:H	2.14	0.56
2:C:771:VAL:HG23	2:C:792:ILE:CD1	2.36	0.56
3:D:116:TYR:HB3	3:D:298:VAL:HG11	1.88	0.56
3:D:460:LEU:HD11	3:D:472:ALA:HB1	1.87	0.56
5:F:253:MET:HE2	5:F:300:GLN:CB	2.28	0.56
1:A:55:ARG:HH12	1:A:161:ARG:CZ	2.19	0.56
2:C:239:ILE:CG2	2:C:253:LEU:HD22	2.35	0.56
3:D:1071:ASP:N	3:D:1072:GLY:HA2	2.20	0.56
2:C:622:GLU:HB3	2:C:703:GLU:HB2	1.88	0.56
2:C:609:LEU:HD12	2:C:708:LYS:HE3	1.87	0.56
2:C:935:TRP:HA	2:C:983:THR:H	1.71	0.56
2:C:981:GLY:O	2:C:982:SER:OG	2.24	0.56
3:D:271:ASP:HA	3:D:303:GLN:NE2	2.20	0.56
2:C:1015:THR:OG1	3:D:731:SER:OG	2.24	0.55
2:C:102:ARG:CG	2:C:125:PHE:HB2	2.36	0.55
3:D:735:VAL:HG22	3:D:798:ILE:HD11	1.88	0.55
2:C:1068:GLN:NE2	3:D:1249:LEU:HD13	2.22	0.55
2:C:752:ASP:OD1	2:C:857:ASN:ND2	2.39	0.55
2:C:755:LEU:HD21	2:C:800:LYS:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:852:LEU:HD23	2:C:856:VAL:HG12	1.87	0.55
3:D:468:ASN:OD1	3:D:470:LYS:HB2	2.05	0.55
8:O:6:DA:H1'	8:O:7:DC:H5'	1.88	0.55
9:P:11:DA:H2'	9:P:12:DA:C8	2.42	0.55
1:B:113:PRO:O	1:B:116:VAL:HG22	2.06	0.55
2:C:233:GLY:HA2	2:C:261:THR:CB	2.37	0.55
2:C:148:PHE:HE1	2:C:380:ILE:HD11	1.71	0.55
5:F:274:ASP:OD1	7:J:89:ARG:NH2	2.34	0.55
5:F:394:LEU:HB2	5:F:464:TYR:CE1	2.41	0.55
1:T:260:SER:O	1:T:264:LEU:HG	2.07	0.55
2:C:221:ARG:HG3	2:C:222:ARG:HG3	1.87	0.55
3:D:1054:VAL:CG2	3:D:1065:ILE:HG23	2.37	0.55
3:D:599:TYR:CB	3:D:610:GLY:HA3	2.35	0.55
5:F:234:LEU:HD23	5:F:270:VAL:HG21	1.88	0.55
1:A:24:GLU:CD	1:A:191:LYS:HD3	2.27	0.55
2:C:437:LEU:HB2	2:C:704:MET:HE1	1.89	0.55
3:D:920:PHE:HE1	3:D:945:ASP:HA	1.71	0.55
4:E:29:PRO:HB2	4:E:33:THR:HG23	1.89	0.55
1:A:5:GLN:HG3	1:A:25:PRO:CG	2.36	0.55
2:C:896:PRO:HB2	2:C:1001:LEU:HD13	1.87	0.55
2:C:614:ALA:HB1	2:C:615:PRO:HD2	1.88	0.55
2:C:911:HIS:O	2:C:914:PRO:HD2	2.06	0.55
5:F:181:ALA:O	5:F:185:VAL:HG23	2.07	0.55
2:C:440:LEU:HD12	2:C:440:LEU:O	2.07	0.55
2:C:747:GLU:HG3	2:C:859:LEU:HD21	1.88	0.55
3:D:579:LEU:CD2	3:D:807:THR:HB	2.37	0.55
1:A:40:ARG:HH11	1:B:33:THR:CG2	2.19	0.55
2:C:398:GLN:HB3	2:C:403:ILE:CG2	2.37	0.55
2:C:370:ARG:HH22	2:C:452:GLY:HA3	1.72	0.55
2:C:448:ALA:HB1	2:C:454:LEU:HD21	1.88	0.55
2:C:626:ALA:HB1	2:C:699:THR:HG21	1.89	0.55
2:C:945:ASP:O	2:C:948:SER:OG	2.22	0.55
3:D:1037:GLU:HG2	3:D:1039:ARG:NH1	2.22	0.55
3:D:693:ALA:O	3:D:697:ASN:HB2	2.05	0.55
3:D:951:LEU:C	3:D:956:ILE:HD11	2.26	0.55
5:F:179:LEU:HB3	5:F:183:GLU:HB2	1.89	0.55
5:F:194:GLY:HA2	5:F:222:ILE:HG22	1.88	0.55
1:B:59:VAL:O	1:B:60:LEU:HD13	2.07	0.55
2:C:426:GLN:OE1	2:C:450:GLY:HA2	2.06	0.55
2:C:714:ILE:HG22	2:C:714:ILE:O	2.07	0.55
2:C:525:ASP:OD1	2:C:525:ASP:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:931:ALA:HB1	2:C:961:SER:O	2.07	0.55
3:D:1119:PRO:HA	3:D:1122:VAL:HG12	1.89	0.55
3:D:1009:LEU:CD1	3:D:1146:GLN:HG3	2.33	0.55
3:D:878:ASP:OD1	3:D:1215:SER:HB2	2.07	0.55
3:D:665:THR:HG21	3:D:682:PHE:CE2	2.42	0.54
4:E:26:TYR:HE1	4:E:29:PRO:HD3	1.73	0.54
1:A:12:GLU:HG2	1:A:13:THR:N	2.20	0.54
1:A:46:ILE:HD12	1:A:210:SER:OG	2.07	0.54
2:C:203:LEU:HD11	2:C:217:ILE:HB	1.89	0.54
2:C:169:GLN:O	2:C:369:LEU:HD12	2.06	0.54
2:C:390:VAL:O	2:C:394:ARG:HB2	2.07	0.54
3:D:844:THR:H	3:D:847:GLU:HB2	1.71	0.54
3:D:912:ASP:OD1	3:D:913:ALA:N	2.40	0.54
2:C:496:ARG:HH21	2:C:521:TYR:CB	2.19	0.54
2:C:712:VAL:HG11	2:C:925:THR:HG23	1.89	0.54
2:C:727:ILE:HG13	2:C:907:ILE:HB	1.89	0.54
3:D:1056:LEU:HD21	3:D:1063:PHE:CD1	2.42	0.54
3:D:74:ILE:HD12	7:J:42:VAL:HG13	1.89	0.54
9:P:11:DA:H2''	9:P:12:DA:C5'	2.37	0.54
5:F:167:ARG:O	5:F:171:LYS:HG3	2.07	0.54
5:F:291:GLN:HG3	5:F:292:ALA:N	2.22	0.54
7:J:31:ARG:HG2	7:J:41:ASP:OD1	2.08	0.54
9:P:17:DT:O5'	1:T:290:GLY:HA3	2.07	0.54
2:C:1129:LEU:HA	2:C:1134:ALA:O	2.07	0.54
2:C:1128:VAL:HG11	2:C:1138:MET:HE2	1.89	0.54
2:C:30:VAL:HG11	2:C:954:LEU:HG	1.89	0.54
2:C:510:VAL:HG23	2:C:514:VAL:C	2.28	0.54
1:A:130:ASP:OD1	1:A:130:ASP:N	2.39	0.54
1:B:34:LEU:O	1:B:38:LEU:HD23	2.07	0.54
2:C:560:GLU:OE1	2:C:560:GLU:HA	2.07	0.54
2:C:716:PRO:O	3:D:724:THR:HB	2.07	0.54
3:D:1118:ASP:HB3	3:D:1121:GLU:HB2	1.88	0.54
3:D:448:ALA:HB1	3:D:491:ILE:HD11	1.90	0.54
2:C:720:HIS:O	3:D:432:VAL:HG11	2.08	0.54
2:C:758:GLU:CG	2:C:798:THR:HG22	2.29	0.54
3:D:357:LEU:HD13	3:D:366:ILE:HG22	1.89	0.54
3:D:556:ARG:O	3:D:560:LEU:HB2	2.08	0.54
1:A:56:ILE:HB	1:A:59:VAL:CG2	2.37	0.54
2:C:128:ALA:CB	2:C:405:PRO:HB3	2.38	0.54
2:C:919:ILE:HD12	2:C:919:ILE:H	1.72	0.54
3:D:161:ALA:HB2	14:D:2104:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:225:THR:HG21	3:D:244:LEU:HD11	1.90	0.54
3:D:468:ASN:ND2	5:F:463:ASP:OD2	2.41	0.54
5:F:370:ASP:N	5:F:370:ASP:OD2	2.29	0.54
11:C:1207:EDO:O2	5:F:322:ARG:HD2	2.07	0.54
3:D:578:ARG:HB2	11:D:2007:EDO:C2	2.38	0.54
3:D:138:SER:HB3	3:D:253:THR:OG1	2.06	0.54
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.73	0.54
1:B:22:VAL:HA	1:B:192:LEU:O	2.07	0.54
2:C:178:PHE:O	2:C:358:VAL:HG13	2.08	0.54
3:D:453:LYS:HB3	3:D:454:PRO:HD3	1.90	0.54
3:D:910:ILE:HG23	3:D:910:ILE:O	2.08	0.54
1:B:50:ALA:HB3	1:B:168:TYR:CD2	2.42	0.53
1:B:66:VAL:HG12	1:B:69:VAL:HG22	1.90	0.53
2:C:716:PRO:HD3	2:C:910:THR:OG1	2.08	0.53
2:C:896:PRO:O	2:C:904:VAL:HG22	2.07	0.53
3:D:240:LEU:HD23	3:D:244:LEU:HG	1.91	0.53
1:B:183:VAL:HG13	3:D:488:GLU:OE2	2.08	0.53
2:C:132:ASN:O	2:C:136:GLY:N	2.39	0.53
2:C:493:VAL:HG12	2:C:494:TYR:CD1	2.43	0.53
2:C:780:ILE:HD12	2:C:781:VAL:O	2.08	0.53
2:C:1034:ALA:HB2	3:D:447:MET:HG3	1.90	0.53
3:D:747:ARG:O	3:D:751:GLU:HG3	2.08	0.53
5:F:215:GLN:O	5:F:219:MET:HG2	2.09	0.53
1:A:18:ARG:HB2	1:A:196:VAL:O	2.09	0.53
2:C:506:PRO:HB2	2:C:572:VAL:HG11	1.89	0.53
2:C:710:LEU:O	2:C:1018:TYR:HA	2.07	0.53
2:C:876:LEU:HD13	2:C:886:ILE:HG13	1.91	0.53
3:D:1009:LEU:HB3	3:D:1029:LEU:HD13	1.90	0.53
3:D:330:LEU:HD22	3:D:330:LEU:N	2.24	0.53
3:D:920:PHE:CE1	3:D:945:ASP:HA	2.43	0.53
2:C:240:VAL:HA	2:C:250:MET:SD	2.49	0.53
2:C:32:PHE:O	2:C:34:LYS:HD2	2.09	0.53
2:C:728:LEU:HD22	2:C:906:ILE:HG22	1.90	0.53
3:D:461:VAL:HG23	3:D:472:ALA:HB2	1.91	0.53
3:D:592:VAL:HG11	11:D:2011:EDO:H12	1.91	0.53
5:F:176:VAL:HG12	5:F:177:ALA:N	2.20	0.53
1:A:12:GLU:O	1:A:19:SER:HB2	2.07	0.53
2:C:280:LYS:HB3	2:C:280:LYS:NZ	2.24	0.53
3:D:1181:LEU:CD1	3:D:1213:LYS:HE2	2.38	0.53
3:D:278:ARG:HA	3:D:281:ILE:HD11	1.90	0.53
3:D:642:PRO:HG3	3:D:661:TRP:CD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:938:GLU:OE1	3:D:938:GLU:N	2.33	0.53
1:A:193:ILE:O	1:A:193:ILE:HD12	2.09	0.53
2:C:1127:GLU:OE1	3:D:11:ARG:NH2	2.35	0.53
2:C:729:SER:HA	2:C:895:MET:HE1	1.90	0.53
2:C:946:TRP:CE2	2:C:978:GLY:HA3	2.44	0.53
3:D:274:ALA:O	3:D:278:ARG:HG2	2.09	0.53
3:D:691:VAL:O	3:D:695:ILE:HG13	2.07	0.53
4:E:86:GLU:OE1	4:E:91:ILE:HG12	2.07	0.53
2:C:1103:ILE:N	10:C:1206:SO4:O3	2.41	0.53
2:C:299:LEU:CB	2:C:323:THR:HB	2.36	0.53
3:D:1119:PRO:HA	3:D:1122:VAL:CG1	2.38	0.53
3:D:687:MET:HE2	3:D:695:ILE:CD1	2.38	0.53
3:D:58:TRP:HZ3	3:D:71:LYS:HB2	1.74	0.53
4:E:26:TYR:CE1	4:E:29:PRO:HD3	2.44	0.53
5:F:423:GLN:O	5:F:423:GLN:HG3	2.09	0.53
1:A:192:LEU:HD12	1:A:192:LEU:O	2.09	0.53
2:C:100:ASP:OD2	2:C:102:ARG:NH2	2.41	0.53
2:C:476:PRO:O	3:D:856:ARG:NH2	2.42	0.53
2:C:721:ASN:HD22	2:C:727:ILE:HD11	1.74	0.53
2:C:951:PRO:HB2	2:C:954:LEU:CB	2.24	0.53
3:D:924:LEU:HD12	3:D:937:ILE:HG22	1.91	0.53
4:E:77:GLY:HA2	4:E:79:LEU:HD23	1.91	0.53
5:F:272:LYS:HE3	8:O:25:DC:OP1	2.08	0.53
1:B:84:VAL:HB	1:B:199:LYS:CD	2.35	0.53
2:C:652:MET:HE2	2:C:658:ARG:HD2	1.91	0.53
3:D:6:PHE:CD1	3:D:1257:LYS:HE3	2.44	0.53
5:F:465:LEU:HD23	5:F:466:ASP:N	2.23	0.53
1:A:129:ASN:H	1:A:129:ASN:HD22	1.55	0.53
1:B:112:PRO:CB	1:B:116:VAL:HG23	2.37	0.53
2:C:591:ASP:OD2	2:C:880:HIS:ND1	2.40	0.53
2:C:710:LEU:HD23	2:C:732:LEU:HD11	1.91	0.53
2:C:788:ARG:N	2:C:791:ASP:OD2	2.39	0.53
2:C:935:TRP:CA	2:C:983:THR:HG23	2.39	0.53
2:C:984:LEU:CB	2:C:991:VAL:HG22	2.39	0.53
5:F:317:LEU:HD12	5:F:351:ILE:HG21	1.91	0.53
1:B:94:THR:HA	1:B:138:LEU:O	2.09	0.52
2:C:1103:ILE:HD12	3:D:548:SER:HA	1.89	0.52
2:C:510:VAL:HG11	2:C:567:VAL:HG12	1.91	0.52
1:A:106:THR:HA	1:A:125:ILE:HD13	1.91	0.52
1:B:56:ILE:HD12	1:B:56:ILE:O	2.09	0.52
2:C:652:MET:CE	2:C:658:ARG:HD2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:665:LYS:NZ	2:C:677:GLN:O	2.41	0.52
2:C:720:HIS:CE1	2:C:888:LYS:HD3	2.43	0.52
3:D:1089:VAL:HG13	3:D:1098:GLY:C	2.30	0.52
3:D:1168:ILE:HD11	3:D:1182:THR:HG21	1.90	0.52
3:D:336:ALA:HA	5:F:359:ILE:O	2.09	0.52
3:D:799:ILE:CG2	3:D:803:LYS:HE2	2.39	0.52
1:B:151:GLN:OE1	1:B:151:GLN:N	2.37	0.52
2:C:921:GLN:HB2	2:C:1019:MET:HE1	1.90	0.52
3:D:498:LEU:HD11	3:D:543:VAL:HG22	1.92	0.52
3:D:656:LYS:HB2	3:D:659:ASP:CB	2.40	0.52
1:A:137:GLU:C	1:A:138:LEU:HD12	2.30	0.52
2:C:224:PRO:HG2	2:C:227:VAL:HG11	1.91	0.52
3:D:573:PRO:HG2	3:D:576:MET:HE3	1.91	0.52
1:A:108:GLY:HA2	1:A:121:PRO:HB3	1.90	0.52
2:C:196:ILE:HG23	2:C:196:ILE:O	2.10	0.52
2:C:199:ARG:NH2	2:C:295:LYS:O	2.41	0.52
2:C:510:VAL:HG12	2:C:568:ASP:C	2.29	0.52
2:C:545:PHE:HD2	2:C:564:ALA:HB1	1.70	0.52
3:D:819:MET:CE	3:D:821:GLY:HA2	2.39	0.52
7:J:96:GLU:O	7:J:100:GLU:HG3	2.09	0.52
2:C:711:LEU:HD23	2:C:904:VAL:CA	2.32	0.52
3:D:937:ILE:CD1	3:D:951:LEU:HG	2.37	0.52
4:E:58:ALA:HB2	4:E:89:LEU:HA	1.90	0.52
5:F:164:ASP:OD1	5:F:166:VAL:HG22	2.09	0.52
5:F:430:ILE:O	5:F:433:VAL:HG13	2.09	0.52
1:B:95:MET:CB	1:B:110:ILE:HD11	2.40	0.52
2:C:534:GLN:NE2	2:C:534:GLN:HA	2.24	0.52
2:C:714:ILE:HD13	2:C:922:ILE:CD1	2.40	0.52
3:D:1251:GLU:OE1	3:D:1251:GLU:N	2.38	0.52
4:E:55:ALA:O	4:E:59:ARG:HG3	2.10	0.52
5:F:358:PRO:O	5:F:359:ILE:HD13	2.09	0.52
1:B:180:ALA:HA	1:B:189:PHE:O	2.09	0.52
1:B:198:THR:HG21	1:B:202:ILE:HG23	1.91	0.52
2:C:467:HIS:ND1	2:C:468:PRO:HD2	2.25	0.52
2:C:723:GLU:O	2:C:724:ASP:HB2	2.10	0.52
2:C:805:LEU:HD22	2:C:805:LEU:H	1.74	0.52
3:D:35:ASN:OD1	3:D:37:ARG:N	2.36	0.52
1:B:162:ILE:CG2	3:D:607:PRO:HG2	2.40	0.52
2:C:593:ALA:HB2	3:D:852:THR:HG22	1.92	0.52
3:D:25:TYR:C	7:J:57:ARG:HG3	2.29	0.52
2:C:792:ILE:HD12	2:C:792:ILE:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:796:LYS:HB3	2:C:826:THR:O	2.09	0.52
2:C:1074:TYR:CZ	3:D:1258:LEU:HD21	2.45	0.52
3:D:612:TYR:HB2	3:D:635:VAL:HG13	1.92	0.52
2:C:398:GLN:HB3	2:C:403:ILE:HG22	1.92	0.52
2:C:479:THR:HG22	2:C:597:LEU:CD1	2.40	0.52
2:C:609:LEU:HD23	2:C:740:SER:HB3	1.91	0.52
3:D:682:PHE:CE2	3:D:684:ASN:HB2	2.45	0.52
3:D:578:ARG:HB2	11:D:2007:EDO:H21	1.92	0.51
3:D:130:TYR:O	3:D:372:ARG:HD3	2.09	0.51
2:C:540:ASP:O	2:C:543:GLY:N	2.37	0.51
2:C:572:VAL:H	2:C:576:GLN:NE2	2.09	0.51
3:D:527:LEU:HD21	3:D:581:MET:CE	2.40	0.51
3:D:716:LYS:HE3	3:D:717:ASP:OD1	2.10	0.51
1:A:138:LEU:HD12	1:A:138:LEU:N	2.25	0.51
1:B:30:PHE:HA	1:B:33:THR:HG23	1.92	0.51
1:B:85:VAL:HG23	1:B:117:THR:C	2.30	0.51
3:D:143:MET:CE	3:D:251:TYR:HA	2.41	0.51
1:B:34:LEU:HD11	1:B:192:LEU:HD22	1.91	0.51
2:C:1112:PHE:CE2	3:D:1255:ILE:HG22	2.46	0.51
2:C:291:PHE:O	2:C:297:TYR:HB3	2.11	0.51
2:C:505:THR:CG2	2:C:506:PRO:HD2	2.41	0.51
2:C:602:MET:HE1	2:C:883:LYS:CB	2.33	0.51
2:C:875:LYS:C	2:C:876:LEU:HD12	2.30	0.51
1:A:40:ARG:HD3	1:B:33:THR:CB	2.40	0.51
1:A:219:PHE:HE1	1:B:38:LEU:HD21	1.76	0.51
2:C:1078:GLU:HG3	2:C:1082:ILE:HD11	1.91	0.51
2:C:231:ALA:HB1	2:C:265:LEU:CD1	2.40	0.51
2:C:269:TYR:CD2	2:C:278:PRO:HB3	2.46	0.51
2:C:623:LEU:HG	2:C:624:ARG:N	2.25	0.51
3:D:155:MET:CE	3:D:219:LEU:HB3	2.41	0.51
3:D:238:GLU:HA	3:D:241:TYR:HB3	1.92	0.51
3:D:799:ILE:HG21	3:D:803:LYS:HE2	1.93	0.51
5:F:385:ALA:O	5:F:389:VAL:HG23	2.11	0.51
8:O:31:DT:H6	8:O:31:DT:H5'	1.75	0.51
2:C:441:THR:OG1	2:C:604:ARG:HD3	2.11	0.51
2:C:676:ASN:OD1	2:C:677:GLN:N	2.44	0.51
5:F:254:ALA:HB3	5:F:257:ASP:OD2	2.11	0.51
2:C:215:VAL:N	2:C:223:GLN:O	2.44	0.51
3:D:1054:VAL:HG12	3:D:1104:ASP:O	2.11	0.51
3:D:411:GLY:O	3:D:415:GLN:HB3	2.11	0.51
3:D:498:LEU:CD1	3:D:543:VAL:HG22	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:736:LEU:HB2	3:D:792:TYR:CE2	2.45	0.51
3:D:76:GLU:H	3:D:76:GLU:CD	2.14	0.51
5:F:462:ARG:HH12	5:F:465:LEU:HB2	1.74	0.51
1:B:28:PRO:HD3	1:B:189:PHE:CD1	2.46	0.51
2:C:560:GLU:CG	2:C:561:PHE:H	2.23	0.51
2:C:763:ASP:CB	2:C:821:ARG:HH22	2.18	0.51
3:D:1034:GLU:OE2	3:D:1041:PRO:HA	2.11	0.51
3:D:745:LEU:O	3:D:749:GLU:HG2	2.11	0.51
1:B:87:SER:HB3	1:B:89:ASP:OD1	2.11	0.51
2:C:710:LEU:CD2	2:C:1021:ILE:HD11	2.32	0.51
2:C:714:ILE:O	2:C:910:THR:OG1	2.25	0.51
2:C:936:ASN:ND2	2:C:937:ILE:O	2.44	0.51
3:D:1088:ARG:HG2	3:D:1089:VAL:N	2.22	0.51
3:D:150:THR:O	3:D:154:GLU:HG3	2.10	0.51
3:D:915:VAL:O	3:D:920:PHE:HD2	1.94	0.51
1:A:68:GLY:CA	1:A:129:ASN:HD21	2.24	0.50
1:B:39:ARG:O	1:B:43:LEU:HB2	2.10	0.50
2:C:169:GLN:HB2	2:C:427:LEU:HD21	1.93	0.50
3:D:432:VAL:CG2	3:D:434:PRO:HD3	2.32	0.50
3:D:704:PRO:HD2	3:D:707:VAL:HG21	1.92	0.50
3:D:740:GLN:H	3:D:740:GLN:NE2	2.08	0.50
1:A:9:LEU:HD23	1:B:221:LEU:O	2.11	0.50
1:B:73:VAL:O	1:B:77:ILE:HG13	2.11	0.50
2:C:154:LYS:HD2	2:C:630:GLY:HA3	1.92	0.50
2:C:892:VAL:HG22	2:C:903:PRO:HG2	1.94	0.50
3:D:488:GLU:CG	3:D:516:LEU:HD12	2.41	0.50
2:C:193:VAL:HG12	2:C:205:PHE:HB2	1.92	0.50
3:D:58:TRP:CG	3:D:68:VAL:HG22	2.47	0.50
1:A:177:LYS:HG2	1:A:193:ILE:HD11	1.93	0.50
1:A:2:LEU:HD12	1:B:143:GLY:CA	2.41	0.50
1:B:17:ASN:OD1	1:B:17:ASN:N	2.38	0.50
2:C:1001:LEU:HD21	2:C:1016:VAL:HG11	1.94	0.50
3:D:281:ILE:HG22	3:D:289:LYS:HG3	1.93	0.50
3:D:43:LYS:O	3:D:44:ASP:HB2	2.11	0.50
2:C:1026:HIS:HB3	2:C:1031:LYS:CE	2.41	0.50
2:C:442:HIS:O	2:C:445:ARG:HB2	2.11	0.50
2:C:446:LEU:HD23	2:C:446:LEU:N	2.25	0.50
2:C:449:LEU:N	2:C:449:LEU:HD12	2.27	0.50
1:B:74:THR:HG21	3:D:608:GLU:OE1	2.12	0.50
3:D:759:TYR:CE1	3:D:766:HIS:HA	2.47	0.50
3:D:822:LEU:HD22	3:D:831:ILE:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:904:GLY:HA3	3:D:910:ILE:CG2	2.41	0.50
5:F:268:ARG:HD3	5:F:288:TRP:CH2	2.46	0.50
1:B:52:THR:O	1:B:164:VAL:HG22	2.11	0.50
2:C:1028:VAL:HG12	3:D:429:VAL:HG11	1.93	0.50
2:C:1035:ARG:CZ	2:C:1047:PRO:HB3	2.41	0.50
3:D:1136:VAL:HG22	3:D:1155:ILE:HG22	1.93	0.50
3:D:66:LYS:O	3:D:66:LYS:HG2	2.11	0.50
2:C:176:VAL:O	2:C:176:VAL:HG23	2.11	0.50
7:J:97:LEU:HD23	7:J:97:LEU:O	2.10	0.50
2:C:846:ARG:N	2:C:857:ASN:O	2.44	0.50
3:D:249:GLY:HA2	3:D:252:PHE:CE2	2.47	0.50
3:D:505:HIS:ND1	3:D:507:LEU:HB2	2.27	0.50
4:E:57:ARG:HD3	4:E:57:ARG:O	2.11	0.50
8:O:15:DT:H6	8:O:15:DT:OP2	1.94	0.50
1:A:211:ALA:O	1:A:215:LEU:HB2	2.11	0.50
1:B:77:ILE:HG22	1:B:81:LYS:HE3	1.93	0.50
2:C:1035:ARG:NH2	2:C:1047:PRO:HB3	2.27	0.50
2:C:1048:LEU:O	2:C:1055:GLY:HA3	2.12	0.50
2:C:336:LEU:HD23	2:C:336:LEU:O	2.11	0.50
2:C:627:ILE:HD12	2:C:628:ASP:N	2.27	0.50
2:C:70:GLU:CD	2:C:70:GLU:H	2.15	0.50
3:D:937:ILE:HD12	3:D:951:LEU:CG	2.38	0.50
4:E:84:LEU:HB2	4:E:85:GLN:NE2	2.22	0.50
7:J:91:VAL:HA	7:J:94:LEU:HD12	1.94	0.50
1:A:192:LEU:HD12	1:A:192:LEU:C	2.32	0.49
2:C:265:LEU:CD2	2:C:284:GLN:HA	2.39	0.49
2:C:774:ASP:HA	2:C:782:ARG:NH2	2.27	0.49
3:D:1044:LYS:HE3	3:D:1118:ASP:HB2	1.93	0.49
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.93	0.49
3:D:70:PHE:HB2	3:D:73:ILE:HD13	1.94	0.49
3:D:70:PHE:O	3:D:82:VAL:HG11	2.12	0.49
5:F:166:VAL:O	5:F:170:LEU:HG	2.12	0.49
5:F:289:ILE:O	5:F:293:ILE:HG13	2.12	0.49
5:F:324:LEU:HD23	5:F:328:LEU:CD1	2.38	0.49
3:D:20:ILE:HG23	3:D:318:PRO:HB3	1.92	0.49
2:C:477:ILE:HD11	3:D:852:THR:HG21	1.94	0.49
5:F:201:LEU:CD2	5:F:211:LEU:HD11	2.41	0.49
5:F:449:MET:O	5:F:453:ARG:HG3	2.12	0.49
8:O:19:DA:H2'	8:O:20:DT:C6	2.47	0.49
1:A:79:ASN:O	1:A:123:MET:HE1	2.11	0.49
2:C:54:TRP:HD1	2:C:61:TRP:CZ2	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:771:VAL:HG22	2:C:772:LEU:CD1	2.27	0.49
2:C:797:VAL:CG1	2:C:823:VAL:HB	2.42	0.49
3:D:231:PRO:O	3:D:232:LYS:HB2	2.12	0.49
3:D:287:GLN:CG	3:D:288:LYS:HZ2	2.26	0.49
3:D:48:CYS:SG	3:D:50:LYS:HB3	2.52	0.49
3:D:567:SER:HB3	3:D:574:LEU:CD1	2.41	0.49
3:D:608:GLU:O	3:D:609:GLN:HB2	2.11	0.49
3:D:744:ILE:O	3:D:748:HIS:HD2	1.96	0.49
3:D:890:CYS:SG	3:D:892:THR:HG22	2.52	0.49
5:F:199:GLN:HG2	7:J:82:TRP:CZ2	2.48	0.49
1:B:97:LEU:HD23	1:B:136:VAL:HG11	1.94	0.49
2:C:23:VAL:HB	2:C:26:ALA:HB2	1.94	0.49
3:D:1062:PHE:CD1	3:D:1080:LYS:HB3	2.47	0.49
3:D:1123:LEU:HB2	3:D:1131:VAL:HG21	1.95	0.49
2:C:239:ILE:HG21	2:C:253:LEU:HD22	1.95	0.49
3:D:362:ALA:HB3	3:D:367:VAL:CG2	2.42	0.49
8:O:6:DA:C1'	8:O:7:DC:H5'	2.43	0.49
1:B:230:GLU:OE1	1:B:231:HIS:N	2.44	0.49
2:C:634:VAL:HG13	2:C:691:GLN:O	2.13	0.49
2:C:691:GLN:HG2	2:C:692:VAL:H	1.76	0.49
2:C:718:GLU:H	3:D:724:THR:HG21	1.78	0.49
3:D:819:MET:HE2	3:D:821:GLY:HA2	1.93	0.49
3:D:945:ASP:N	3:D:946:PRO:HD2	2.27	0.49
5:F:338:ALA:HB1	5:F:343:ILE:O	2.12	0.49
1:B:137:GLU:C	1:B:138:LEU:HD12	2.33	0.49
2:C:250:MET:HA	2:C:253:LEU:CD2	2.41	0.49
2:C:302:VAL:HG11	2:C:368:ARG:HD2	1.93	0.49
2:C:566:GLN:OE1	2:C:566:GLN:HA	2.13	0.49
2:C:913:VAL:HB	2:C:914:PRO:HD3	1.93	0.49
3:D:1153:LYS:O	3:D:1157:VAL:HG23	2.13	0.49
3:D:602:ALA:HB3	3:D:607:PRO:O	2.13	0.49
3:D:752:ALA:HB1	3:D:773:LEU:CD2	2.43	0.49
3:D:923:THR:O	3:D:961:VAL:HG23	2.12	0.49
2:C:1045:GLN:HG2	2:C:1087:THR:CG2	2.39	0.49
2:C:534:GLN:HE21	2:C:534:GLN:CA	2.24	0.49
2:C:560:GLU:HG3	2:C:561:PHE:N	2.28	0.49
2:C:648:TYR:CD2	2:C:650:THR:HG23	2.48	0.49
3:D:873:THR:O	3:D:877:VAL:HG23	2.13	0.49
9:P:15:DC:C6	9:P:16:DT:H72	2.48	0.49
2:C:916:ARG:NH2	10:C:1201:SO4:O1	2.45	0.49
2:C:102:ARG:O	2:C:124:LEU:HD23	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:510:VAL:HG12	2:C:568:ASP:O	2.13	0.49
1:A:63:PHE:CE1	2:C:741:ILE:HD13	2.47	0.49
5:F:199:GLN:HG2	7:J:82:TRP:CE2	2.47	0.49
5:F:324:LEU:HB3	5:F:332:PRO:HG3	1.95	0.49
1:B:105:VAL:HG12	1:B:125:ILE:HG21	1.94	0.49
2:C:1128:VAL:HG11	2:C:1138:MET:HE3	1.94	0.49
2:C:150:MET:CE	2:C:150:MET:HA	2.42	0.49
2:C:404:THR:HG23	2:C:406:GLN:H	1.77	0.49
2:C:508:ARG:HD3	2:C:515:VAL:CG1	2.41	0.49
2:C:680:ILE:HG12	2:C:693:ILE:O	2.13	0.49
2:C:698:CYS:O	2:C:705:ALA:N	2.42	0.49
3:D:1054:VAL:HG11	3:D:1100:LEU:HD21	1.95	0.49
3:D:1252:ASN:HB3	3:D:1257:LYS:HB3	1.94	0.49
3:D:911:ARG:NH1	3:D:949:ASP:OD1	2.32	0.49
5:F:173:ILE:HG22	5:F:238:LEU:CD1	2.43	0.49
1:B:4:SER:OG	1:B:5:GLN:N	2.45	0.48
2:C:1084:SER:OG	2:C:1085:ASP:N	2.46	0.48
2:C:423:GLY:O	2:C:424:THR:OG1	2.26	0.48
2:C:29:ARG:HD3	2:C:964:ALA:HB2	1.95	0.48
2:C:926:HIS:CE1	2:C:997:GLY:HA3	2.47	0.48
3:D:1122:VAL:HG23	3:D:1126:GLN:NE2	2.27	0.48
5:F:345:PRO:HA	5:F:348:VAL:HG13	1.94	0.48
7:J:90:SER:N	7:J:93:GLU:OE1	2.35	0.48
1:B:102:PRO:CG	1:B:131:LYS:H	2.26	0.48
1:B:196:VAL:HG13	1:B:196:VAL:O	2.12	0.48
1:B:32:TYR:CE1	2:C:1005:ARG:HD3	2.48	0.48
2:C:510:VAL:CG1	2:C:567:VAL:HG12	2.42	0.48
2:C:531:VAL:HG22	2:C:552:VAL:CG1	2.43	0.48
2:C:598:MET:O	2:C:602:MET:HG3	2.13	0.48
3:D:1057:GLU:HB2	3:D:1064:LYS:HB3	1.94	0.48
2:C:477:ILE:CD1	3:D:852:THR:HG21	2.43	0.48
8:O:31:DT:C6	8:O:31:DT:H5'	2.48	0.48
2:C:174:PRO:O	2:C:303:GLY:HA2	2.13	0.48
2:C:788:ARG:O	2:C:830:VAL:HG11	2.13	0.48
2:C:751:ARG:HG2	2:C:856:VAL:HG22	1.93	0.48
5:F:253:MET:HE3	5:F:297:MET:CA	2.30	0.48
1:B:87:SER:HB3	1:B:116:VAL:HG12	1.96	0.48
2:C:272:LEU:C	2:C:274:PRO:HD3	2.34	0.48
3:D:452:PHE:CE1	3:D:491:ILE:HG12	2.48	0.48
5:F:170:LEU:HA	5:F:173:ILE:HG12	1.96	0.48
5:F:277:LYS:HB3	5:F:279:TYR:CD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:911:HIS:NE2	3:D:580:ASP:OD1	2.46	0.48
3:D:103:HIS:CE1	3:D:105:TRP:HB2	2.49	0.48
3:D:739:PRO:HD3	3:D:791:PHE:CE2	2.49	0.48
4:E:81:GLU:OE1	4:E:81:GLU:HA	2.12	0.48
2:C:250:MET:O	2:C:253:LEU:HG	2.14	0.48
2:C:575:ARG:NH2	2:C:966:PRO:HB2	2.29	0.48
2:C:704:MET:CE	2:C:706:LEU:HD21	2.44	0.48
2:C:727:ILE:HD12	2:C:907:ILE:HD12	1.94	0.48
3:D:972:GLY:HA2	10:D:2004:SO4:O2	2.14	0.48
3:D:641:ARG:O	3:D:682:PHE:HB2	2.13	0.48
1:A:146:TYR:CG	2:C:734:GLU:HG2	2.48	0.48
2:C:204:GLU:HB2	2:C:216:ARG:NH1	2.28	0.48
2:C:236:ASN:HA	2:C:239:ILE:HD12	1.95	0.48
2:C:343:GLN:NE2	2:C:345:SER:O	2.47	0.48
3:D:26:GLY:HA3	3:D:51:ILE:HG23	1.95	0.48
3:D:599:TYR:HA	3:D:610:GLY:CA	2.44	0.48
5:F:214:GLN:HE21	5:F:214:GLN:HA	1.79	0.48
1:A:27:GLU:OE2	1:B:144:ARG:NH2	2.47	0.48
1:A:40:ARG:CZ	1:B:33:THR:HG22	2.44	0.48
2:C:70:GLU:N	2:C:70:GLU:OE1	2.46	0.48
2:C:712:VAL:CG1	2:C:925:THR:HG23	2.44	0.48
3:D:721:TYR:CZ	3:D:725:ARG:NH1	2.81	0.48
5:F:211:LEU:HB2	5:F:216:ARG:HD2	1.95	0.48
7:J:74:LYS:HG3	7:J:74:LYS:O	2.14	0.48
1:B:113:PRO:HD2	1:B:116:VAL:HG21	1.96	0.48
2:C:1070:TYR:CD1	3:D:559:MET:HG2	2.48	0.48
2:C:516:THR:HG23	2:C:518:GLN:H	1.79	0.48
2:C:678:ARG:O	2:C:694:ALA:HB1	2.13	0.48
2:C:935:TRP:C	2:C:983:THR:HG23	2.34	0.48
3:D:480:ARG:HB3	3:D:482:GLN:OE1	2.13	0.48
2:C:533:ALA:CB	2:C:570:MET:HG3	2.43	0.48
2:C:650:THR:HG22	2:C:660:SER:CB	2.44	0.48
3:D:1123:LEU:HD22	3:D:1208:LEU:HB2	1.95	0.48
3:D:58:TRP:CZ3	3:D:71:LYS:HE3	2.49	0.48
5:F:306:ILE:CG2	5:F:310:MET:HB3	2.44	0.48
1:B:111:VAL:HG13	1:B:111:VAL:O	2.14	0.47
2:C:572:VAL:O	2:C:573:SER:HB3	2.14	0.47
2:C:614:ALA:HA	2:C:705:ALA:CB	2.44	0.47
2:C:876:LEU:N	2:C:876:LEU:HD12	2.28	0.47
2:C:224:PRO:HD2	2:C:227:VAL:CG2	2.44	0.47
2:C:935:TRP:HB2	2:C:982:SER:CB	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:HD21	3:D:581:MET:HE3	1.95	0.47
3:D:664:GLU:O	3:D:664:GLU:HG3	2.15	0.47
7:J:40:PHE:HZ	7:J:58:ASN:HB2	1.79	0.47
8:O:6:DA:H2"	8:O:7:DC:OP2	2.14	0.47
1:A:210:SER:HB3	1:B:229:SER:HB2	1.96	0.47
1:A:39:ARG:O	1:A:43:LEU:HD13	2.14	0.47
1:B:99:LYS:HD3	1:B:109:ASP:OD2	2.14	0.47
2:C:530:HIS:HB3	2:C:568:ASP:OD2	2.14	0.47
2:C:642:GLU:HG2	2:C:643:GLU:HG3	1.96	0.47
3:D:116:TYR:CB	3:D:298:VAL:HG11	2.43	0.47
3:D:155:MET:HE3	3:D:219:LEU:HB3	1.96	0.47
3:D:527:LEU:CD1	3:D:712:VAL:HG12	2.44	0.47
3:D:736:LEU:N	3:D:792:TYR:OH	2.26	0.47
3:D:935:VAL:O	3:D:935:VAL:HG12	2.13	0.47
5:F:196:TYR:HA	7:J:82:TRP:CZ3	2.49	0.47
8:O:15:DT:H1'	8:O:16:DT:H5"	1.95	0.47
1:A:66:VAL:HB	1:A:69:VAL:CG2	2.41	0.47
1:B:22:VAL:HG12	1:B:193:ILE:CD1	2.45	0.47
2:C:167:VAL:HG13	2:C:445:ARG:O	2.15	0.47
1:B:32:TYR:CZ	2:C:1005:ARG:HD3	2.49	0.47
2:C:1045:GLN:HG3	2:C:1090:ARG:HH21	1.79	0.47
2:C:1084:SER:OG	3:D:420:LYS:HD3	2.15	0.47
2:C:236:ASN:HA	2:C:239:ILE:CD1	2.44	0.47
3:D:799:ILE:HG23	3:D:803:LYS:HG3	1.95	0.47
5:F:338:ALA:HB2	5:F:345:PRO:HA	1.97	0.47
7:J:40:PHE:CZ	7:J:58:ASN:HB2	2.49	0.47
5:F:274:ASP:CG	7:J:89:ARG:HH22	2.15	0.47
2:C:106:VAL:HG11	2:C:120:TYR:CE1	2.49	0.47
3:D:505:HIS:CD2	3:D:1004:GLU:HG3	2.49	0.47
3:D:646:LEU:HD23	3:D:646:LEU:O	2.15	0.47
8:O:4:DT:H2"	8:O:5:DG:C8	2.49	0.47
1:A:82:GLY:CA	1:A:123:MET:HE1	2.44	0.47
1:B:22:VAL:CG1	1:B:193:ILE:HD12	2.44	0.47
2:C:1028:VAL:HG12	3:D:429:VAL:HG12	1.95	0.47
2:C:148:PHE:CE1	2:C:380:ILE:HD11	2.50	0.47
2:C:732:LEU:HA	2:C:737:VAL:HG12	1.94	0.47
2:C:997:GLY:O	2:C:1015:THR:HG23	2.14	0.47
3:D:694:ARG:CZ	3:D:694:ARG:HB3	2.45	0.47
3:D:875:ARG:HH22	3:D:1033:GLN:CD	2.18	0.47
5:F:234:LEU:CD2	5:F:270:VAL:HG21	2.44	0.47
2:C:224:PRO:HB2	2:C:227:VAL:CG1	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LEU:CD2	2:C:323:THR:HG22	2.44	0.47
2:C:334:GLU:O	2:C:338:ARG:HG2	2.15	0.47
2:C:572:VAL:HG22	2:C:576:GLN:NE2	2.29	0.47
3:D:1081:LEU:HB3	3:D:1113:MET:CE	2.45	0.47
3:D:117:LEU:HD13	3:D:118:LEU:HD23	1.97	0.47
3:D:268:PHE:CZ	3:D:273:GLU:HG3	2.50	0.47
8:O:28:DT:H2'	8:O:29:DA:C8	2.49	0.47
1:A:111:VAL:CG2	1:A:111:VAL:O	2.62	0.47
1:A:54:ILE:C	1:A:54:ILE:HD12	2.35	0.47
2:C:1137:GLU:OE1	2:C:1137:GLU:N	2.44	0.47
2:C:199:ARG:HG2	2:C:200:GLY:N	2.30	0.47
2:C:571:ASP:HB3	2:C:576:GLN:HE21	1.79	0.47
3:D:39:LEU:HD13	3:D:335:PHE:HZ	1.79	0.47
3:D:590:THR:CG2	3:D:630:ARG:HE	2.28	0.47
3:D:915:VAL:HG23	3:D:920:PHE:CE2	2.50	0.47
1:A:9:LEU:HB2	1:A:23:ILE:HG12	1.96	0.47
1:B:60:LEU:HD22	1:B:60:LEU:N	2.29	0.47
2:C:141:GLN:OE1	2:C:406:GLN:HG2	2.15	0.47
5:F:373:LEU:O	5:F:373:LEU:HD23	2.15	0.47
1:B:213:GLY:HA2	1:B:216:VAL:HG12	1.97	0.47
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.50	0.47
2:C:712:VAL:HA	2:C:906:ILE:HG13	1.96	0.47
2:C:85:SER:HA	2:C:86:PRO:HA	1.70	0.47
3:D:1088:ARG:HA	3:D:1114:GLU:OE1	2.15	0.47
3:D:1128:PRO:HG3	3:D:1206:PRO:CB	2.45	0.47
3:D:822:LEU:HD23	3:D:834:PRO:CA	2.42	0.47
2:C:412:ARG:HD2	5:F:322:ARG:NE	2.30	0.47
3:D:22:ASN:HA	7:J:57:ARG:HH12	1.79	0.47
1:B:52:THR:HG21	1:B:141:GLU:OE2	2.14	0.46
1:A:40:ARG:CD	1:B:33:THR:HG22	2.40	0.46
2:C:32:PHE:HE1	2:C:963:VAL:CG1	2.28	0.46
2:C:1032:ILE:HG21	3:D:520:LYS:HD3	1.96	0.46
3:D:88:ARG:O	3:D:322:PRO:HD2	2.15	0.46
7:J:28:GLN:CG	7:J:46:ASP:HA	2.44	0.46
1:B:89:ASP:O	1:B:90:ASP:HB2	2.14	0.46
2:C:174:PRO:HA	2:C:196:ILE:HG23	1.97	0.46
2:C:224:PRO:O	2:C:226:THR:N	2.48	0.46
2:C:727:ILE:HA	2:C:888:LYS:O	2.15	0.46
3:D:278:ARG:HH11	3:D:278:ARG:HG3	1.80	0.46
3:D:28:VAL:HG22	3:D:28:VAL:O	2.15	0.46
3:D:642:PRO:HD3	3:D:656:LYS:CE	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:682:PHE:HE2	3:D:684:ASN:HB2	1.80	0.46
4:E:40:LEU:HB3	4:E:50:LEU:HD11	1.98	0.46
1:A:43:LEU:HD11	1:A:174:VAL:HB	1.96	0.46
1:A:36:ASN:CB	2:C:1007:GLY:HA3	2.44	0.46
1:B:147:VAL:O	1:B:147:VAL:HG13	2.16	0.46
1:B:226:ASN:O	1:B:227:ALA:HB3	2.15	0.46
2:C:217:ILE:HG13	2:C:217:ILE:O	2.14	0.46
2:C:461:LEU:N	2:C:461:LEU:HD23	2.31	0.46
2:C:640:VAL:HG22	2:C:641:ILE:N	2.31	0.46
2:C:984:LEU:CB	2:C:991:VAL:CG2	2.93	0.46
3:D:119:ASP:C	3:D:120:LEU:HD12	2.36	0.46
3:D:650:LEU:HD13	3:D:651:PHE:CE2	2.49	0.46
3:D:668:GLY:HA2	3:D:671:MET:HE2	1.97	0.46
3:D:825:ASN:CB	3:D:826:PRO:HD2	2.46	0.46
3:D:961:VAL:HG22	3:D:962:ARG:N	2.30	0.46
5:F:394:LEU:HB2	5:F:464:TYR:CD1	2.51	0.46
5:F:448:THR:O	5:F:452:LEU:HD22	2.15	0.46
1:A:113:PRO:HD2	1:A:116:VAL:CG2	2.43	0.46
2:C:41:VAL:HG13	2:C:493:VAL:CG1	2.45	0.46
2:C:35:LEU:HD13	2:C:969:ASP:OD2	2.15	0.46
8:O:11:DA:H2''	8:O:12:DG:C5'	2.45	0.46
1:B:18:ARG:HG3	1:B:197:GLU:HG3	1.98	0.46
2:C:565:ASP:OD1	2:C:566:GLN:N	2.48	0.46
2:C:851:GLU:C	2:C:852:LEU:HD12	2.35	0.46
3:D:214:ARG:O	3:D:218:ARG:HG3	2.14	0.46
1:A:8:THR:O	1:A:23:ILE:HA	2.16	0.46
2:C:882:ASN:HD21	2:C:1019:MET:CE	2.29	0.46
2:C:227:VAL:HG23	2:C:268:ILE:HD11	1.97	0.46
2:C:269:TYR:CD1	2:C:286:LEU:HD22	2.50	0.46
2:C:494:TYR:HB3	2:C:506:PRO:CG	2.40	0.46
2:C:578:VAL:HG13	2:C:582:THR:CG2	2.45	0.46
2:C:623:LEU:H	2:C:623:LEU:HD23	1.81	0.46
3:D:1170:ASP:O	3:D:1202:ALA:HA	2.15	0.46
3:D:1249:LEU:HA	3:D:1260:PRO:HD2	1.98	0.46
5:F:201:LEU:HD21	5:F:211:LEU:HD11	1.98	0.46
5:F:321:GLN:O	5:F:325:LEU:HB2	2.16	0.46
1:B:158:GLU:HB3	1:B:161:ARG:HB2	1.97	0.46
2:C:434:ASN:O	2:C:608:PRO:HD3	2.16	0.46
2:C:435:ASN:HB2	2:C:436:PRO:HD2	1.98	0.46
2:C:508:ARG:HD2	2:C:570:MET:HE3	1.97	0.46
2:C:805:LEU:HD22	2:C:805:LEU:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:589:GLU:HB3	2:C:968:PHE:CD1	2.51	0.46
2:C:885:VAL:HG22	3:D:536:PHE:O	2.15	0.46
3:D:735:VAL:HG22	3:D:798:ILE:CD1	2.45	0.46
3:D:740:GLN:OE1	3:D:787:ALA:HB1	2.16	0.46
5:F:409:GLU:HG2	5:F:448:THR:HG22	1.98	0.46
1:A:112:PRO:HB2	1:A:116:VAL:O	2.16	0.46
2:C:344:THR:HG22	2:C:344:THR:O	2.16	0.46
2:C:454:LEU:HD23	2:C:454:LEU:O	2.16	0.46
3:D:612:TYR:OH	3:D:627:LEU:HG	2.16	0.46
1:T:279:THR:HG23	1:T:282:ASP:H	1.80	0.46
2:C:898:LEU:HD23	2:C:1001:LEU:CD2	2.46	0.46
2:C:1126:VAL:O	2:C:1126:VAL:HG23	2.16	0.46
2:C:215:VAL:HG22	2:C:225:VAL:N	2.29	0.46
3:D:900:LEU:O	3:D:901:ALA:HB2	2.15	0.46
7:J:88:ARG:HG3	7:J:89:ARG:N	2.31	0.46
1:B:87:SER:OG	1:B:140:VAL:HG11	2.16	0.46
2:C:427:LEU:HD12	2:C:427:LEU:N	2.31	0.46
3:D:131:PHE:C	3:D:256:MET:HE1	2.36	0.46
3:D:603:THR:HG22	3:D:604:LYS:CG	2.38	0.46
8:O:12:DG:H1'	8:O:13:DT:H5''	1.97	0.46
9:P:3:DC:H2''	9:P:4:DA:C8	2.51	0.46
2:C:1043:ILE:HD13	3:D:412:ARG:HH22	1.81	0.45
2:C:55:LEU:HD22	2:C:376:ILE:HB	1.98	0.45
2:C:708:LYS:HG3	2:C:737:VAL:HG23	1.98	0.45
1:A:152:ASN:HD21	2:C:837:LYS:HZ3	1.64	0.45
2:C:716:PRO:HB3	2:C:909:ASN:OD1	2.16	0.45
3:D:91:ARG:O	3:D:321:PRO:HG3	2.16	0.45
5:F:272:LYS:HE2	7:J:84:MET:HE2	1.99	0.45
5:F:310:MET:O	5:F:314:ILE:HG13	2.16	0.45
9:P:4:DA:H2''	9:P:5:DC:C6	2.52	0.45
1:B:151:GLN:HG2	1:B:151:GLN:O	2.17	0.45
2:C:240:VAL:HA	2:C:250:MET:CE	2.45	0.45
2:C:614:ALA:H	2:C:700:GLN:NE2	2.14	0.45
2:C:777:GLU:H	2:C:777:GLU:CD	2.18	0.45
3:D:1062:PHE:CE1	3:D:1080:LYS:HB3	2.51	0.45
3:D:1165:ARG:HD2	3:D:1209:MET:CE	2.46	0.45
3:D:285:LYS:HA	3:D:289:LYS:HB2	1.99	0.45
3:D:31:PRO:HB3	3:D:348:ILE:HG23	1.99	0.45
3:D:929:VAL:O	3:D:929:VAL:HG23	2.16	0.45
4:E:39:GLU:OE1	4:E:97:HIS:NE2	2.36	0.45
5:F:180:ASN:OD1	5:F:182:GLU:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:231:ASN:O	5:F:235:GLU:HG3	2.16	0.45
1:T:269:VAL:HG23	1:T:269:VAL:O	2.16	0.45
1:A:84:VAL:HG12	1:A:120:ASN:CG	2.37	0.45
2:C:967:VAL:HG23	2:C:968:PHE:N	2.31	0.45
3:D:1140:GLN:NE2	3:D:1155:ILE:HD12	2.32	0.45
3:D:115:GLY:O	3:D:119:ASP:N	2.50	0.45
3:D:373:MET:SD	5:F:256:LEU:HB3	2.56	0.45
2:C:754:LYS:HD3	3:D:39:LEU:CD1	2.46	0.45
5:F:325:LEU:HD23	5:F:325:LEU:O	2.15	0.45
5:F:409:GLU:O	5:F:413:VAL:HG23	2.17	0.45
2:C:126:VAL:HG12	2:C:127:THR:N	2.31	0.45
2:C:186:THR:HG23	2:C:188:LYS:H	1.81	0.45
2:C:310:LYS:HE3	2:C:335:TYR:CE2	2.52	0.45
2:C:709:ASN:C	2:C:710:LEU:HD12	2.36	0.45
2:C:708:LYS:HG3	2:C:737:VAL:CG2	2.46	0.45
3:D:1034:GLU:OE2	3:D:1042:ARG:N	2.50	0.45
3:D:1129:ARG:O	3:D:1133:ILE:HG12	2.16	0.45
3:D:582:VAL:HB	3:D:806:ALA:HB2	1.99	0.45
3:D:568:PRO:HB3	3:D:983:ALA:HB2	1.98	0.45
1:B:182:ARG:O	1:B:186:ARG:O	2.35	0.45
2:C:299:LEU:HD23	2:C:323:THR:HG22	1.99	0.45
2:C:580:VAL:HG13	2:C:621:MET:HE2	1.98	0.45
2:C:765:PRO:CD	2:C:825:ASP:HB2	2.44	0.45
3:D:12:ILE:HG12	3:D:1221:TRP:CZ2	2.51	0.45
3:D:550:GLU:O	3:D:554:GLU:HG3	2.16	0.45
1:A:18:ARG:HA	1:A:204:PRO:HG3	1.99	0.45
1:B:138:LEU:N	1:B:138:LEU:HD12	2.31	0.45
2:C:475:CYS:HB2	2:C:579:SER:HB3	1.99	0.45
2:C:738:LEU:HB2	2:C:870:ILE:HB	1.99	0.45
3:D:711:THR:O	3:D:715:LEU:HG	2.17	0.45
7:J:106:LYS:CE	7:J:106:LYS:HA	2.19	0.45
1:A:147:VAL:HG12	1:A:168:TYR:HE2	1.81	0.45
2:C:648:TYR:CE2	2:C:650:THR:HG23	2.51	0.45
3:D:320:ILE:CG1	3:D:321:PRO:HD2	2.46	0.45
3:D:863:ALA:O	3:D:866:THR:HG22	2.17	0.45
5:F:164:ASP:OD1	5:F:165:SER:N	2.50	0.45
7:J:58:ASN:HD21	7:J:60:LEU:HD12	1.81	0.45
9:P:4:DA:H2"	9:P:5:DC:H6	1.82	0.45
1:A:125:ILE:N	1:A:125:ILE:HD12	2.31	0.45
1:A:54:ILE:O	1:A:54:ILE:HD12	2.17	0.45
1:B:174:VAL:HA	1:B:195:ASP:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PHE:HE1	1:B:44:SER:HB3	1.81	0.45
2:C:372:VAL:O	2:C:376:ILE:HG12	2.17	0.45
2:C:531:VAL:CG1	2:C:552:VAL:HG13	2.36	0.45
2:C:945:ASP:N	2:C:945:ASP:OD1	2.48	0.45
3:D:1132:GLN:CG	3:D:1163:LEU:HD12	2.46	0.45
3:D:47:PHE:CD1	3:D:322:PRO:HB3	2.52	0.45
5:F:440:ARG:O	5:F:444:ILE:HG13	2.16	0.45
7:J:106:LYS:CA	7:J:106:LYS:HE2	2.26	0.45
1:B:68:GLY:O	1:B:129:ASN:N	2.44	0.45
2:C:454:LEU:HD12	2:C:459:ALA:CB	2.47	0.45
3:D:276:SER:O	3:D:280:VAL:HG23	2.17	0.45
3:D:114:LEU:HG	3:D:312:MET:HE2	1.99	0.45
5:F:404:THR:CB	5:F:457:ARG:HH21	2.30	0.45
8:O:11:DA:C2'	8:O:12:DG:H5''	2.46	0.45
2:C:197:PRO:HG3	2:C:297:TYR:CE1	2.51	0.45
2:C:44:LEU:HD13	2:C:440:LEU:HD21	1.98	0.45
3:D:246:ASP:OD1	3:D:246:ASP:N	2.46	0.45
3:D:507:LEU:HD12	3:D:507:LEU:HA	1.82	0.45
3:D:581:MET:HE2	3:D:716:LYS:CA	2.36	0.45
3:D:602:ALA:CB	3:D:607:PRO:O	2.65	0.45
3:D:641:ARG:HA	3:D:656:LYS:HZ1	1.81	0.45
5:F:348:VAL:O	5:F:352:GLN:HG3	2.17	0.45
1:A:215:LEU:HA	1:A:215:LEU:HD12	1.87	0.44
2:C:1048:LEU:HD23	2:C:1048:LEU:N	2.19	0.44
2:C:229:LEU:O	2:C:229:LEU:HD12	2.17	0.44
2:C:712:VAL:HG12	2:C:1017:GLY:O	2.18	0.44
2:C:772:LEU:HA	2:C:775:LEU:HD22	1.98	0.44
2:C:949:LYS:O	2:C:949:LYS:HG2	2.17	0.44
3:D:191:SER:O	3:D:195:ARG:HG2	2.17	0.44
3:D:203:ARG:HA	3:D:203:ARG:NE	2.31	0.44
3:D:460:LEU:HD12	3:D:460:LEU:C	2.38	0.44
3:D:599:TYR:CA	3:D:610:GLY:HA3	2.48	0.44
3:D:884:ILE:HD11	3:D:886:ARG:CD	2.47	0.44
5:F:465:LEU:O	5:F:466:ASP:HB2	2.16	0.44
5:F:295:ARG:NH2	8:O:24:DG:O6	2.50	0.44
1:A:149:ALA:HB2	1:A:164:VAL:C	2.38	0.44
1:A:54:ILE:CD1	1:A:162:ILE:HB	2.47	0.44
1:B:213:GLY:HA2	1:B:216:VAL:CG1	2.48	0.44
2:C:132:ASN:CG	2:C:135:THR:HG22	2.37	0.44
2:C:231:ALA:HB1	2:C:287:LEU:HD11	1.99	0.44
2:C:51:SER:OG	2:C:371:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:575:ARG:HE	2:C:967:VAL:CG2	2.24	0.44
3:D:49:GLU:OE1	3:D:61:TYR:HD1	2.00	0.44
3:D:801:ILE:HG22	3:D:807:THR:O	2.16	0.44
5:F:317:LEU:HD23	5:F:317:LEU:O	2.17	0.44
2:C:299:LEU:HD12	2:C:299:LEU:C	2.37	0.44
2:C:885:VAL:CG1	3:D:538:GLY:HA2	2.47	0.44
3:D:173:ARG:HH22	3:D:201:GLY:HA2	1.80	0.44
5:F:244:LEU:HD12	5:F:289:ILE:CG2	2.48	0.44
1:B:41:THR:HG22	1:B:211:ALA:CB	2.47	0.44
2:C:199:ARG:HB3	2:C:199:ARG:CZ	2.47	0.44
2:C:335:TYR:HD1	2:C:335:TYR:O	2.00	0.44
2:C:704:MET:HE3	2:C:706:LEU:HD21	2.00	0.44
2:C:744:GLU:HG3	2:C:834:GLU:OE2	2.18	0.44
3:D:1056:LEU:HD23	3:D:1057:GLU:H	1.82	0.44
3:D:525:HIS:O	3:D:528:VAL:HG22	2.18	0.44
1:B:77:ILE:O	1:B:81:LYS:HG3	2.17	0.44
2:C:1031:LYS:NZ	10:C:1203:SO4:S	2.90	0.44
2:C:404:THR:HG23	2:C:406:GLN:N	2.32	0.44
2:C:587:PHE:CD2	2:C:923:LEU:HB2	2.53	0.44
3:D:1181:LEU:HD11	3:D:1213:LYS:HE2	1.99	0.44
3:D:1266:SER:CA	3:D:1269:ARG:NH1	2.79	0.44
5:F:214:GLN:NE2	5:F:214:GLN:HA	2.33	0.44
3:D:79:GLY:HA2	7:J:54:TRP:CH2	2.53	0.44
1:A:93:VAL:HG22	1:A:113:PRO:HG2	2.00	0.44
1:B:105:VAL:HB	1:B:125:ILE:HG23	1.99	0.44
1:B:185:GLN:HE21	1:B:185:GLN:HB2	1.51	0.44
1:B:29:GLY:HA2	1:B:190:ASP:OD2	2.17	0.44
2:C:203:LEU:CD1	2:C:217:ILE:HB	2.47	0.44
2:C:406:GLN:OE1	5:F:326:GLN:HG2	2.17	0.44
3:D:190:LYS:HD2	3:D:192:ASP:H	1.82	0.44
3:D:573:PRO:HG2	3:D:576:MET:HE2	2.00	0.44
5:F:308:VAL:HG23	5:F:309:HIS:N	2.33	0.44
5:F:324:LEU:CD2	5:F:328:LEU:HD22	2.48	0.44
1:A:57:ASP:N	1:A:57:ASP:OD1	2.49	0.44
1:B:32:TYR:CZ	2:C:1005:ARG:NH1	2.86	0.44
1:B:99:LYS:HE2	1:B:99:LYS:HB3	1.73	0.44
2:C:34:LYS:HD2	2:C:34:LYS:N	2.33	0.44
8:O:14:DG:H3'	1:T:258:VAL:CG1	2.45	0.44
2:C:44:LEU:CD1	2:C:440:LEU:HD21	2.48	0.44
2:C:586:PRO:O	2:C:880:HIS:HE1	1.99	0.44
2:C:721:ASN:ND2	2:C:727:ILE:HD11	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1042:ARG:H	3:D:1042:ARG:HG2	1.64	0.44
3:D:1152:ASP:O	3:D:1156:GLU:HG3	2.18	0.44
3:D:277:LEU:CD2	3:D:292:ALA:HB1	2.47	0.44
3:D:962:ARG:HB3	3:D:977:CYS:HA	1.98	0.44
4:E:80:VAL:O	4:E:82:PRO:HD3	2.17	0.44
5:F:320:ILE:HG22	5:F:337:LEU:HD12	2.00	0.44
7:J:92:GLU:OE1	7:J:92:GLU:N	2.39	0.44
2:C:128:ALA:HB2	2:C:143:VAL:HG21	1.99	0.44
2:C:302:VAL:HG11	2:C:368:ARG:CD	2.48	0.44
3:D:1054:VAL:HG23	3:D:1065:ILE:HG23	2.00	0.44
3:D:1168:ILE:CD1	3:D:1176:PHE:HB3	2.41	0.44
3:D:137:THR:HG23	3:D:253:THR:OG1	2.18	0.44
3:D:222:ILE:HG23	3:D:244:LEU:HD23	2.00	0.44
3:D:599:TYR:CZ	3:D:601:ALA:HB2	2.53	0.44
3:D:737:VAL:HG13	3:D:738:PRO:HD2	2.00	0.44
3:D:706:ILE:CD1	4:E:36:PRO:HB3	2.47	0.44
1:A:147:VAL:HG13	1:A:147:VAL:O	2.18	0.43
2:C:1138:MET:O	2:C:1139:ARG:HG3	2.18	0.43
2:C:158:ILE:HD12	2:C:158:ILE:N	2.32	0.43
2:C:372:VAL:HG13	2:C:373:GLY:N	2.33	0.43
2:C:47:VAL:HG23	2:C:497:VAL:HG21	2.00	0.43
2:C:664:ARG:HB2	2:C:677:GLN:OE1	2.18	0.43
2:C:77:LEU:HA	2:C:77:LEU:HD23	1.85	0.43
2:C:726:ILE:HG23	2:C:908:LEU:HD23	2.00	0.43
3:D:1056:LEU:HD23	3:D:1057:GLU:N	2.32	0.43
5:F:241:VAL:HG22	5:F:289:ILE:HD13	2.00	0.43
7:J:69:VAL:O	7:J:69:VAL:HG12	2.17	0.43
9:P:13:DC:H2"	9:P:14:DA:C8	2.53	0.43
1:A:34:LEU:HD11	1:B:218:LEU:CD1	2.45	0.43
2:C:1015:THR:HG1	3:D:731:SER:HG	1.65	0.43
2:C:992:MET:HB3	2:C:992:MET:HE2	1.81	0.43
3:D:34:ILE:O	5:F:304:ILE:HG23	2.18	0.43
3:D:354:LEU:O	3:D:358:ILE:HG12	2.19	0.43
3:D:46:LEU:O	3:D:47:PHE:HB2	2.18	0.43
3:D:988:VAL:HG23	3:D:992:GLU:HG3	1.99	0.43
4:E:57:ARG:HH22	4:E:76:VAL:HG13	1.83	0.43
1:A:9:LEU:HD23	1:B:221:LEU:C	2.38	0.43
2:C:1045:GLN:CG	2:C:1090:ARG:HH21	2.32	0.43
2:C:1057:GLN:O	3:D:421:ARG:HA	2.17	0.43
2:C:445:ARG:NE	12:C:1205:SRN:O6	2.31	0.43
2:C:228:LEU:HA	2:C:228:LEU:HD23	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:PRO:HG3	2:C:577:MET:HE3	2.01	0.43
3:D:885:VAL:O	3:D:990:ILE:O	2.36	0.43
7:J:65:ILE:HG22	7:J:65:ILE:O	2.19	0.43
2:C:53:GLU:O	2:C:57:GLY:N	2.52	0.43
3:D:1009:LEU:HD12	3:D:1146:GLN:CG	2.38	0.43
3:D:612:TYR:HB2	3:D:635:VAL:CG1	2.48	0.43
3:D:813:THR:HG22	3:D:813:THR:O	2.17	0.43
1:B:139:VAL:HG21	1:B:161:ARG:HH21	1.83	0.43
2:C:361:ILE:N	2:C:361:ILE:HD12	2.28	0.43
2:C:891:PRO:CB	2:C:893:GLU:HG2	2.37	0.43
3:D:1004:GLU:N	3:D:1005:PRO:HD2	2.34	0.43
3:D:591:LEU:HD22	3:D:592:VAL:N	2.33	0.43
5:F:440:ARG:NH1	5:F:443:GLN:OE1	2.38	0.43
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.70	0.43
2:C:1043:ILE:HG23	2:C:1044:THR:N	2.31	0.43
2:C:398:GLN:HE21	2:C:398:GLN:HB3	1.57	0.43
2:C:563:SER:O	2:C:564:ALA:HB3	2.18	0.43
2:C:780:ILE:HG13	2:C:780:ILE:O	2.19	0.43
2:C:797:VAL:HG13	2:C:824:ARG:O	2.18	0.43
3:D:796:ASN:HD22	3:D:799:ILE:H	1.66	0.43
5:F:277:LYS:HB3	5:F:279:TYR:CE2	2.54	0.43
1:A:47:PRO:O	1:A:170:PRO:HG2	2.18	0.43
2:C:879:ARG:NH2	2:C:1020:TYR:HB3	2.34	0.43
12:C:1205:SRN:H152	12:C:1205:SRN:H181	1.70	0.43
2:C:126:VAL:HG23	2:C:145:MET:HG2	2.01	0.43
2:C:217:ILE:CD1	2:C:272:LEU:HD21	2.49	0.43
2:C:291:PHE:HA	2:C:297:TYR:HB2	2.00	0.43
2:C:299:LEU:HD23	2:C:323:THR:CG2	2.49	0.43
2:C:800:LYS:HG3	2:C:801:GLY:N	2.34	0.43
3:D:1161:GLN:HA	3:D:1164:ARG:HD3	2.00	0.43
3:D:869:SER:HB2	3:D:1029:LEU:HD21	2.00	0.43
1:A:112:PRO:HB2	1:A:116:VAL:HG23	2.00	0.43
1:B:171:VAL:O	1:B:171:VAL:HG23	2.19	0.43
2:C:29:ARG:HG2	2:C:964:ALA:HB2	2.00	0.43
2:C:910:THR:O	2:C:914:PRO:HD3	2.19	0.43
2:C:930:VAL:HG12	2:C:935:TRP:CE3	2.53	0.43
2:C:950:LEU:CB	2:C:951:PRO:HD2	2.48	0.43
2:C:718:GLU:H	3:D:724:THR:CG2	2.32	0.43
5:F:359:ILE:HG22	5:F:360:SER:N	2.33	0.43
5:F:359:ILE:HG22	5:F:360:SER:H	1.84	0.43
2:C:728:LEU:HB2	2:C:889:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:723:ALA:O	3:D:726:SER:HB3	2.19	0.43
5:F:179:LEU:CD1	5:F:187:LEU:HD12	2.49	0.43
1:A:210:SER:HA	1:B:229:SER:HB2	2.00	0.42
1:B:211:ALA:O	1:B:215:LEU:HB2	2.18	0.42
2:C:338:ARG:HB2	2:C:356:VAL:HG21	2.00	0.42
3:D:1009:LEU:HD23	3:D:1029:LEU:HD12	2.00	0.42
3:D:1037:GLU:HG2	3:D:1039:ARG:CZ	2.49	0.42
3:D:1050:VAL:HG22	3:D:1051:ALA:H	1.83	0.42
3:D:1168:ILE:HD13	3:D:1176:PHE:CG	2.54	0.42
3:D:1276:THR:HG22	4:E:102:GLU:CG	2.47	0.42
3:D:651:PHE:C	3:D:653:ASN:H	2.22	0.42
3:D:921:ALA:HB3	3:D:1151:HIS:NE2	2.34	0.42
4:E:28:THR:HG23	4:E:28:THR:O	2.19	0.42
1:A:84:VAL:HG13	1:A:84:VAL:O	2.19	0.42
2:C:649:ILE:HD13	2:C:693:ILE:HG22	2.01	0.42
3:D:331:ASP:N	3:D:331:ASP:OD1	2.52	0.42
3:D:687:MET:CE	3:D:695:ILE:HD11	2.49	0.42
3:D:716:LYS:HB3	3:D:716:LYS:HE2	1.84	0.42
2:C:1012:TYR:CG	3:D:727:GLY:HA3	2.54	0.42
5:F:246:LYS:HB3	5:F:246:LYS:HE2	1.80	0.42
1:A:113:PRO:O	1:A:116:VAL:HG22	2.19	0.42
1:A:167:ILE:HD11	2:C:734:GLU:HB3	2.01	0.42
1:A:50:ALA:HB3	1:A:168:TYR:CE1	2.54	0.42
1:A:36:ASN:HB3	2:C:1007:GLY:HA3	2.00	0.42
2:C:772:LEU:N	2:C:772:LEU:HD12	2.34	0.42
3:D:170:LEU:HD11	3:D:209:ARG:HB2	2.02	0.42
5:F:268:ARG:HD3	5:F:288:TRP:CZ2	2.54	0.42
1:T:279:THR:HG23	1:T:282:ASP:CB	2.49	0.42
1:A:11:GLU:HG2	1:A:12:GLU:H	1.83	0.42
1:B:95:MET:HE3	1:B:110:ILE:HD13	2.00	0.42
3:D:590:THR:HG23	3:D:630:ARG:HE	1.84	0.42
5:F:462:ARG:HD3	5:F:462:ARG:C	2.38	0.42
1:A:146:TYR:HD2	1:A:167:ILE:HG12	1.85	0.42
1:B:84:VAL:HG22	1:B:119:HIS:HB2	2.00	0.42
2:C:613:GLU:HB3	2:C:708:LYS:CD	2.50	0.42
2:C:922:ILE:O	2:C:925:THR:HB	2.19	0.42
3:D:880:SER:HB3	3:D:1158:ILE:HD13	2.02	0.42
1:B:96:TYR:O	1:B:110:ILE:HG13	2.19	0.42
1:A:2:LEU:HD13	1:B:142:ARG:CB	2.50	0.42
1:B:150:VAL:O	1:B:150:VAL:HG13	2.19	0.42
2:C:193:VAL:CG1	2:C:336:LEU:HD12	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:HIS:HD2	2:C:469:SER:OG	2.03	0.42
2:C:584:MET:CA	2:C:619:THR:HG21	2.37	0.42
3:D:50:LYS:HE2	7:J:55:LEU:HB3	2.02	0.42
3:D:884:ILE:HD11	3:D:886:ARG:HD3	2.02	0.42
5:F:258:LEU:HD22	5:F:293:ILE:HG23	2.01	0.42
8:O:1:DG:H2''	8:O:2:DC:H5'	2.00	0.42
2:C:1036:SER:HB3	3:D:450:GLU:O	2.20	0.42
2:C:180:GLU:O	2:C:180:GLU:HG3	2.19	0.42
2:C:217:ILE:HD11	2:C:272:LEU:HD21	2.01	0.42
2:C:794:VAL:HG21	2:C:860:VAL:CG1	2.49	0.42
2:C:976:LEU:HA	2:C:976:LEU:HD23	1.83	0.42
3:D:92:MET:HG2	3:D:321:PRO:HD3	2.01	0.42
3:D:899:THR:HA	3:D:958:THR:HG22	2.00	0.42
3:D:706:ILE:CD1	4:E:36:PRO:HA	2.50	0.42
8:O:16:DT:H6	8:O:16:DT:H5'	1.84	0.42
1:B:56:ILE:HG23	1:B:136:VAL:HG23	2.01	0.42
2:C:1037:THR:HG22	2:C:1038:GLY:N	2.35	0.42
2:C:560:GLU:CG	2:C:561:PHE:N	2.83	0.42
2:C:986:ASN:OD1	2:C:986:ASN:N	2.52	0.42
3:D:269:ASP:HB3	3:D:272:ALA:CB	2.42	0.42
3:D:656:LYS:CD	3:D:656:LYS:H	2.33	0.42
5:F:174:GLY:HA2	5:F:239:ARG:CZ	2.49	0.42
5:F:345:PRO:HA	5:F:348:VAL:CG1	2.49	0.42
1:A:9:LEU:HD12	1:A:22:VAL:O	2.20	0.42
1:B:30:PHE:HA	1:B:33:THR:CG2	2.49	0.42
1:B:52:THR:OG1	1:B:141:GLU:HG2	2.18	0.42
2:C:1035:ARG:HD3	2:C:1056:GLY:CA	2.50	0.42
2:C:1108:ILE:N	2:C:1108:ILE:HD12	2.28	0.42
2:C:421:PHE:O	2:C:425:SER:CB	2.65	0.42
2:C:926:HIS:O	2:C:930:VAL:HG23	2.20	0.42
2:C:936:ASN:N	2:C:983:THR:HG23	2.35	0.42
3:D:927:ASP:OD1	3:D:938:GLU:HA	2.19	0.42
5:F:366:GLY:C	5:F:369:GLY:H	2.23	0.42
5:F:416:ARG:HA	5:F:430:ILE:HD11	2.02	0.42
1:B:143:GLY:HA3	1:B:168:TYR:CE1	2.55	0.42
1:B:41:THR:HG22	1:B:211:ALA:HB1	2.00	0.42
2:C:445:ARG:HH11	2:C:445:ARG:CG	2.33	0.42
2:C:626:ALA:HB3	2:C:702:GLY:O	2.20	0.42
3:D:417:LEU:HD12	3:D:417:LEU:HA	1.75	0.42
2:C:723:GLU:HB3	3:D:536:PHE:HD1	1.85	0.42
3:D:890:CYS:O	3:D:891:GLU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:283:THR:OG1	8:O:29:DA:H8	2.03	0.42
1:A:172:LEU:HD23	1:A:172:LEU:C	2.41	0.41
1:B:147:VAL:HG11	1:B:168:TYR:CZ	2.55	0.41
2:C:1093:VAL:O	2:C:1097:ILE:HG13	2.20	0.41
12:C:1205:SRN:C4	12:C:1205:SRN:O1	2.66	0.41
2:C:481:GLU:HG2	2:C:597:LEU:CD2	2.50	0.41
3:D:1035:LEU:HD11	3:D:1138:GLU:HB3	2.02	0.41
3:D:417:LEU:CG	3:D:1254:ILE:HG23	2.42	0.41
3:D:58:TRP:HA	3:D:82:VAL:HG23	2.01	0.41
5:F:313:VAL:CG2	5:F:351:ILE:HD13	2.50	0.41
3:D:397:ARG:HH21	5:F:360:SER:CB	2.33	0.41
5:F:426:THR:OG1	5:F:429:GLU:HG3	2.20	0.41
1:A:11:GLU:OE1	1:A:205:ARG:HD3	2.18	0.41
1:B:74:THR:O	1:B:78:LEU:HG	2.20	0.41
2:C:294:GLU:OE1	2:C:295:LYS:N	2.53	0.41
2:C:170:LEU:N	2:C:447:SER:O	2.43	0.41
2:C:691:GLN:HG2	2:C:692:VAL:N	2.35	0.41
2:C:859:LEU:HD13	2:C:859:LEU:C	2.40	0.41
3:D:582:VAL:CG1	3:D:806:ALA:HB2	2.49	0.41
3:D:656:LYS:HB2	3:D:659:ASP:O	2.20	0.41
5:F:338:ALA:HB2	5:F:348:VAL:CG1	2.47	0.41
1:B:18:ARG:CG	1:B:197:GLU:HG3	2.50	0.41
2:C:367:ARG:NH2	2:C:448:ALA:HB2	2.35	0.41
2:C:801:GLY:O	2:C:802:GLU:C	2.58	0.41
3:D:1050:VAL:HG22	3:D:1051:ALA:N	2.34	0.41
3:D:1117:ALA:O	3:D:1119:PRO:HD3	2.20	0.41
3:D:1121:GLU:OE2	3:D:1124:ARG:NH2	2.35	0.41
3:D:413:PHE:CD2	3:D:1226:SER:HB3	2.54	0.41
2:C:911:HIS:CE1	3:D:580:ASP:HA	2.55	0.41
3:D:650:LEU:HB3	3:D:651:PHE:CD2	2.55	0.41
2:C:973:GLU:CA	3:D:732:MET:HE3	2.50	0.41
5:F:269:ALA:O	5:F:273:PHE:HB2	2.20	0.41
5:F:371:SER:HG	5:F:376:PHE:HZ	1.65	0.41
1:A:50:ALA:HB3	1:A:168:TYR:CD1	2.55	0.41
1:B:105:VAL:HG12	1:B:125:ILE:CG2	2.50	0.41
2:C:644:VAL:O	2:C:644:VAL:HG23	2.19	0.41
2:C:747:GLU:CG	2:C:859:LEU:HD21	2.50	0.41
2:C:992:MET:HA	2:C:992:MET:CE	2.50	0.41
3:D:1132:GLN:HG3	3:D:1163:LEU:CD1	2.50	0.41
3:D:114:LEU:HG	3:D:312:MET:CE	2.51	0.41
3:D:320:ILE:HG12	3:D:321:PRO:CD	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:613:SER:N	3:D:617:GLU:OE1	2.50	0.41
3:D:1271:ILE:HG12	4:E:105:GLU:HA	2.02	0.41
5:F:321:GLN:NE2	5:F:331:GLU:OE2	2.54	0.41
5:F:272:LYS:HB2	7:J:84:MET:CE	2.50	0.41
1:B:183:VAL:HG13	3:D:488:GLU:CD	2.41	0.41
1:A:219:PHE:CE1	1:B:38:LEU:HD21	2.54	0.41
1:B:71:GLU:HB3	1:B:76:ILE:HG13	2.01	0.41
2:C:126:VAL:HG12	2:C:127:THR:H	1.85	0.41
2:C:601:ASN:O	2:C:605:GLN:HG3	2.21	0.41
2:C:441:THR:CB	2:C:604:ARG:HD3	2.51	0.41
2:C:822:GLU:H	2:C:822:GLU:CD	2.24	0.41
2:C:1043:ILE:HD13	3:D:412:ARG:NH2	2.35	0.41
3:D:83:THR:OG1	3:D:84:ARG:N	2.53	0.41
4:E:57:ARG:HH12	4:E:76:VAL:HG12	1.85	0.41
1:B:96:TYR:CE1	1:B:137:GLU:HG3	2.55	0.41
2:C:199:ARG:HB3	2:C:199:ARG:NH1	2.35	0.41
2:C:445:ARG:HE	12:C:1205:SRN:HO6	1.62	0.41
2:C:572:VAL:HG22	2:C:576:GLN:CD	2.41	0.41
2:C:472:GLY:H	2:C:577:MET:HA	1.86	0.41
2:C:639:GLY:HA3	2:C:653:ALA:HA	2.02	0.41
2:C:959:ALA:O	2:C:960:ASP:HB2	2.20	0.41
3:D:753:ASP:O	3:D:757:ARG:N	2.48	0.41
3:D:860:ALA:O	3:D:863:ALA:HB3	2.21	0.41
4:E:95:GLU:HB3	4:E:101:LEU:CD2	2.51	0.41
5:F:427:LEU:HD12	9:P:20:DG:H2'	2.02	0.41
8:O:19:DA:H2'	8:O:20:DT:H6	1.85	0.41
1:B:200:ASN:ND2	1:B:200:ASN:H	2.17	0.41
1:B:79:ASN:O	1:B:123:MET:HE1	2.21	0.41
2:C:1122:LEU:HD12	2:C:1122:LEU:HA	1.80	0.41
2:C:41:VAL:HG13	2:C:493:VAL:HG12	2.02	0.41
3:D:1045:ALA:HA	3:D:1046:PRO:HD3	1.92	0.41
3:D:1132:GLN:CD	3:D:1163:LEU:HD12	2.41	0.41
3:D:676:LEU:HD12	3:D:676:LEU:H	1.83	0.41
5:F:173:ILE:HG22	5:F:238:LEU:HD13	2.03	0.41
1:B:32:TYR:OH	2:C:1005:ARG:NH1	2.53	0.41
2:C:1117:LYS:HD2	2:C:1117:LYS:HA	1.71	0.41
2:C:51:SER:CB	2:C:371:THR:OG1	2.69	0.41
2:C:641:ILE:CG2	2:C:644:VAL:HG13	2.50	0.41
2:C:433:GLN:HE21	2:C:670:ASN:H	1.68	0.41
3:D:236:VAL:HG12	3:D:236:VAL:O	2.20	0.41
3:D:28:VAL:HG21	3:D:46:LEU:CD2	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:365:ILE:HD13	5:F:235:GLU:HG2	2.02	0.41
3:D:650:LEU:CD1	3:D:661:TRP:HB2	2.51	0.41
7:J:98:LEU:O	7:J:102:LEU:HD13	2.21	0.41
1:B:47:PRO:HB3	1:B:144:ARG:HD2	2.03	0.41
2:C:882:ASN:HD21	2:C:1019:MET:HE1	1.85	0.41
2:C:464:ARG:HG2	2:C:485:ILE:O	2.21	0.41
3:D:183:GLU:O	3:D:187:GLU:HG2	2.21	0.41
3:D:321:PRO:HD2	3:D:324:LEU:HD12	2.02	0.41
3:D:633:ILE:C	3:D:633:ILE:HD12	2.41	0.41
3:D:796:ASN:ND2	3:D:798:ILE:H	2.19	0.41
3:D:54:PRO:HG3	3:D:81:GLU:O	2.20	0.41
3:D:920:PHE:CZ	3:D:948:ILE:HG13	2.56	0.41
5:F:195:LEU:HD21	7:J:81:HIS:CG	2.55	0.41
7:J:98:LEU:HG	7:J:102:LEU:CD1	2.50	0.41
1:B:34:LEU:CD1	1:B:192:LEU:HD22	2.51	0.41
1:B:210:SER:O	1:B:214:THR:HG23	2.20	0.41
1:A:33:THR:HG22	1:B:37:SER:HA	2.03	0.41
1:B:63:PHE:CE1	3:D:604:LYS:HA	2.56	0.41
2:C:1138:MET:C	2:C:1139:ARG:HG3	2.41	0.41
2:C:446:LEU:HD21	2:C:491:LEU:N	2.36	0.41
2:C:554:LYS:O	2:C:557:GLY:HA2	2.20	0.41
2:C:839:ILE:HG22	2:C:840:GLY:N	2.36	0.41
3:D:1208:LEU:HD23	3:D:1208:LEU:HA	1.90	0.41
3:D:237:ASP:OD2	3:D:240:LEU:HB2	2.21	0.41
3:D:143:MET:HG2	3:D:251:TYR:CD1	2.55	0.41
3:D:285:LYS:HG3	3:D:289:LYS:CD	2.51	0.41
3:D:599:TYR:N	3:D:633:ILE:HG22	2.36	0.41
3:D:748:HIS:CE1	3:D:780:ALA:HB2	2.56	0.41
1:T:264:LEU:HB3	1:T:269:VAL:HG21	2.03	0.41
1:A:2:LEU:HD13	1:B:142:ARG:HB3	2.03	0.41
2:C:166:VAL:HA	2:C:427:LEU:O	2.20	0.41
2:C:493:VAL:HG23	2:C:578:VAL:O	2.20	0.41
2:C:614:ALA:CB	2:C:700:GLN:HE21	2.34	0.41
2:C:797:VAL:HG11	2:C:823:VAL:CG2	2.50	0.41
3:D:507:LEU:HB3	3:D:531:ALA:HB1	2.02	0.41
3:D:904:GLY:HA3	3:D:910:ILE:HG21	2.01	0.41
3:D:939:ARG:HG3	3:D:939:ARG:O	2.21	0.41
5:F:230:LYS:O	5:F:234:LEU:HG	2.21	0.41
3:D:67:ARG:NH1	5:F:423:GLN:HA	2.36	0.41
1:A:49:ALA:HB2	1:A:87:SER:H	1.86	0.40
2:C:168:SER:HB2	2:C:369:LEU:HG	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:475:CYS:HA	2:C:577:MET:O	2.21	0.40
2:C:498:ASN:ND2	2:C:500:PHE:HB2	2.36	0.40
2:C:751:ARG:CD	2:C:856:VAL:HG22	2.50	0.40
3:D:1009:LEU:CD2	3:D:1029:LEU:HD12	2.51	0.40
3:D:59:GLU:HG2	3:D:66:LYS:HG3	2.03	0.40
4:E:76:VAL:HG13	4:E:77:GLY:N	2.36	0.40
8:O:16:DT:C6	8:O:16:DT:H5'	2.56	0.40
1:A:100:GLN:HG3	1:A:101:GLY:N	2.36	0.40
1:B:202:ILE:HG12	1:B:206:ASP:HB2	2.03	0.40
2:C:1034:ALA:O	2:C:1054:PHE:HE2	2.04	0.40
2:C:852:LEU:HD22	2:C:856:VAL:O	2.21	0.40
3:D:200:SER:O	3:D:204:GLU:HG3	2.22	0.40
3:D:578:ARG:HA	3:D:582:VAL:HG23	2.03	0.40
3:D:581:MET:HE3	3:D:716:LYS:HB2	2.02	0.40
3:D:751:GLU:O	3:D:755:ILE:HG13	2.21	0.40
5:F:187:LEU:O	5:F:191:ILE:HG13	2.21	0.40
5:F:251:ARG:HB2	5:F:297:MET:HE3	2.02	0.40
5:F:290:ARG:NH1	14:F:603:HOH:O	2.54	0.40
9:P:5:DC:H2''	9:P:6:DA:C8	2.56	0.40
2:C:103:PHE:HE2	2:C:148:PHE:HB3	1.86	0.40
2:C:399:ASP:O	2:C:403:ILE:HG23	2.22	0.40
2:C:445:ARG:HE	12:C:1205:SRN:C24	2.35	0.40
2:C:619:THR:OG1	2:C:620:GLY:N	2.54	0.40
2:C:640:VAL:CG2	2:C:641:ILE:N	2.84	0.40
3:D:1010:THR:O	3:D:1011:MET:CB	2.70	0.40
3:D:1081:LEU:N	3:D:1081:LEU:HD22	2.36	0.40
3:D:650:LEU:HD11	3:D:661:TRP:HB2	2.02	0.40
5:F:173:ILE:HG22	5:F:238:LEU:HD12	2.04	0.40
7:J:77:PRO:HA	7:J:78:PRO:HD3	1.88	0.40
2:C:1012:TYR:HB3	2:C:1013:PRO:HD2	2.03	0.40
2:C:171:VAL:HG12	2:C:172:ARG:N	2.36	0.40
2:C:512:ASN:ND2	2:C:512:ASN:O	2.55	0.40
2:C:481:GLU:HG2	2:C:597:LEU:HD21	2.03	0.40
2:C:844:PHE:HD2	2:C:859:LEU:HD12	1.87	0.40
2:C:876:LEU:HD11	2:C:886:ILE:CD1	2.48	0.40
2:C:31:SER:HA	2:C:964:ALA:O	2.20	0.40
3:D:505:HIS:HD2	3:D:1004:GLU:HG3	1.87	0.40
3:D:302:PHE:CE2	3:D:309:PRO:HA	2.57	0.40
3:D:34:ILE:HG22	3:D:41:PRO:HA	2.02	0.40
3:D:622:MET:HE1	3:D:629:VAL:HG22	2.02	0.40
3:D:704:PRO:HD2	3:D:707:VAL:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:936:ILE:CG2	3:D:951:LEU:HD23	2.52	0.40
8:O:6:DA:H1'	8:O:7:DC:C5'	2.50	0.40
1:B:34:LEU:HD12	1:B:34:LEU:C	2.42	0.40
2:C:1086:ASP:OD1	2:C:1107:GLY:N	2.52	0.40
2:C:1125:ASN:O	3:D:12:ILE:HA	2.22	0.40
2:C:522:LEU:HB3	2:C:526:GLU:HG3	2.03	0.40
2:C:634:VAL:HA	2:C:691:GLN:O	2.22	0.40
2:C:727:ILE:CG2	2:C:888:LYS:HB3	2.49	0.40
1:A:174:VAL:O	2:C:901:GLY:HA3	2.22	0.40
2:C:728:LEU:HD23	2:C:906:ILE:HG22	2.02	0.40
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.87	0.40
3:D:1110:ASP:OD1	3:D:1110:ASP:N	2.54	0.40
3:D:1258:LEU:HD12	3:D:1258:LEU:HA	1.91	0.40
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.93	0.40
2:C:973:GLU:CB	3:D:732:MET:HE3	2.52	0.40
4:E:75:TYR:O	4:E:76:VAL:HB	2.22	0.40
5:F:310:MET:O	5:F:313:VAL:HG13	2.20	0.40
1:T:264:LEU:O	1:T:269:VAL:HG22	2.22	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)
2:C:658:ARG:NH1	3:D:147:GLU:OE1[2_356]	1.96	0.24

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/350 (61%)	202 (94%)	12 (6%)	0	100	100
1	B	231/350 (66%)	211 (91%)	19 (8%)	1 (0%)	34	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	51/350 (15%)	51 (100%)	0	0	100	100
2	C	1093/1169 (94%)	1040 (95%)	52 (5%)	1 (0%)	51	83
3	D	1234/1317 (94%)	1181 (96%)	51 (4%)	2 (0%)	47	79
4	E	72/107 (67%)	66 (92%)	4 (6%)	2 (3%)	5	24
5	F	303/466 (65%)	296 (98%)	7 (2%)	0	100	100
7	J	81/114 (71%)	76 (94%)	5 (6%)	0	100	100
All	All	3279/4223 (78%)	3123 (95%)	150 (5%)	6 (0%)	47	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	76	VAL
3	D	1194	VAL
4	E	78	PRO
1	B	183	VAL
2	C	967	VAL
3	D	935	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/297 (59%)	161 (92%)	13 (8%)	13	41
1	B	173/297 (58%)	153 (88%)	20 (12%)	5	22
1	T	26/297 (9%)	25 (96%)	1 (4%)	33	65
2	C	862/984 (88%)	798 (93%)	64 (7%)	13	41
3	D	989/1095 (90%)	912 (92%)	77 (8%)	12	40
4	E	62/86 (72%)	52 (84%)	10 (16%)	2	10
5	F	251/379 (66%)	233 (93%)	18 (7%)	14	43
7	J	72/98 (74%)	66 (92%)	6 (8%)	11	37
All	All	2609/3533 (74%)	2400 (92%)	209 (8%)	12	39

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	30	PHE
1	A	40	ARG
1	A	51	VAL
1	A	71	GLU
1	A	74	THR
1	A	127	THR
1	A	129	ASN
1	A	130	ASP
1	A	135	GLU
1	A	150	VAL
1	A	159	ILE
1	A	168	TYR
1	B	4	SER
1	B	5	GLN
1	B	17	ASN
1	B	33	THR
1	B	43	LEU
1	B	57	ASP
1	B	60	LEU
1	B	84	VAL
1	B	88	ASP
1	B	89	ASP
1	B	90	ASP
1	B	125	ILE
1	B	144	ARG
1	B	161	ARG
1	B	176	TYR
1	B	185	GLN
1	B	200	ASN
1	B	215	LEU
1	B	230	GLU
1	B	231	HIS
2	C	67	ASP
2	C	70	GLU
2	C	81	LEU
2	C	102	ARG
2	C	119	THR
2	C	124	LEU
2	C	202	TRP
2	C	215	VAL
2	C	236	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	273	ARG
2	C	294	GLU
2	C	299	LEU
2	C	301	ARG
2	C	323	THR
2	C	335	TYR
2	C	364	PHE
2	C	398	GLN
2	C	437	LEU
2	C	443	LYS
2	C	445	ARG
2	C	446	LEU
2	C	454	LEU
2	C	456	ARG
2	C	461	LEU
2	C	520	ASP
2	C	523	THR
2	C	525	ASP
2	C	534	GLN
2	C	546	THR
2	C	568	ASP
2	C	611	ARG
2	C	617	VAL
2	C	658	ARG
2	C	727	ILE
2	C	737	VAL
2	C	753	THR
2	C	754	LYS
2	C	763	ASP
2	C	771	VAL
2	C	775	LEU
2	C	777	GLU
2	C	778	ARG
2	C	780	ILE
2	C	783	ILE
2	C	848	ASP
2	C	872	ASP
2	C	919	ILE
2	C	927	LEU
2	C	936	ASN
2	C	945	ASP
2	C	953	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	954	LEU
2	C	961	SER
2	C	965	THR
2	C	986	ASN
2	C	988	ASP
2	C	1022	LEU
2	C	1045	GLN
2	C	1048	LEU
2	C	1054	PHE
2	C	1085	ASP
2	C	1108	ILE
2	C	1122	LEU
2	C	1138	MET
3	D	7	PHE
3	D	12	ILE
3	D	28	VAL
3	D	51	ILE
3	D	70	PHE
3	D	107	PHE
3	D	144	ARG
3	D	148	LEU
3	D	150	THR
3	D	165	GLN
3	D	187	GLU
3	D	192	ASP
3	D	234	LEU
3	D	238	GLU
3	D	239	VAL
3	D	243	GLU
3	D	246	ASP
3	D	281	ILE
3	D	298	VAL
3	D	304	GLN
3	D	314	LEU
3	D	330	LEU
3	D	365	ILE
3	D	415	GLN
3	D	417	LEU
3	D	449	LEU
3	D	451	LEU
3	D	456	VAL
3	D	467	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	504	LEU
3	D	507	LEU
3	D	558	LEU
3	D	566	LEU
3	D	588	LEU
3	D	591	LEU
3	D	599	TYR
3	D	627	LEU
3	D	635	VAL
3	D	650	LEU
3	D	656	LYS
3	D	666	THR
3	D	667	LEU
3	D	675	LEU
3	D	687	MET
3	D	706	ILE
3	D	724	THR
3	D	740	GLN
3	D	767	THR
3	D	784	VAL
3	D	791	PHE
3	D	799	ILE
3	D	830	PHE
3	D	831	ILE
3	D	841	GLU
3	D	846	LEU
3	D	853	HIS
3	D	862	THR
3	D	876	LEU
3	D	900	LEU
3	D	914	HIS
3	D	930	ASP
3	D	945	ASP
3	D	952	LEU
3	D	1049	ASP
3	D	1056	LEU
3	D	1071	ASP
3	D	1079	ASP
3	D	1086	ARG
3	D	1110	ASP
3	D	1112	LEU
3	D	1183	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1186	GLU
3	D	1190	GLU
3	D	1208	LEU
3	D	1234	LEU
3	D	1243	SER
3	D	1278	GLU
4	E	37	ILE
4	E	50	LEU
4	E	53	TYR
4	E	57	ARG
4	E	75	TYR
4	E	76	VAL
4	E	85	GLN
4	E	101	LEU
4	E	102	GLU
4	E	103	HIS
5	F	182	GLU
5	F	216	ARG
5	F	291	GLN
5	F	310	MET
5	F	313	VAL
5	F	317	LEU
5	F	324	LEU
5	F	348	VAL
5	F	349	LEU
5	F	365	ILE
5	F	370	ASP
5	F	407	GLU
5	F	423	GLN
5	F	433	VAL
5	F	452	LEU
5	F	462	ARG
5	F	465	LEU
5	F	466	ASP
7	J	47	ASP
7	J	55	LEU
7	J	64	LEU
7	J	74	LYS
7	J	104	LEU
7	J	105	ILE
1	T	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	129	ASN
1	A	152	ASN
1	B	5	GLN
1	B	124	HIS
1	B	185	GLN
2	C	48	GLN
2	C	160	ASN
2	C	343	GLN
2	C	398	GLN
2	C	433	GLN
2	C	467	HIS
2	C	484	ASN
2	C	576	GLN
2	C	590	HIS
2	C	700	GLN
2	C	720	HIS
2	C	911	HIS
2	C	936	ASN
2	C	1068	GLN
3	D	165	GLN
3	D	287	GLN
3	D	303	GLN
3	D	416	ASN
3	D	465	HIS
3	D	494	HIS
3	D	515	GLN
3	D	600	GLN
3	D	684	ASN
3	D	692	GLN
3	D	740	GLN
3	D	748	HIS
3	D	778	GLN
3	D	796	ASN
3	D	881	GLN
3	D	888	HIS
3	D	1085	GLN
3	D	1126	GLN
3	D	1140	GLN
3	D	1146	GLN
4	E	62	ASN
4	E	85	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	103	HIS
5	F	214	GLN
5	F	397	GLN
5	F	454	HIS
7	J	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\# Z > 2$
10	SO4	D	2004	-	4,4,4	0.13	0	6,6,6	0.10	0
10	SO4	F	504	-	4,4,4	0.15	0	6,6,6	0.05	0
10	SO4	D	2010	-	4,4,4	0.14	0	6,6,6	0.08	0
10	SO4	F	503	-	4,4,4	0.13	0	6,6,6	0.10	0
10	SO4	C	1206	-	4,4,4	0.14	0	6,6,6	0.08	0
12	SRN	C	1205	-	57,62,62	5.22	32 (56%)	58,84,84	1.79	15 (25%)
10	SO4	C	1201	-	4,4,4	0.14	0	6,6,6	0.08	0
11	EDO	C	1207	-	3,3,3	0.49	0	2,2,2	0.26	0
10	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SO4	D	2006	-	4,4,4	0.15	0	6,6,6	0.09	0
11	EDO	C	1204	-	3,3,3	0.40	0	2,2,2	0.41	0
10	SO4	D	2005	-	4,4,4	0.13	0	6,6,6	0.09	0
11	EDO	D	2011	-	3,3,3	0.46	0	2,2,2	0.27	0
10	SO4	D	2003	-	4,4,4	0.13	0	6,6,6	0.15	0
10	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.07	0
10	SO4	C	1202	-	4,4,4	0.13	0	6,6,6	0.08	0
11	EDO	D	2009	-	3,3,3	0.48	0	2,2,2	0.25	0
11	EDO	D	2008	-	3,3,3	0.43	0	2,2,2	0.35	0
11	EDO	D	2007	-	3,3,3	0.47	0	2,2,2	0.28	0
11	EDO	F	506	-	3,3,3	0.48	0	2,2,2	0.26	0
10	SO4	F	505	-	4,4,4	0.15	0	6,6,6	0.09	0
10	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.11	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
11	EDO	D	2009	-	-	0/1/1/1	-
11	EDO	D	2007	-	-	0/1/1/1	-
11	EDO	D	2008	-	-	0/1/1/1	-
11	EDO	C	1204	-	-	1/1/1/1	-
12	SRN	C	1205	-	-	5/50/105/105	0/2/5/5
11	EDO	C	1207	-	-	0/1/1/1	-
11	EDO	F	506	-	-	0/1/1/1	-
11	EDO	D	2011	-	-	0/1/1/1	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1205	SRN	O3-C8	19.79	1.80	1.44
12	C	1205	SRN	O3-C9	16.07	1.80	1.45
12	C	1205	SRN	C34-C9	-11.15	1.28	1.52
12	C	1205	SRN	C3-C2	9.74	1.59	1.34
12	C	1205	SRN	C34-C35	-8.88	1.33	1.52
12	C	1205	SRN	C4-C5	8.36	1.57	1.36
12	C	1205	SRN	C13-C14	6.72	1.60	1.31
12	C	1205	SRN	C24-C25	6.10	1.57	1.31
12	C	1205	SRN	C6-C7	5.99	1.57	1.33
12	C	1205	SRN	C8-C7	-5.92	1.30	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1205	SRN	O7-C32	5.72	1.53	1.43
12	C	1205	SRN	C12-C13	-5.52	1.31	1.50
12	C	1205	SRN	C10-C9	-5.43	1.43	1.53
12	C	1205	SRN	C28-C29	5.09	1.61	1.31
12	C	1205	SRN	C3-C4	4.98	1.58	1.44
12	C	1205	SRN	C5-C6	4.81	1.58	1.44
12	C	1205	SRN	C11-C10	-4.42	1.44	1.53
12	C	1205	SRN	O8-C12	4.16	1.50	1.43
12	C	1205	SRN	C35-C8	-3.96	1.46	1.53
12	C	1205	SRN	O1-C33	3.94	1.52	1.46
12	C	1205	SRN	C46-C47	3.83	1.45	1.33
12	C	1205	SRN	O1-C1	3.66	1.42	1.34
12	C	1205	SRN	C2-C1	3.62	1.56	1.48
12	C	1205	SRN	C30-C29	3.48	1.60	1.50
12	C	1205	SRN	C33-C47	-3.48	1.44	1.49
12	C	1205	SRN	O7-C31	3.43	1.53	1.44
12	C	1205	SRN	C23-C24	3.27	1.55	1.50
12	C	1205	SRN	C15-C14	2.61	1.58	1.50
12	C	1205	SRN	C31-C46	2.22	1.53	1.50
12	C	1205	SRN	C22-C21	2.13	1.56	1.52
12	C	1205	SRN	O8-C35	2.11	1.49	1.44
12	C	1205	SRN	C20-C19	-2.01	1.49	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1205	SRN	O9-C21-C20	5.19	115.31	109.94
12	C	1205	SRN	C8-C7-C6	-4.22	117.35	125.61
12	C	1205	SRN	C37-C36-C32	3.67	122.03	115.68
12	C	1205	SRN	C6-C5-C4	-3.66	116.66	124.81
12	C	1205	SRN	C9-C34-C35	3.28	113.21	103.73
12	C	1205	SRN	C32-C33-C47	2.79	113.47	110.64
12	C	1205	SRN	C30-C31-C46	-2.55	108.52	113.00
12	C	1205	SRN	C18-C17-C19	-2.39	108.43	111.36
12	C	1205	SRN	C30-C29-C28	-2.36	117.64	126.40
12	C	1205	SRN	O3-C9-C34	2.31	109.66	104.74
12	C	1205	SRN	C15-C16-C17	-2.20	108.56	113.67
12	C	1205	SRN	O9-C16-C17	2.12	113.10	110.65
12	C	1205	SRN	O3-C8-C35	2.12	107.40	104.29
12	C	1205	SRN	C39-C38-C36	-2.07	119.90	127.09
12	C	1205	SRN	C11-C10-C9	-2.01	108.26	111.96

There are no chirality outliers.

All (6) torsion outliers are listed below:

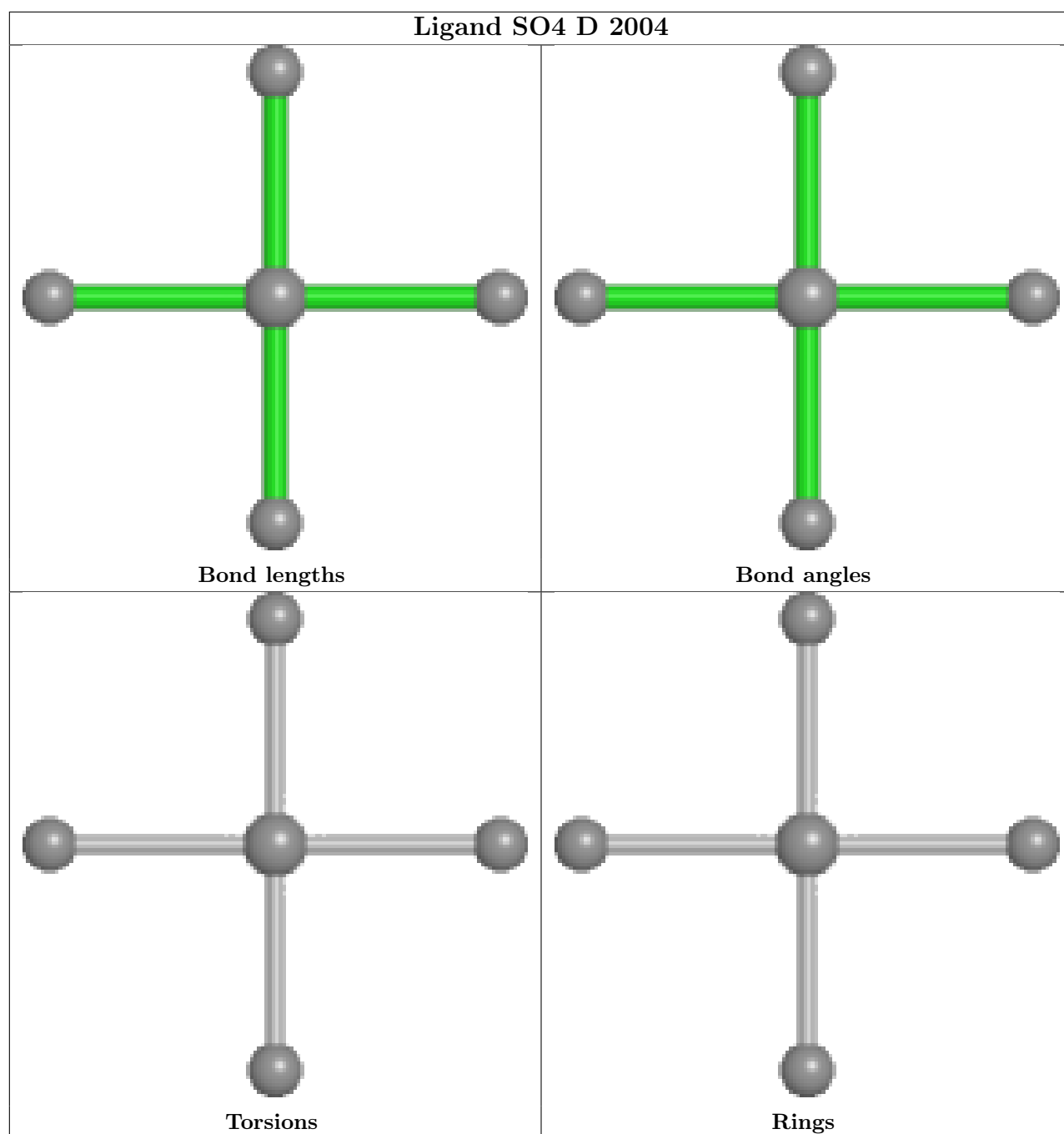
Mol	Chain	Res	Type	Atoms
12	C	1205	SRN	C42-C43-C44-C45
12	C	1205	SRN	C25-C26-C27-C28
12	C	1205	SRN	C14-C15-C16-O9
12	C	1205	SRN	C39-C41-C42-C43
12	C	1205	SRN	C14-C15-C16-C17
11	C	1204	EDO	O1-C1-C2-O2

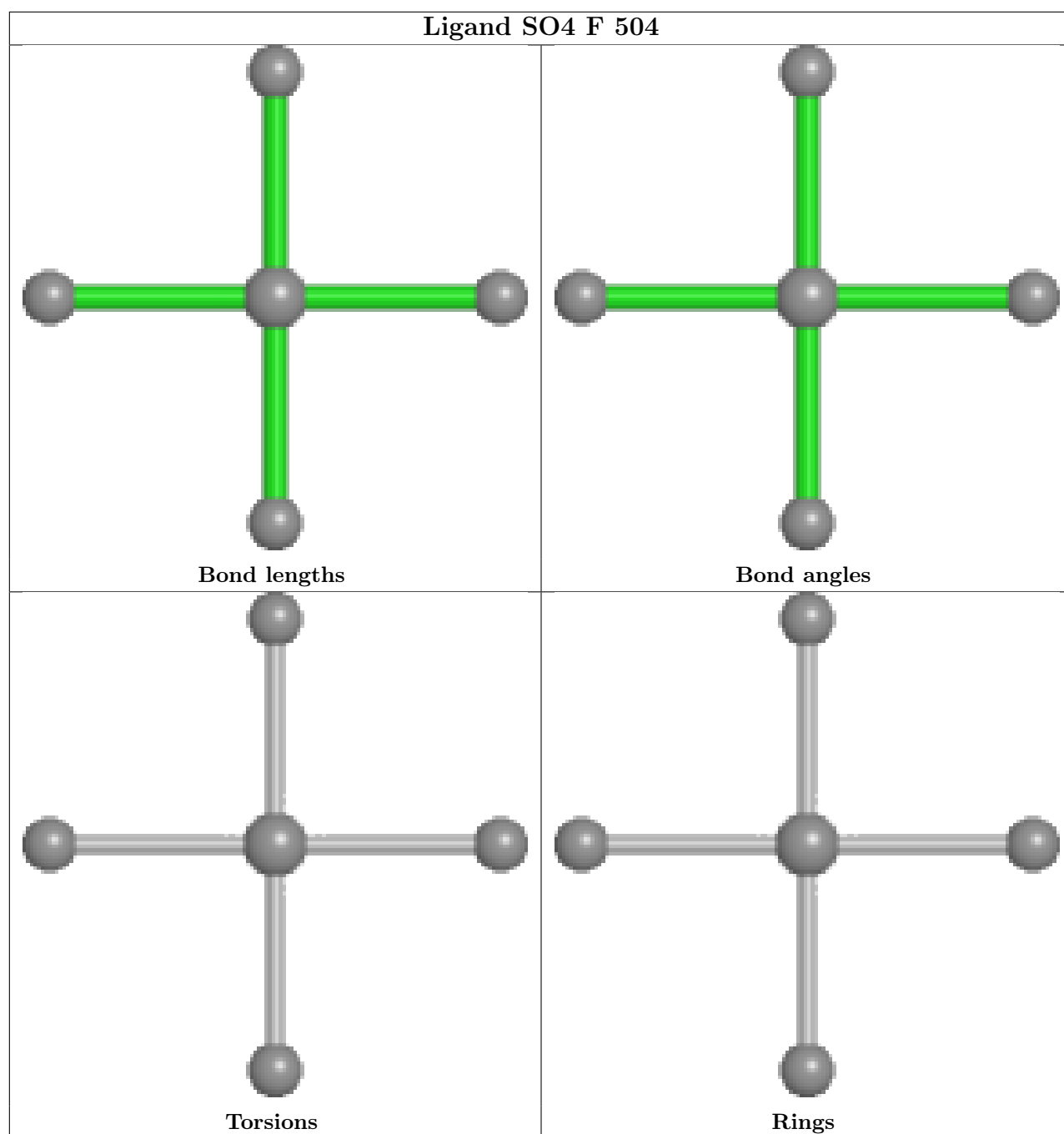
There are no ring outliers.

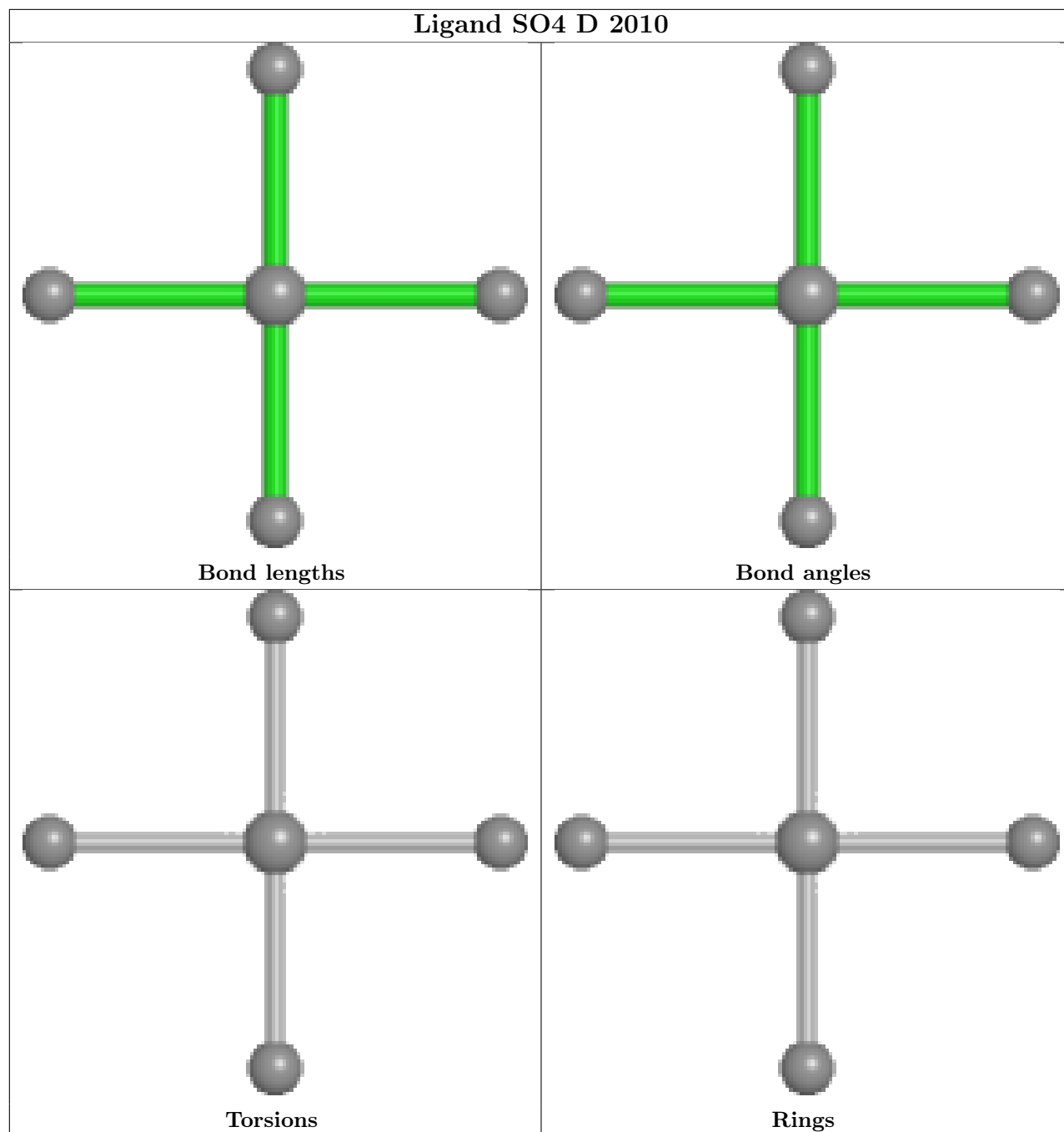
11 monomers are involved in 26 short contacts:

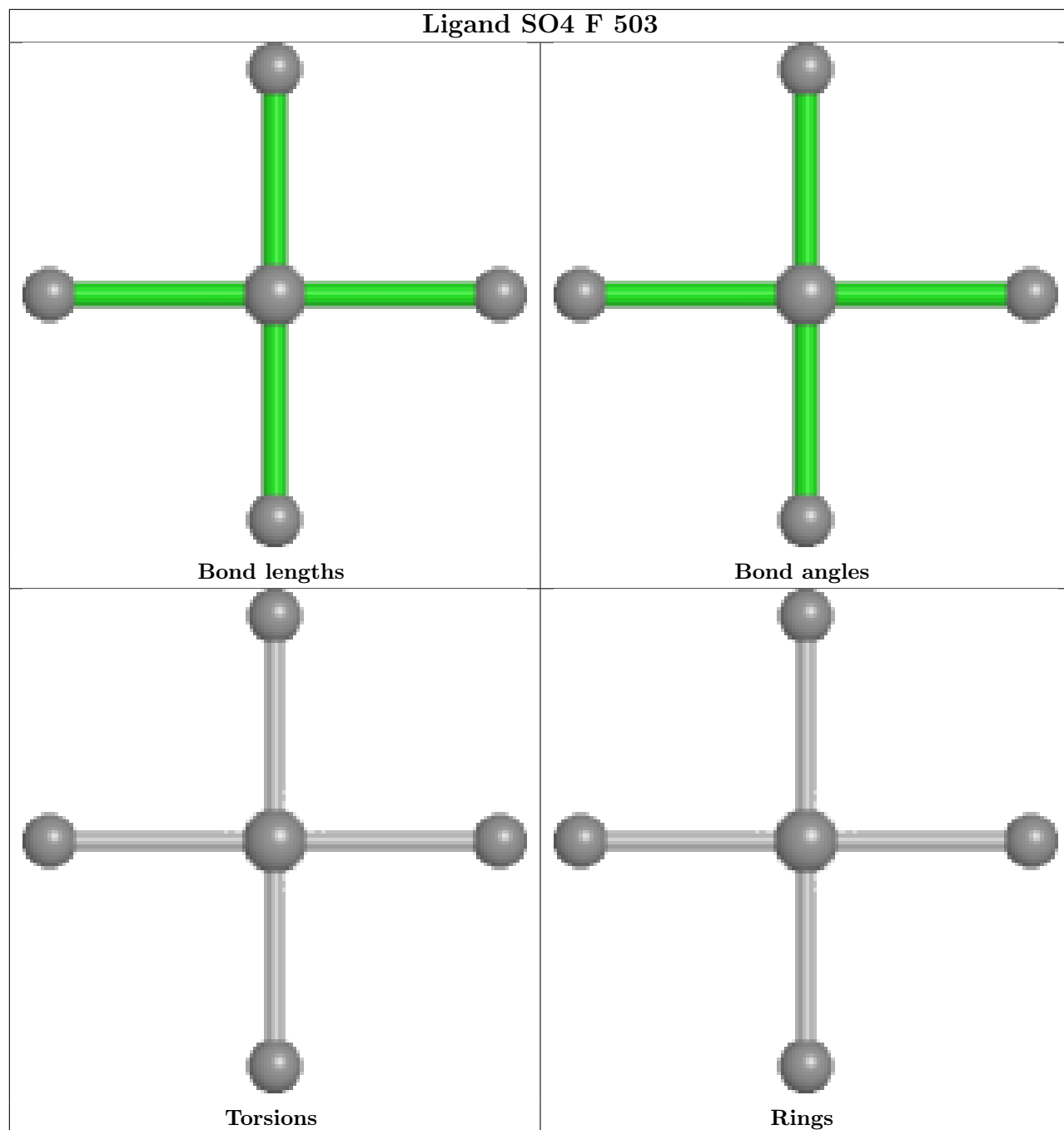
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	2004	SO4	2	0
10	C	1206	SO4	1	0
12	C	1205	SRN	14	0
10	C	1201	SO4	1	0
11	C	1207	EDO	1	0
10	C	1203	SO4	1	0
11	D	2011	EDO	1	0
11	D	2007	EDO	2	0
11	F	506	EDO	1	0
10	F	505	SO4	1	0
10	F	502	SO4	1	0

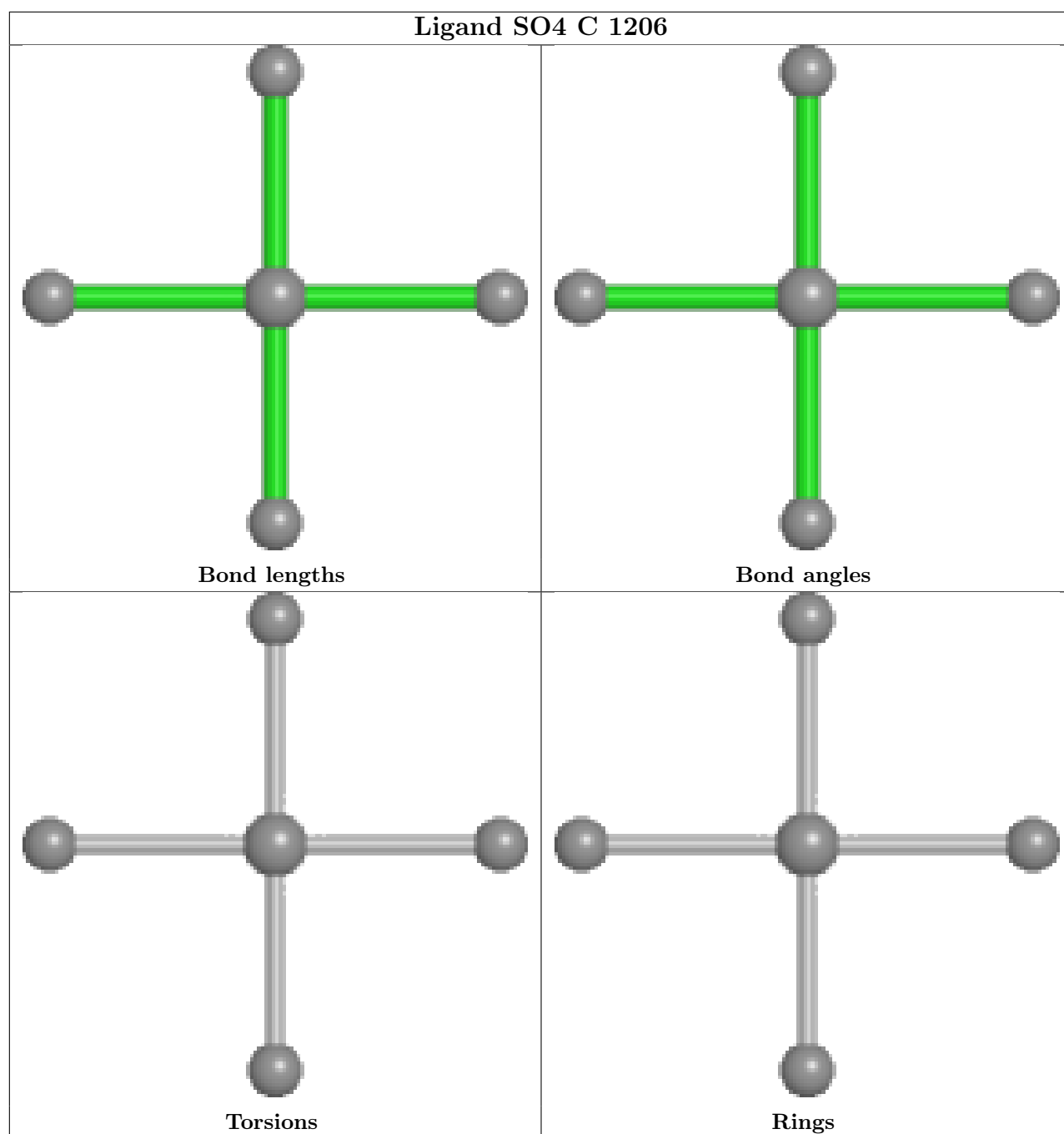
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

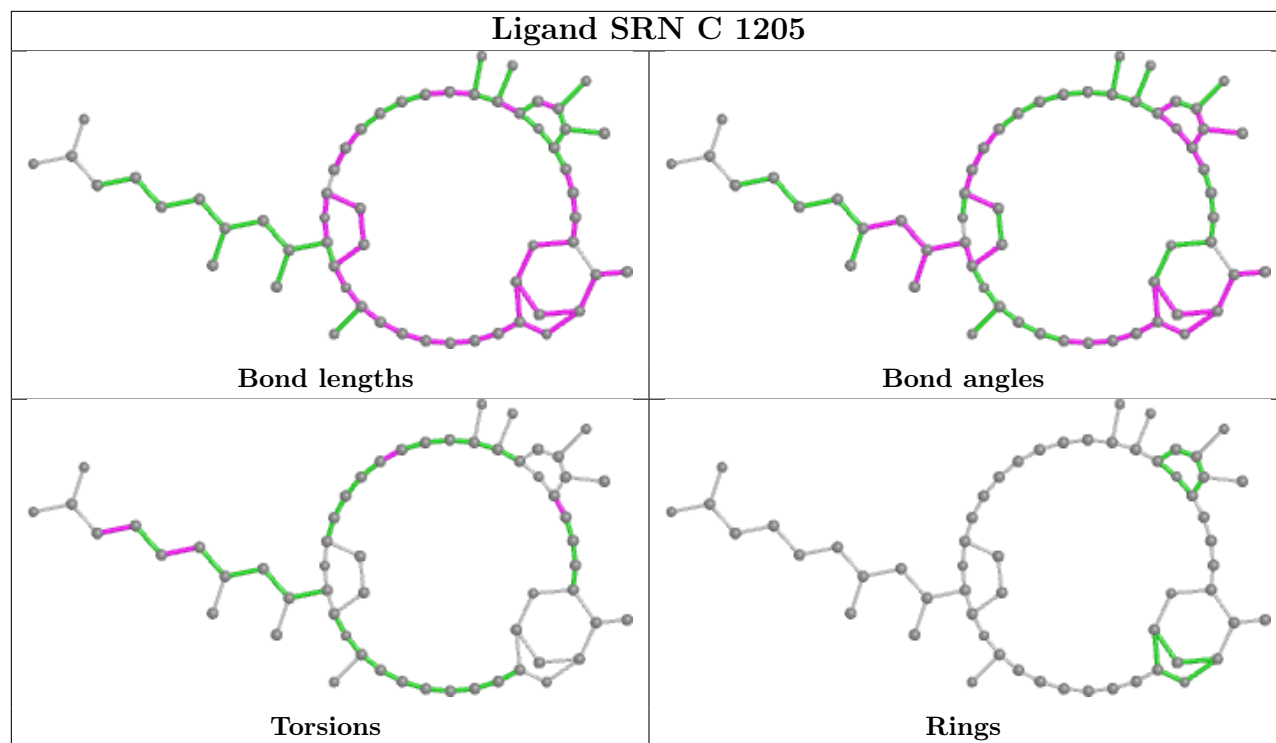


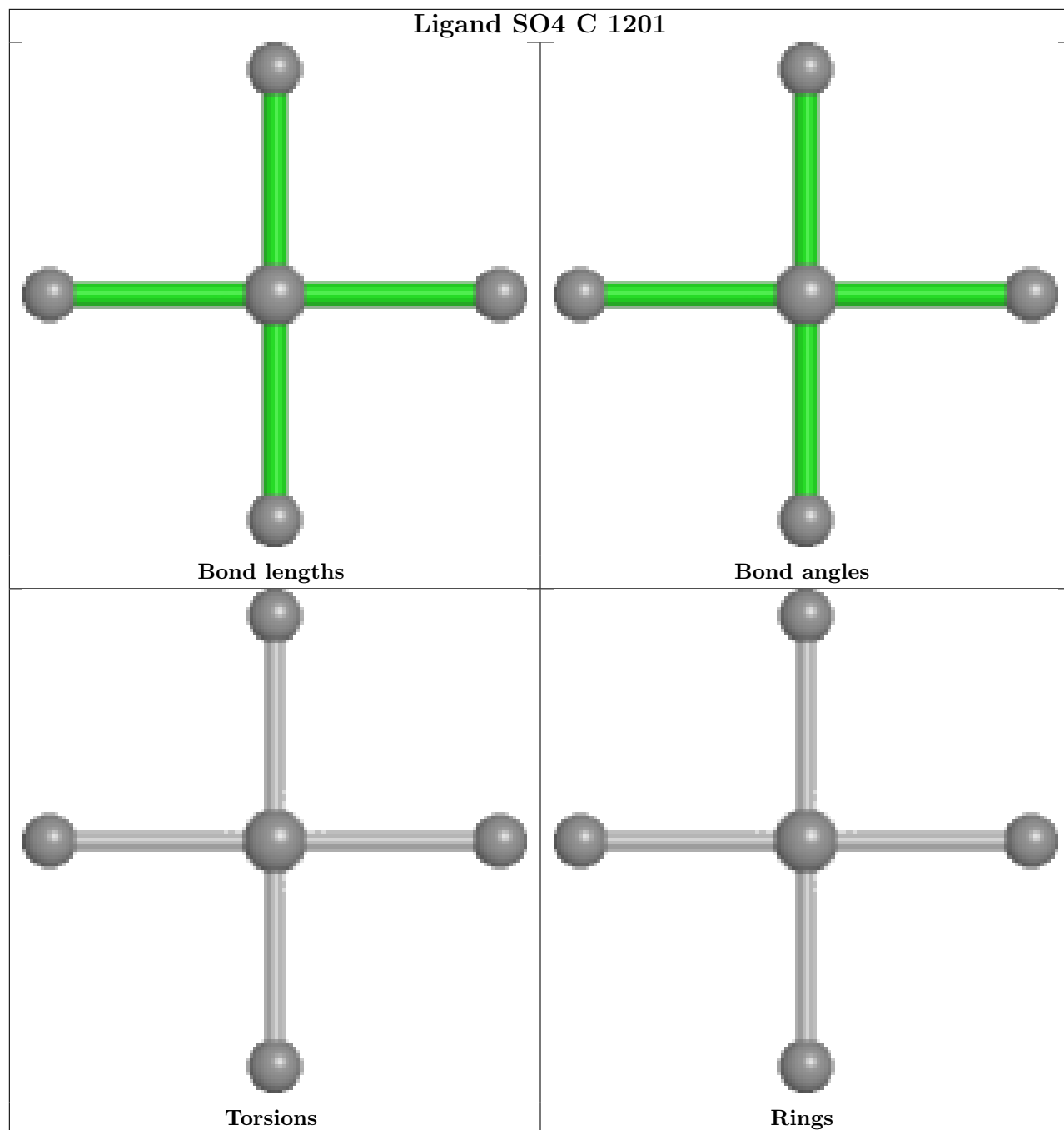


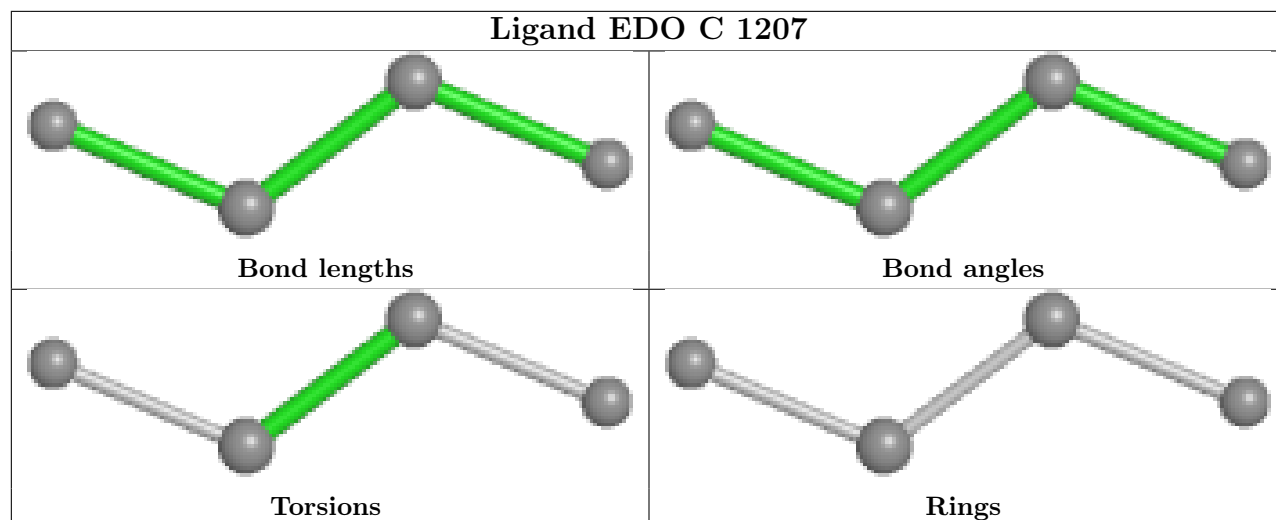


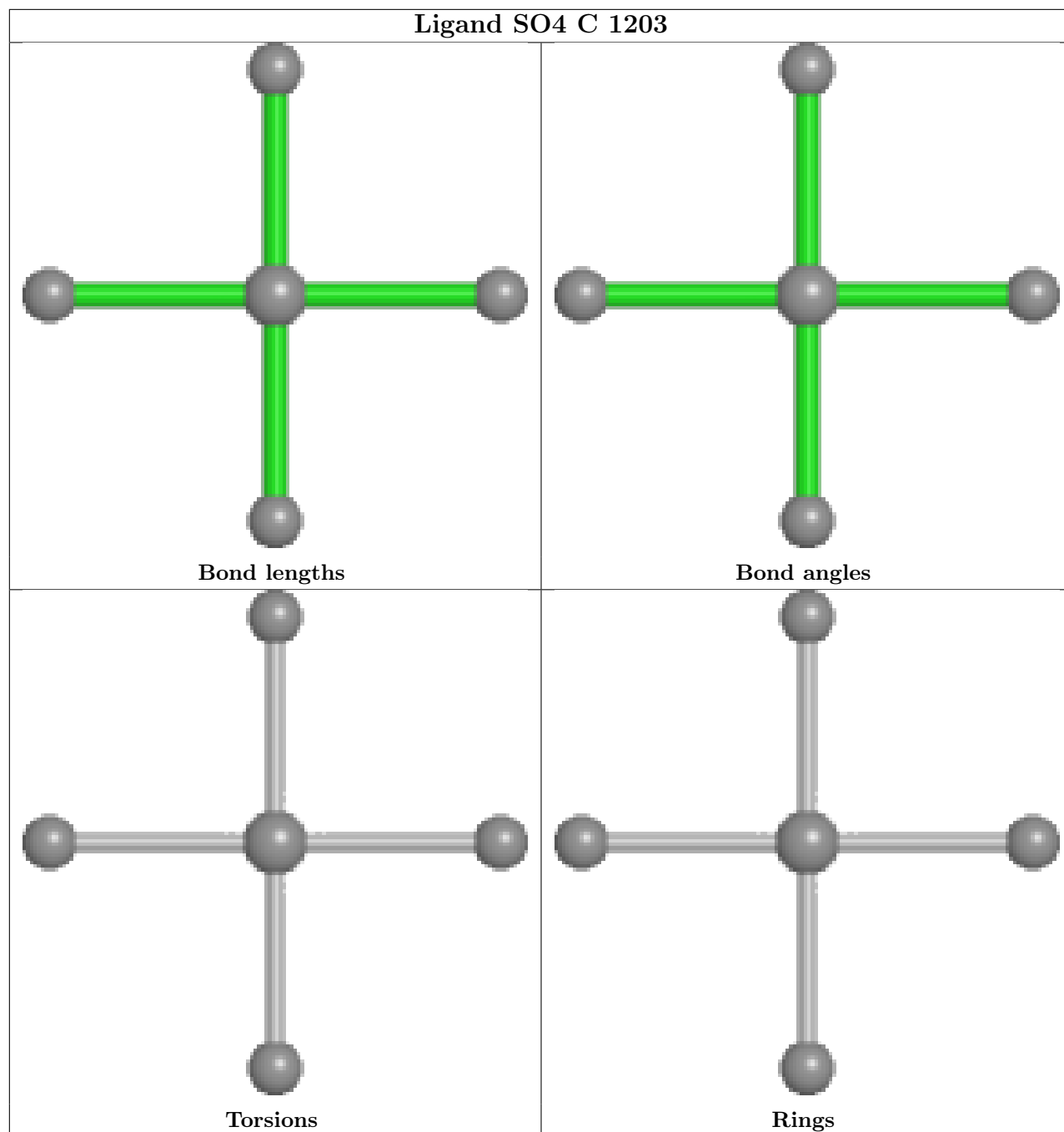


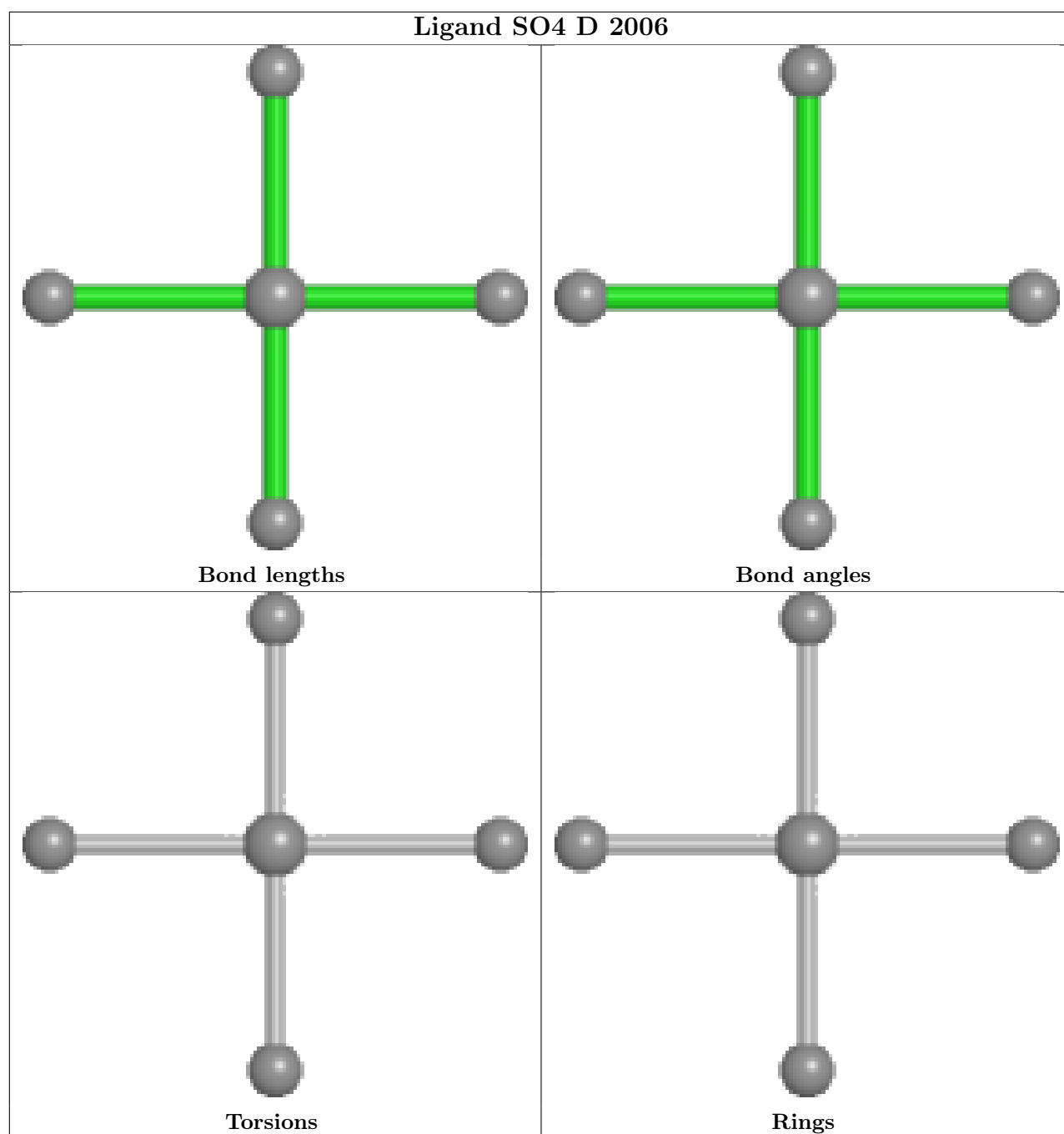


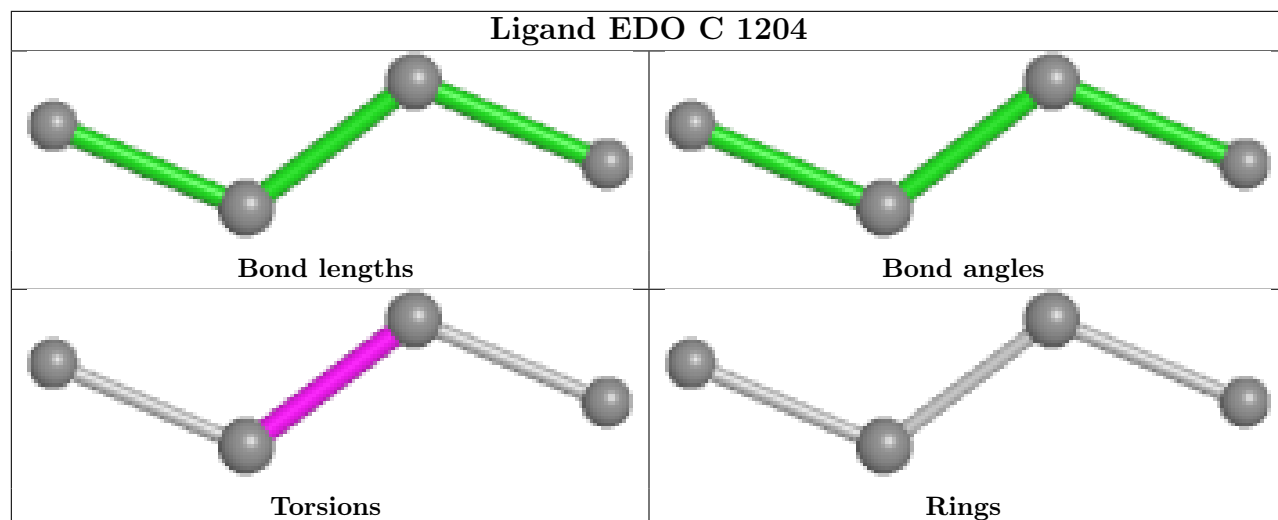


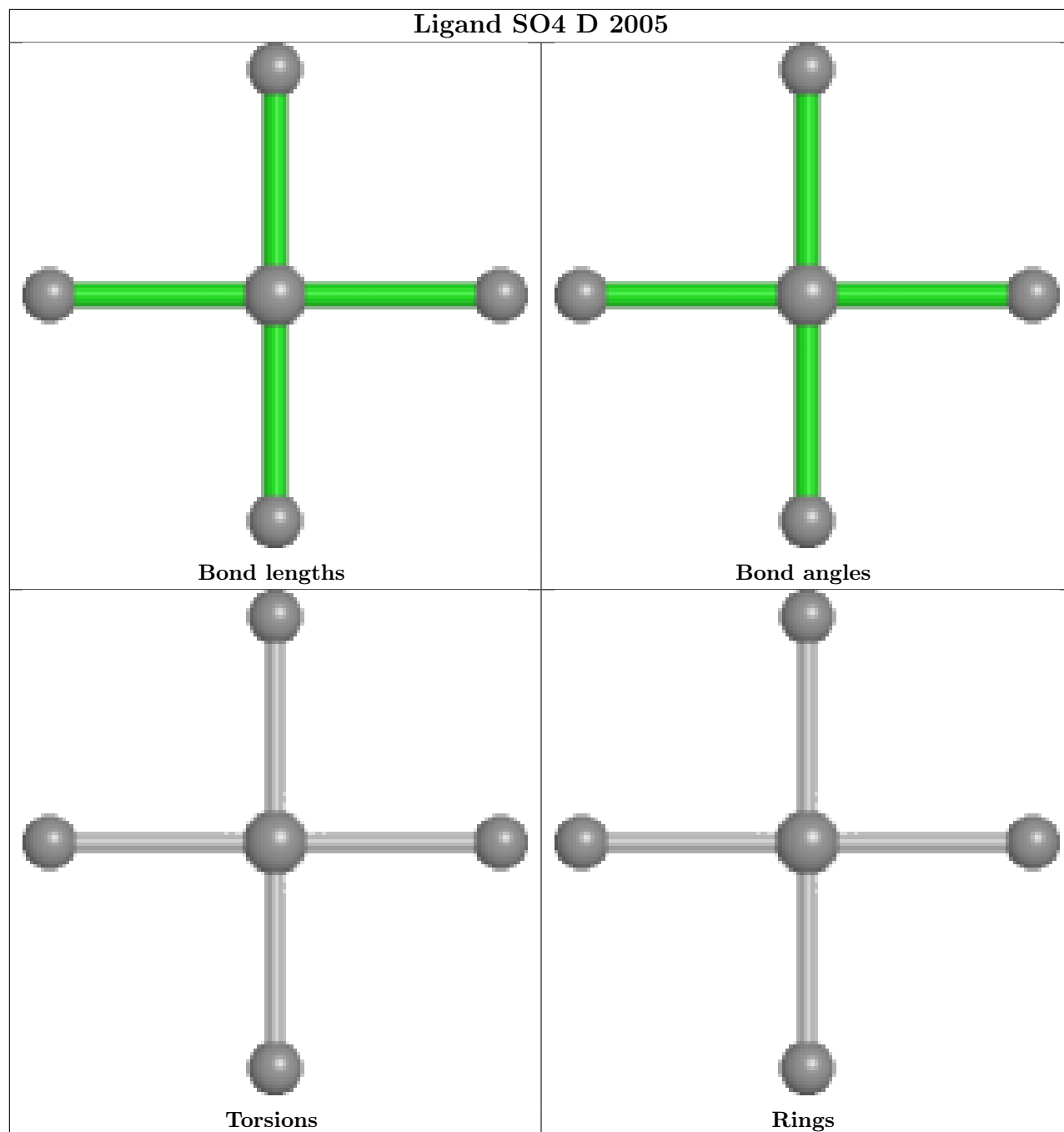


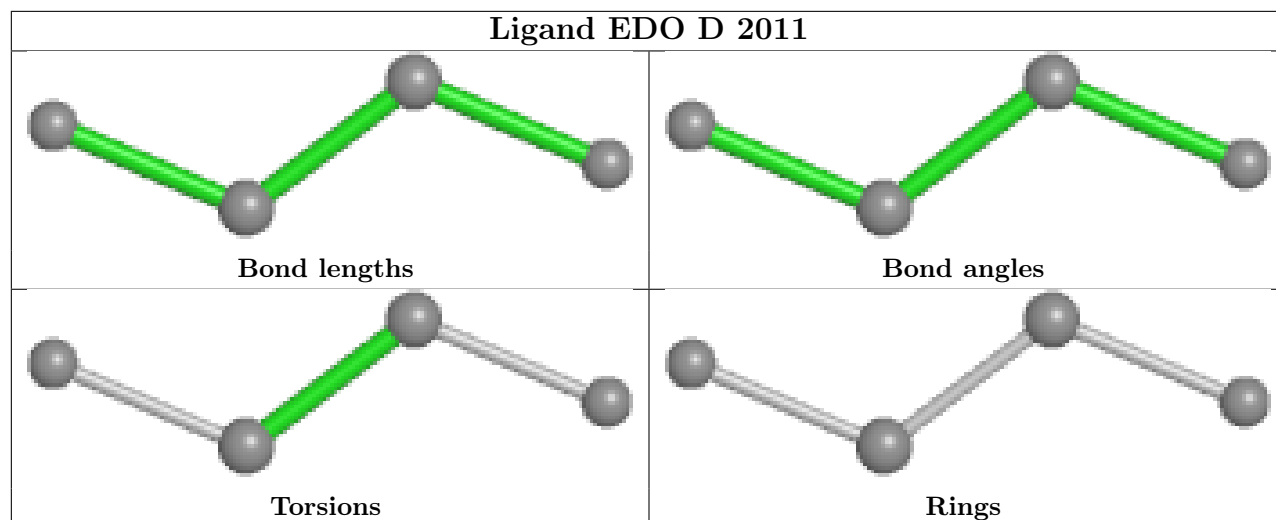


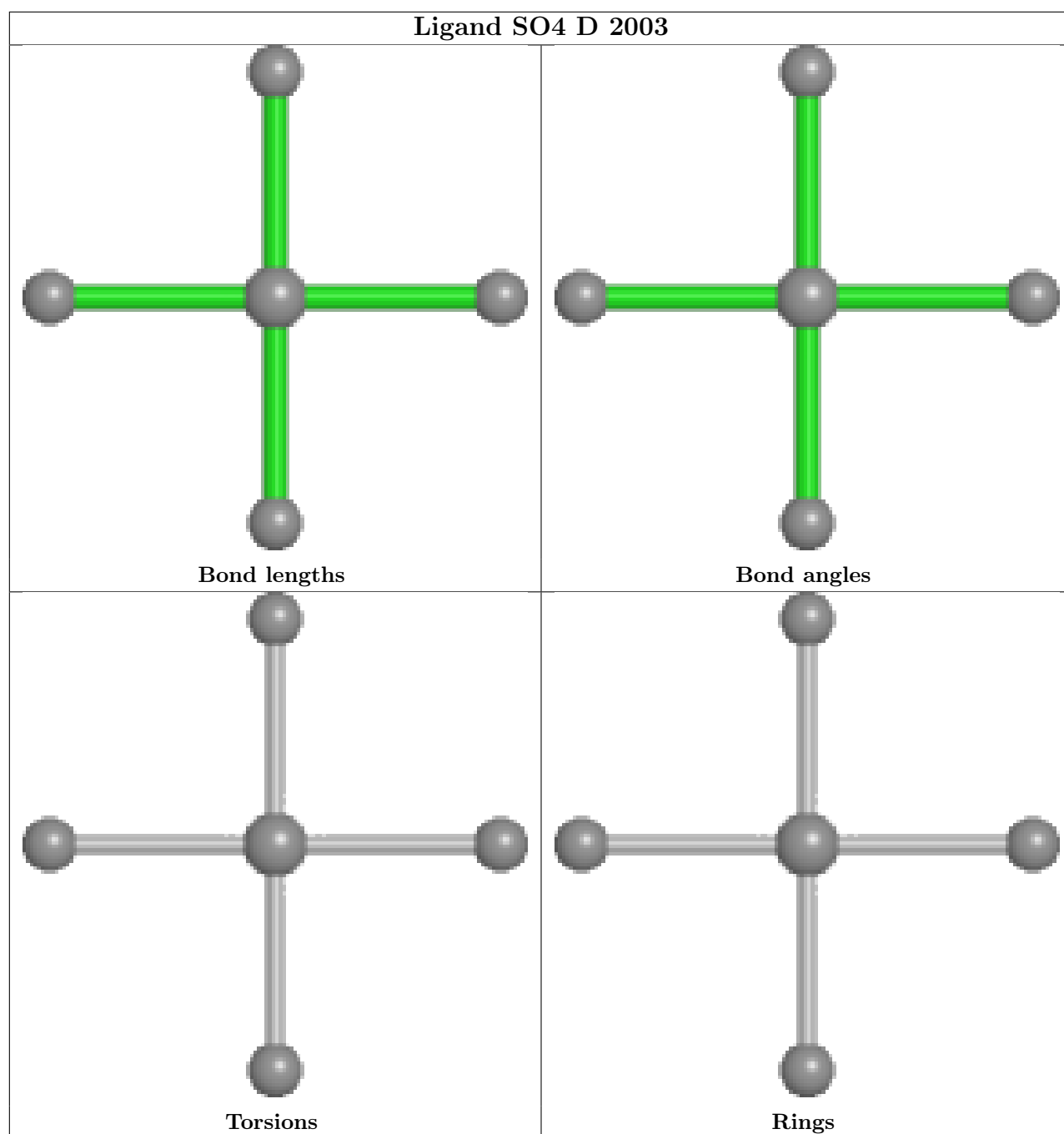


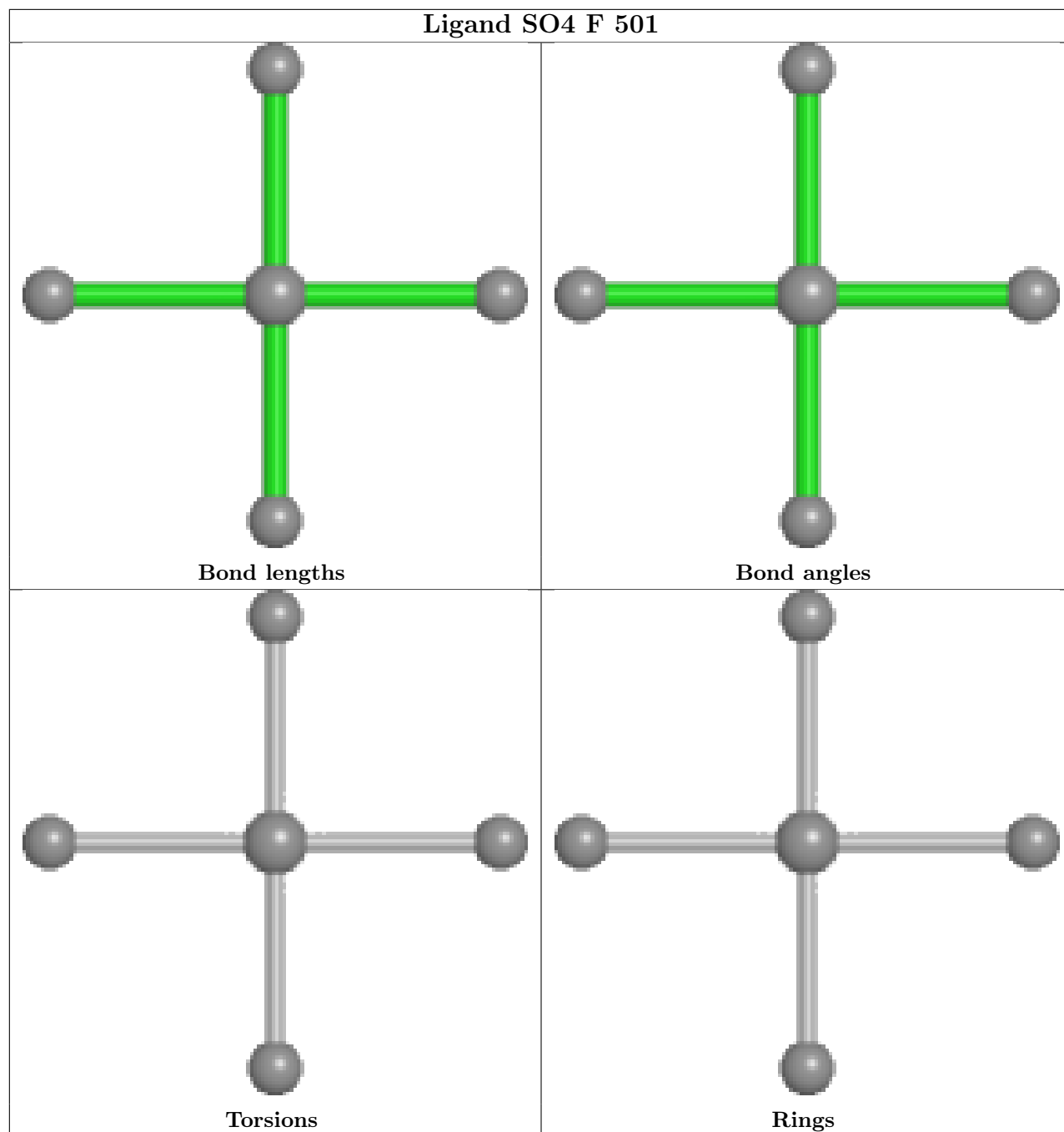


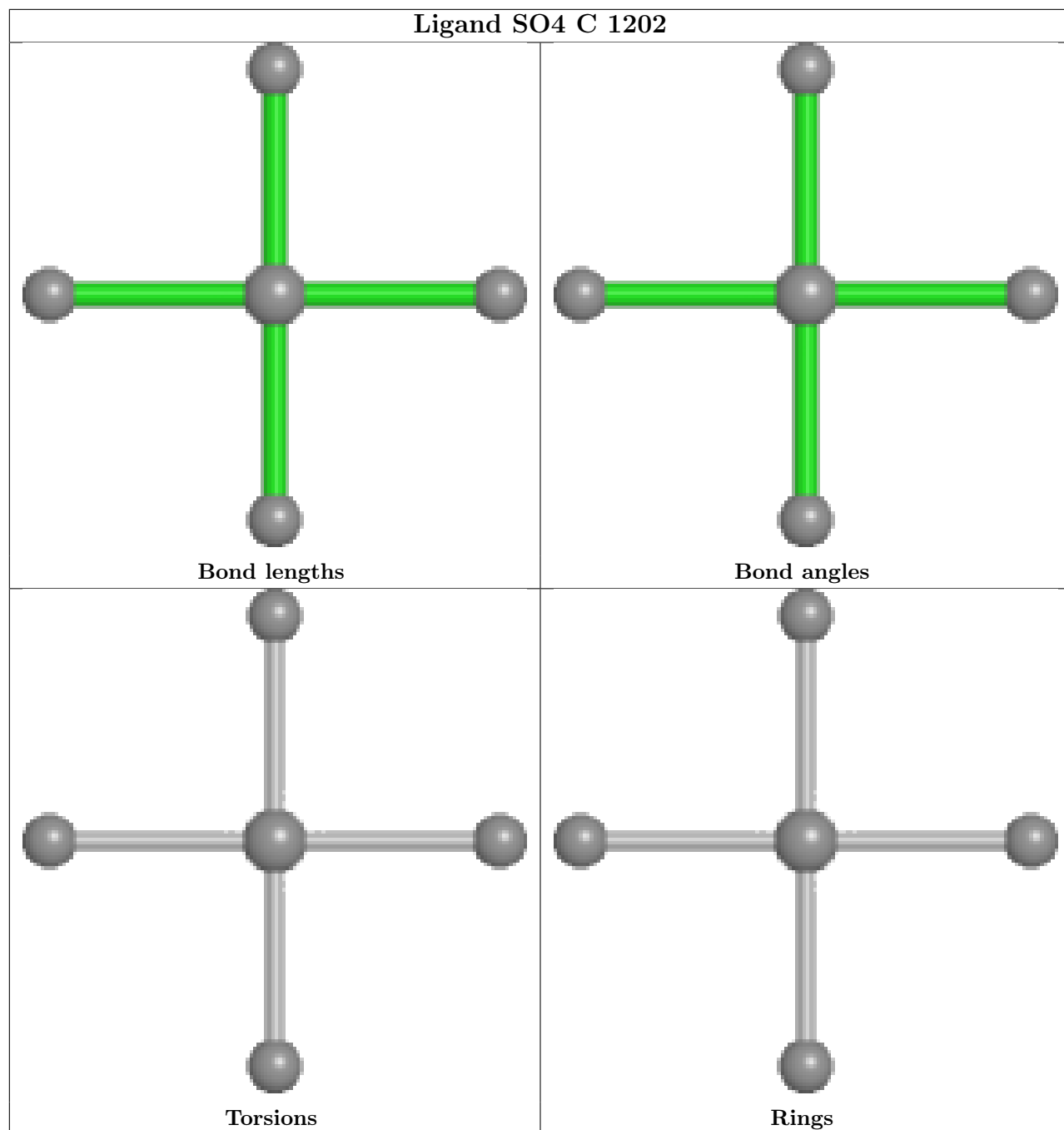


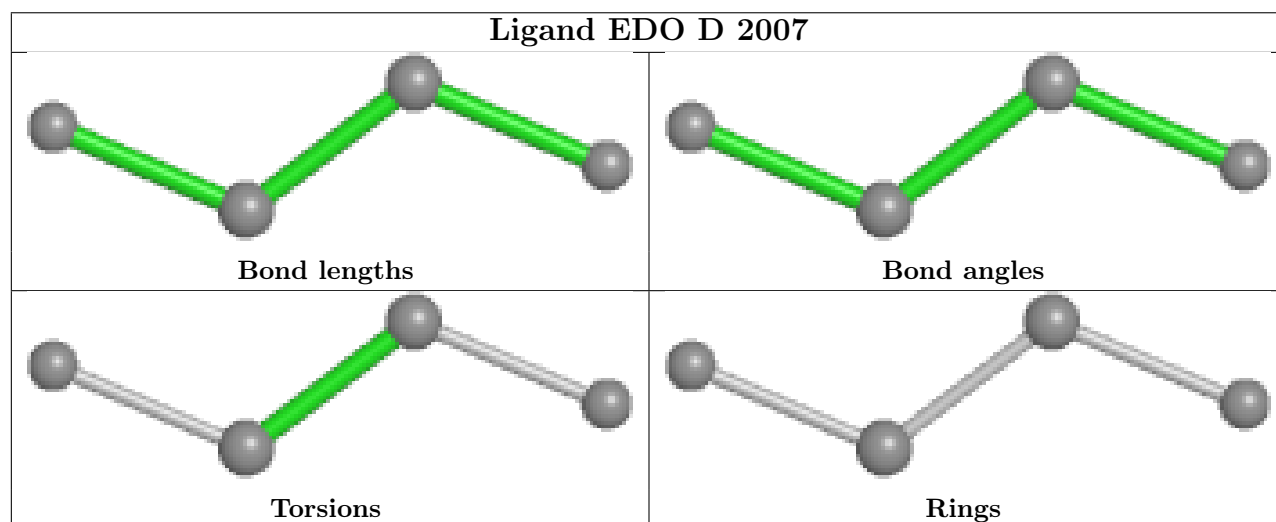
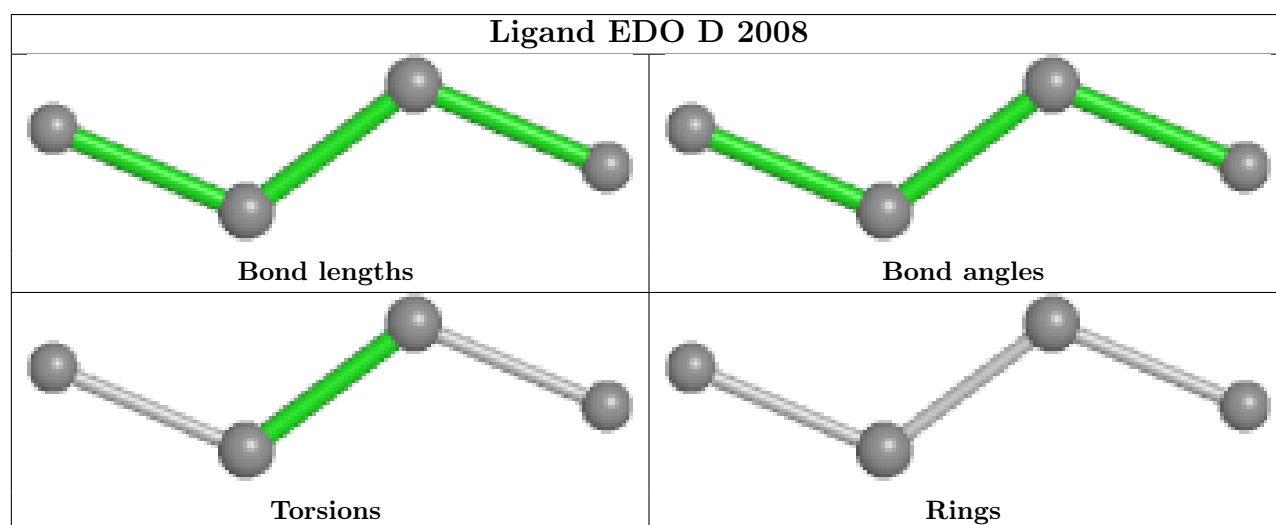
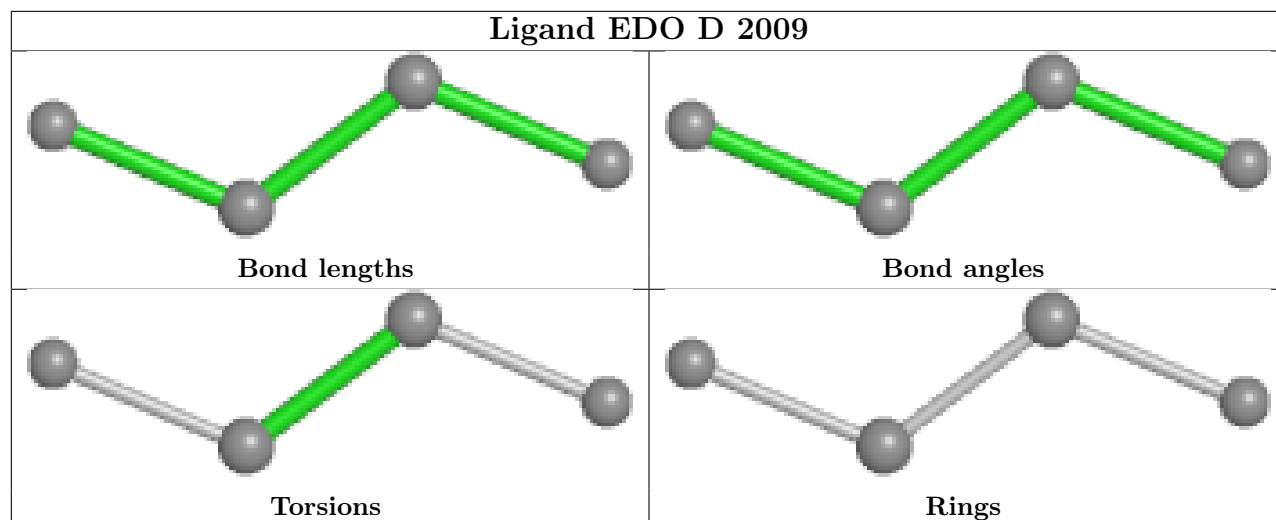


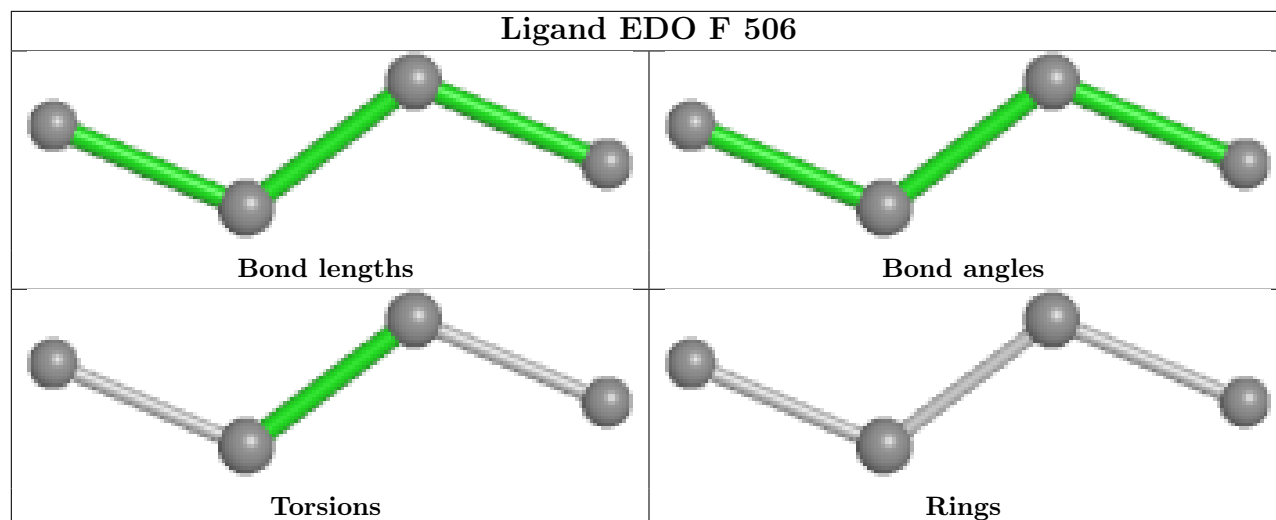


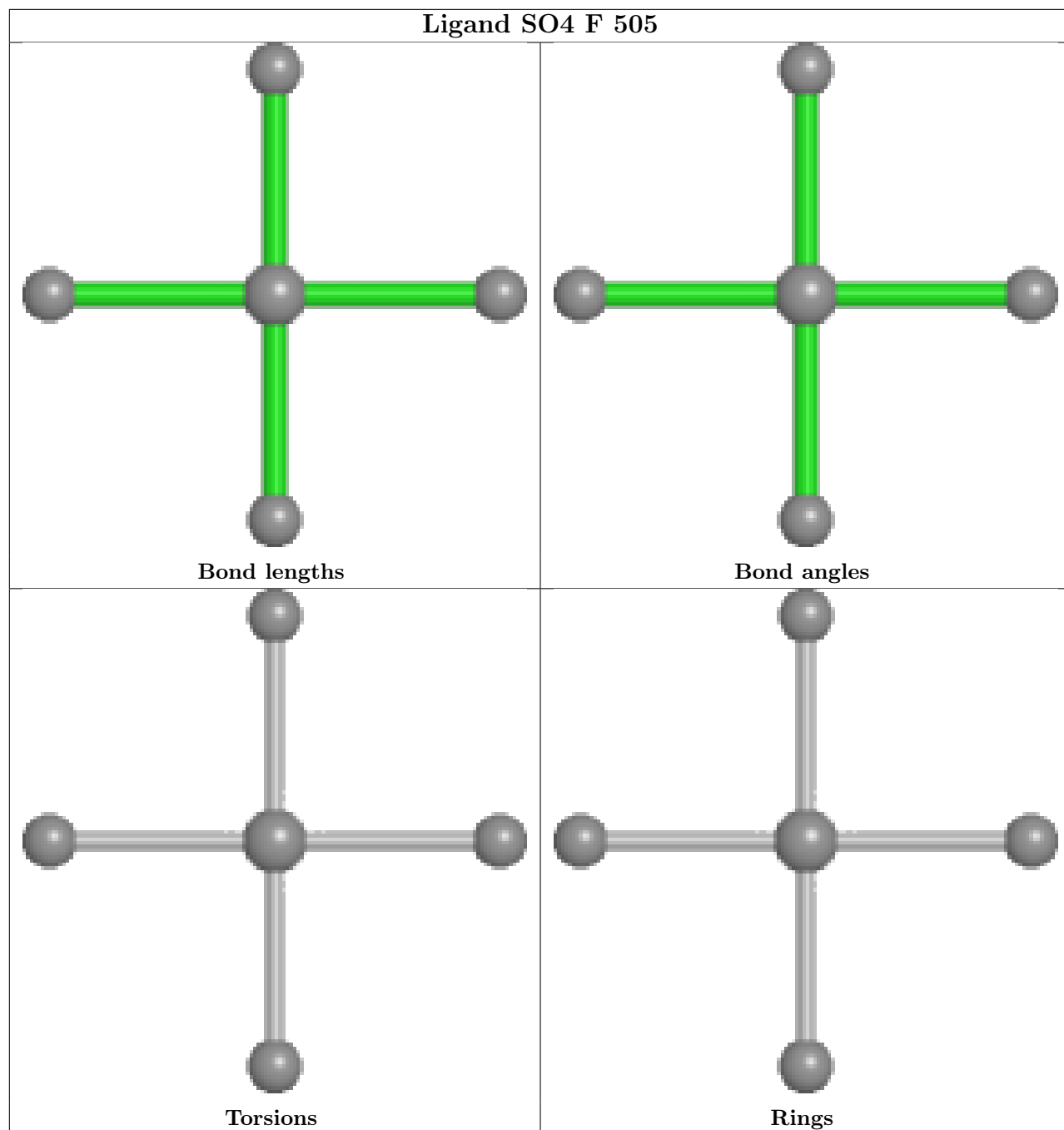


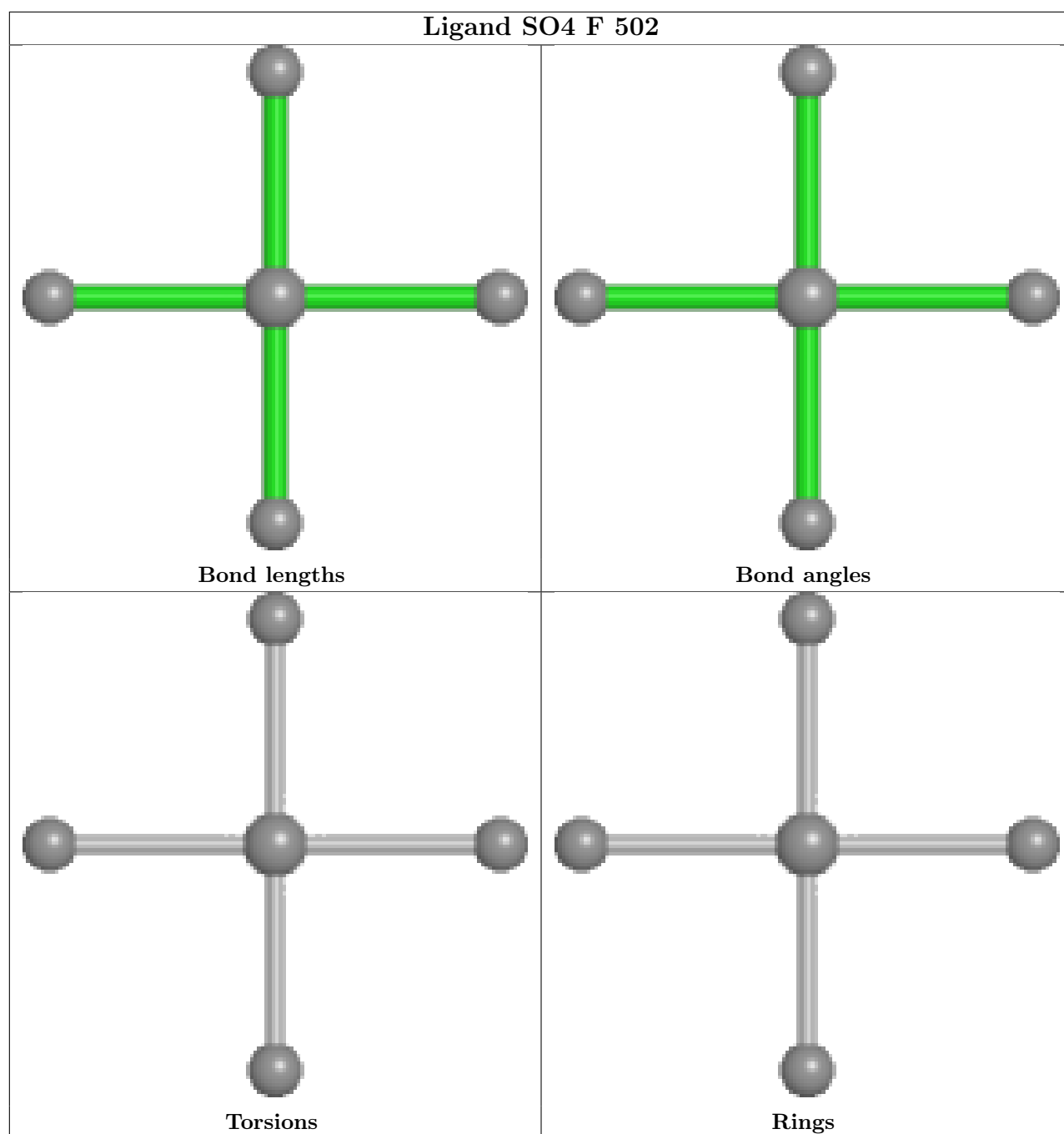












5.7 Other polymers [i](#)

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	A	218/350 (62%)	-0.17	5 (2%) 60 39	76, 105, 138, 165	0
1	B	233/350 (66%)	0.18	7 (3%) 50 27	98, 133, 157, 174	0
1	T	53/350 (15%)	1.32	10 (18%) 1 0	128, 168, 199, 204	0
2	C	1099/1169 (94%)	0.05	37 (3%) 45 24	54, 104, 178, 205	0
3	D	1246/1317 (94%)	-0.12	10 (0%) 86 74	46, 91, 152, 196	0
4	E	76/107 (71%)	-0.07	0 100 100	67, 98, 140, 151	0
5	F	305/466 (65%)	-0.30	0 100 100	50, 90, 142, 186	0
6	G	0/17	-	-	-	-
7	J	83/114 (72%)	-0.26	0 100 100	80, 117, 166, 183	0
8	O	31/31 (100%)	-0.82	0 100 100	64, 81, 105, 111	0
9	P	26/26 (100%)	-0.85	0 100 100	76, 87, 113, 119	0
All	All	3370/4297 (78%)	-0.06	69 (2%) 65 45	46, 101, 169, 205	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	350	GLY	4.6
1	T	263	CYS	4.5
2	C	190	LEU	4.5
2	C	228	LEU	4.3
1	B	1	MET	4.1
1	T	266	ARG	4.1
2	C	354	VAL	3.8
2	C	189	THR	3.7
1	T	267	GLU	3.7
2	C	226	THR	3.6
2	C	352	VAL	3.6
2	C	180	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	297	VAL	3.4
1	A	26	LEU	3.3
2	C	564	ALA	3.3
2	C	302	VAL	3.3
3	D	1178	PRO	3.3
2	C	185	SER	3.3
2	C	181	THR	3.3
1	T	273	GLY	3.0
1	A	2	LEU	2.9
1	A	192	LEU	2.8
2	C	332	THR	2.8
1	A	23	ILE	2.8
2	C	191	HIS	2.7
1	B	21	PHE	2.7
2	C	550	VAL	2.7
3	D	738	PRO	2.7
1	B	110	ILE	2.7
3	D	900	LEU	2.6
2	C	325	THR	2.6
1	B	134	LEU	2.6
2	C	353	GLU	2.6
1	B	138	LEU	2.5
1	T	253	ASP	2.5
2	C	244	GLY	2.5
3	D	1187	PHE	2.5
1	T	293	SER	2.5
2	C	542	ASN	2.4
2	C	254	GLU	2.4
2	C	271	LYS	2.4
2	C	227	VAL	2.4
2	C	243	PHE	2.4
1	A	25	PRO	2.3
2	C	351	GLY	2.3
2	C	355	PRO	2.3
2	C	145	MET	2.3
2	C	349	PRO	2.3
2	C	196	ILE	2.3
2	C	205	PHE	2.3
1	T	268	GLY	2.2
2	C	225	VAL	2.2
3	D	1191	ASN	2.2
3	D	762	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	66	LYS	2.2
2	C	563	SER	2.2
2	C	201	ALA	2.2
1	B	118	VAL	2.2
2	C	182	ILE	2.2
2	C	344	THR	2.2
2	C	277	PRO	2.2
1	T	276	VAL	2.2
2	C	455	SER	2.1
1	B	107	ALA	2.1
3	D	832	PRO	2.1
2	C	224	PRO	2.1
3	D	188	GLY	2.1
3	D	640	LEU	2.0
1	T	261	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	EDO	C	1207	4/4	0.62	0.30	107,129,144,144	0
11	EDO	D	2008	4/4	0.65	0.29	93,111,125,126	0
11	EDO	D	2007	4/4	0.68	0.40	102,123,135,156	0
10	SO4	F	504	5/5	0.78	0.22	133,134,157,163	0
10	SO4	C	1203	5/5	0.80	0.33	114,140,180,183	0
11	EDO	F	506	4/4	0.83	0.32	101,121,130,156	0
11	EDO	D	2009	4/4	0.86	0.36	90,108,124,137	0
11	EDO	D	2011	4/4	0.87	0.25	76,107,133,133	0

Continued on next page...

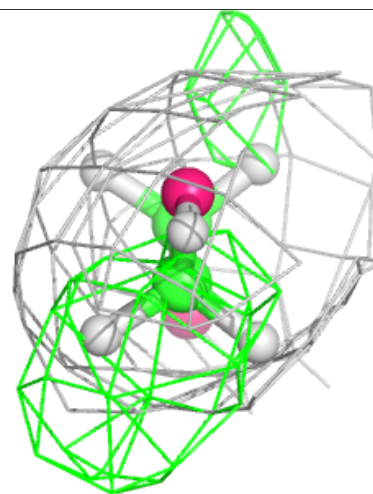
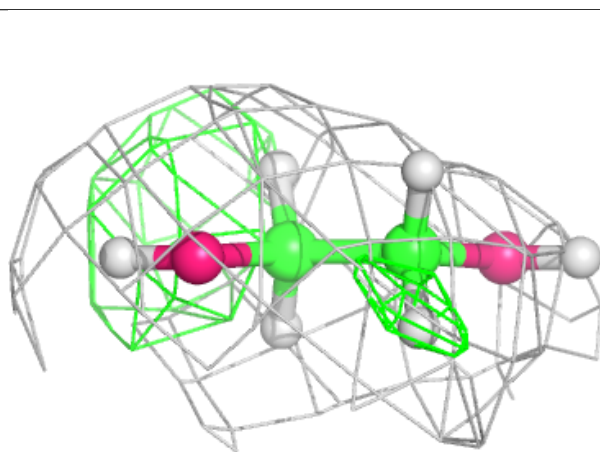
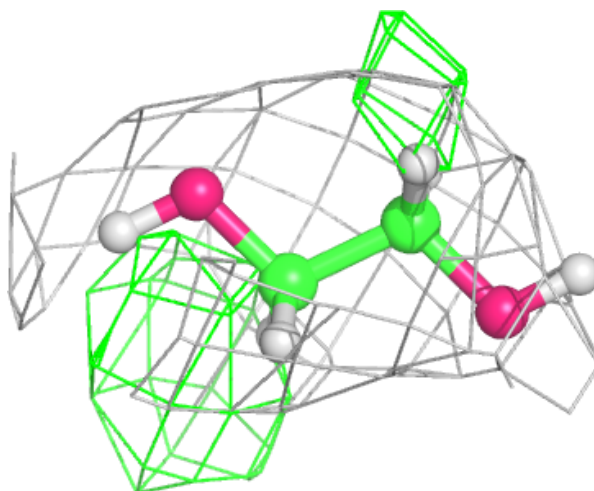
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	SO4	F	505	5/5	0.87	0.56	116,128,134,152	0
10	SO4	C	1202	5/5	0.89	0.10	116,120,146,158	0
10	SO4	D	2006	5/5	0.89	0.14	113,121,139,140	0
10	SO4	C	1206	5/5	0.90	0.26	127,131,156,410	0
10	SO4	F	503	5/5	0.91	0.13	105,109,129,136	0
10	SO4	D	2005	5/5	0.91	0.44	104,115,141,154	0
10	SO4	D	2010	5/5	0.91	0.14	94,120,151,152	0
12	SRN	C	1205	58/58	0.92	0.29	79,97,136,149	0
11	EDO	C	1204	4/4	0.93	0.35	61,88,105,113	0
10	SO4	D	2004	5/5	0.94	0.18	98,103,114,125	0
10	SO4	C	1201	5/5	0.94	0.29	133,138,162,170	0
10	SO4	F	501	5/5	0.95	0.08	122,128,139,153	0
10	SO4	D	2003	5/5	0.96	0.22	74,87,102,109	0
13	ZN	D	2002	1/1	0.96	0.23	134,134,134,134	0
13	ZN	D	2001	1/1	0.98	0.21	77,77,77,77	0
10	SO4	F	502	5/5	0.98	0.15	90,91,130,137	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.

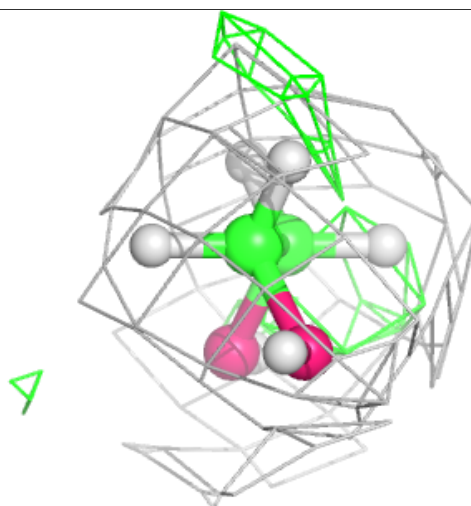
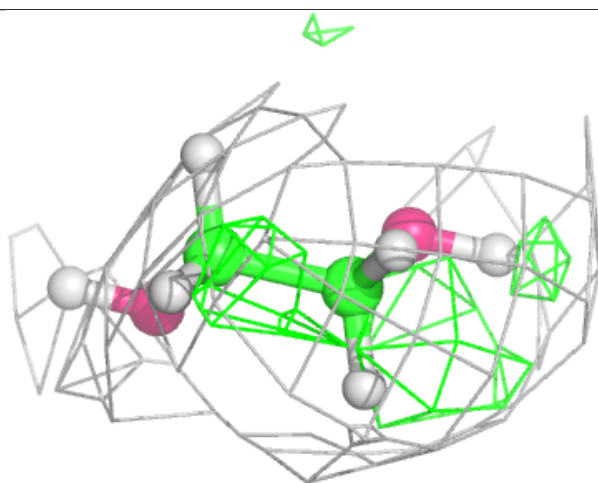
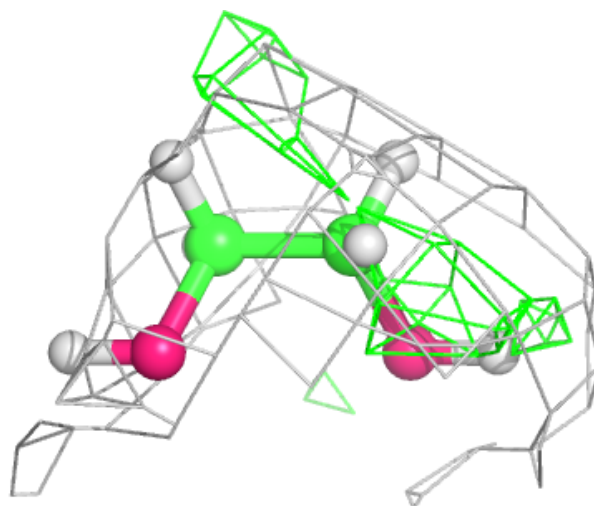
Electron density around EDO C 1207:

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



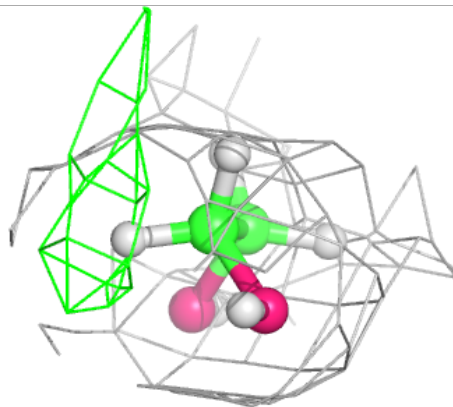
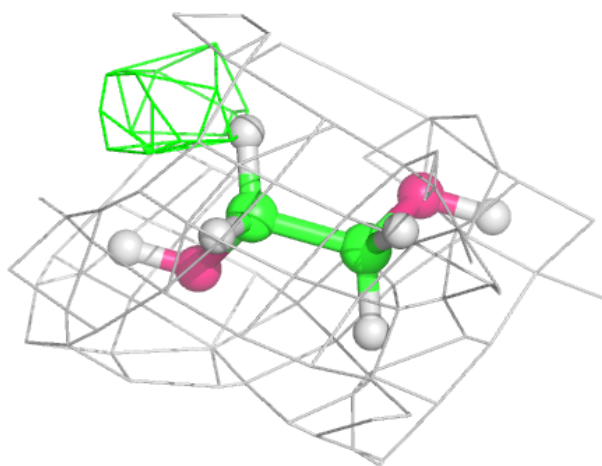
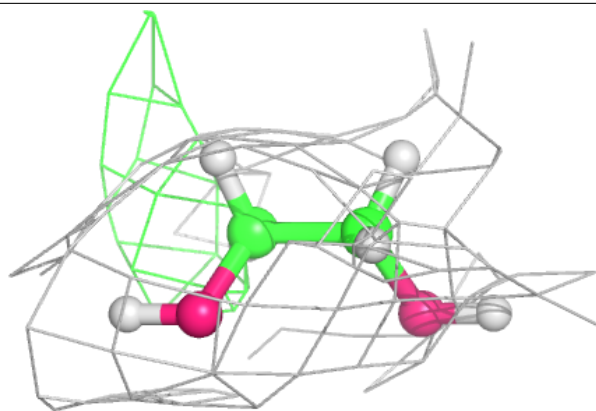
Electron density around EDO D 2008:

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



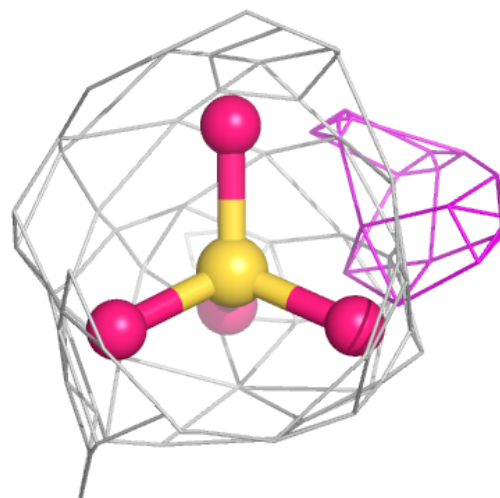
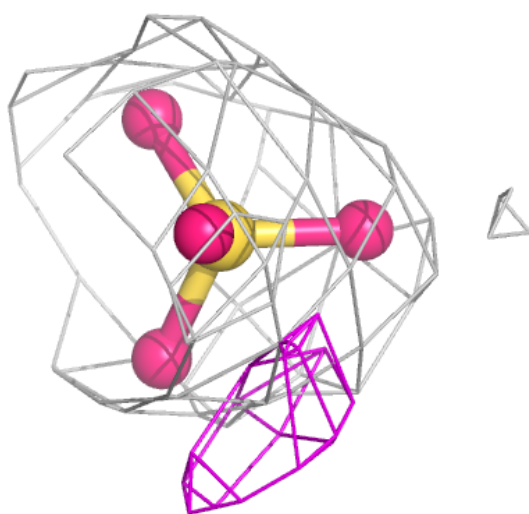
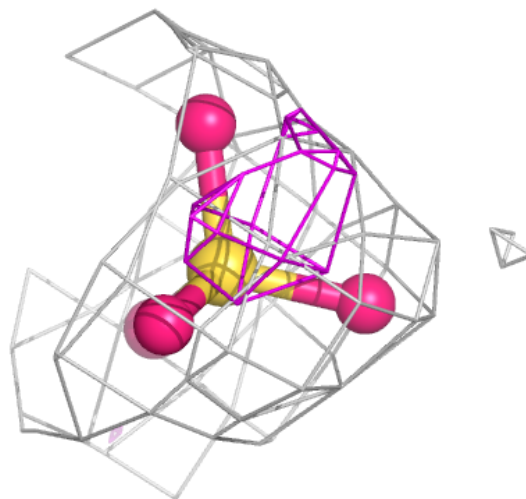
Electron density around EDO D 2007:

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



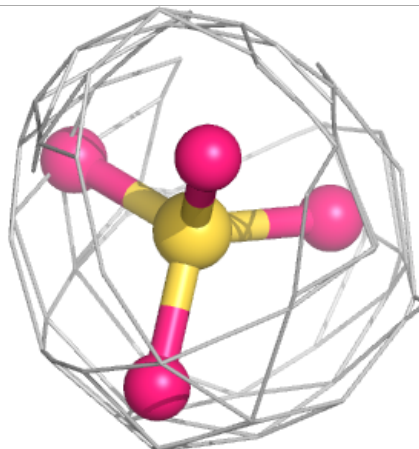
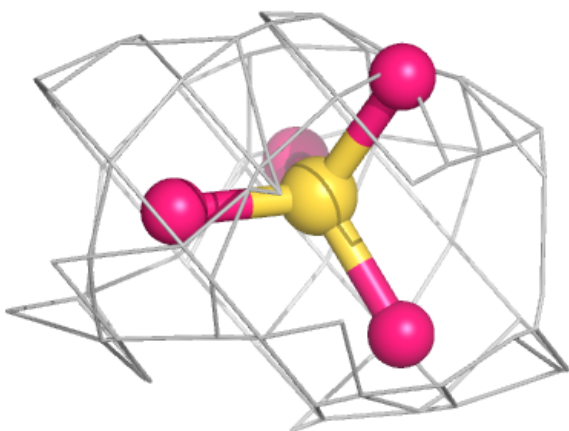
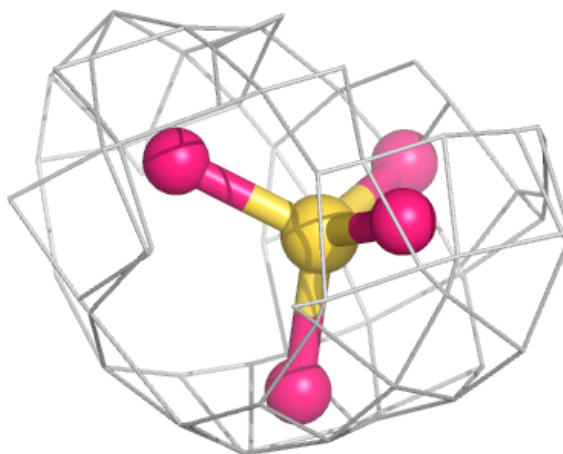
Electron density around SO4 F 504:

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



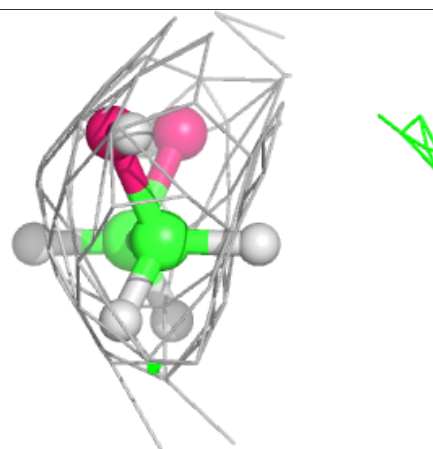
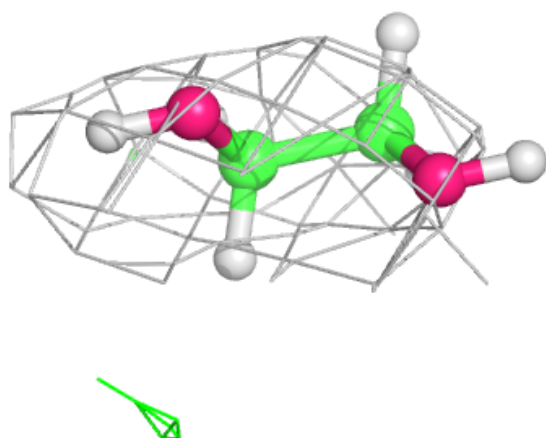
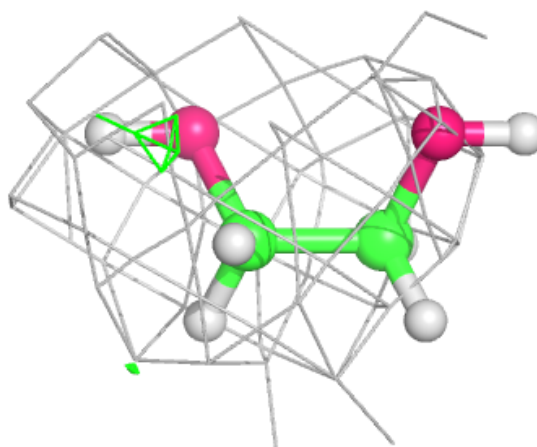
Electron density around SO4 C 1203:

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



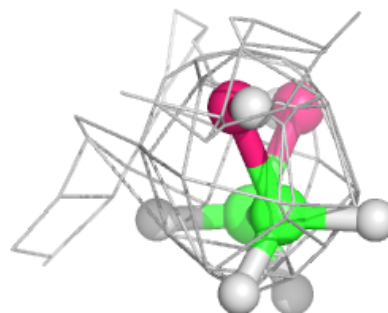
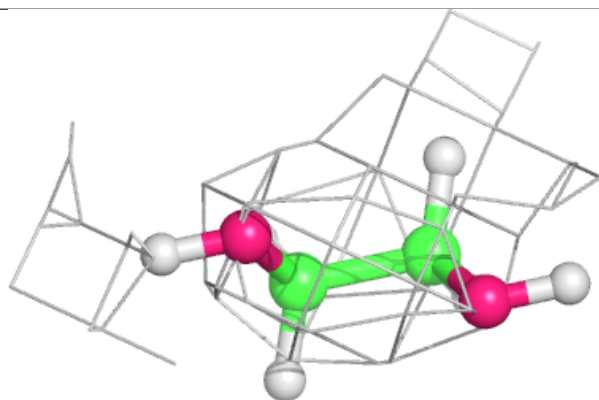
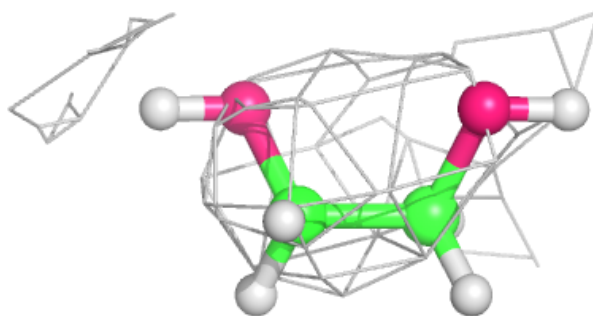
Electron density around EDO F 506:

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

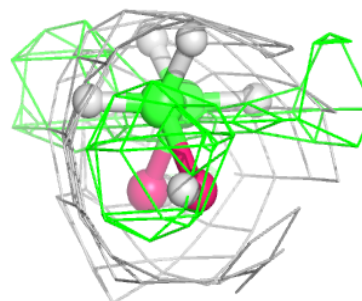
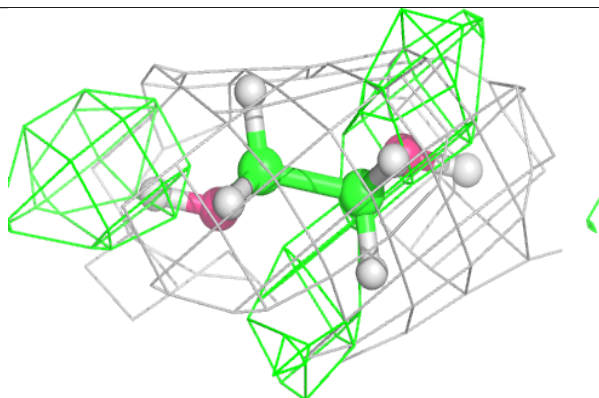
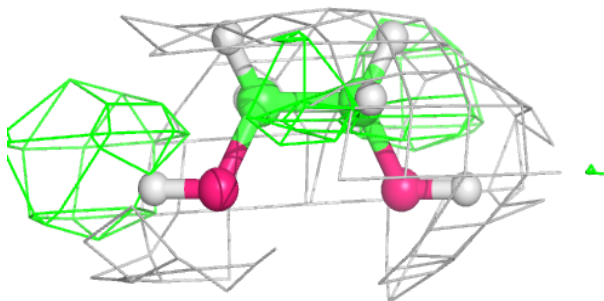


Electron density around EDO D 2009:

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

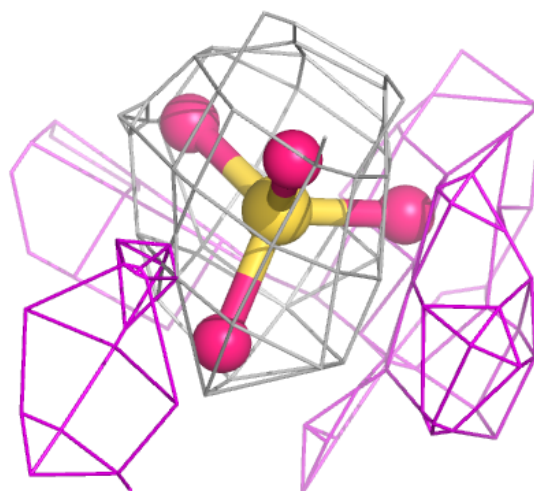
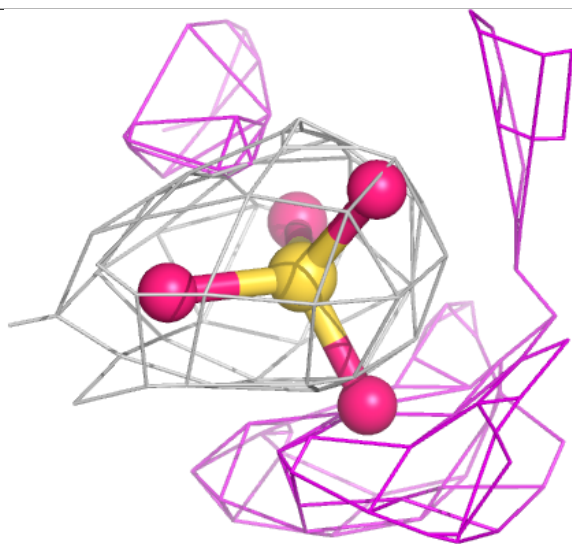
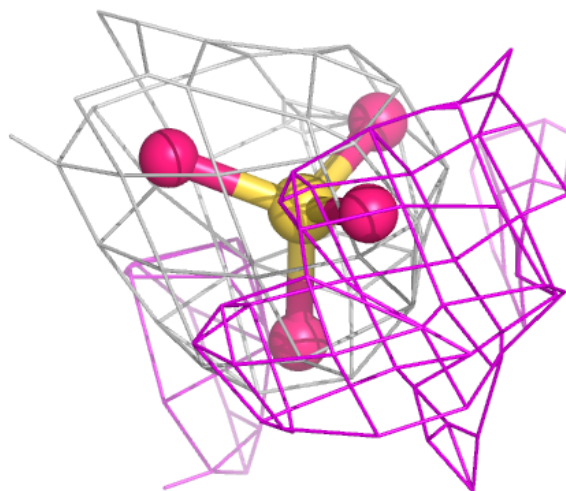
**Electron density around EDO D 2011:**

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



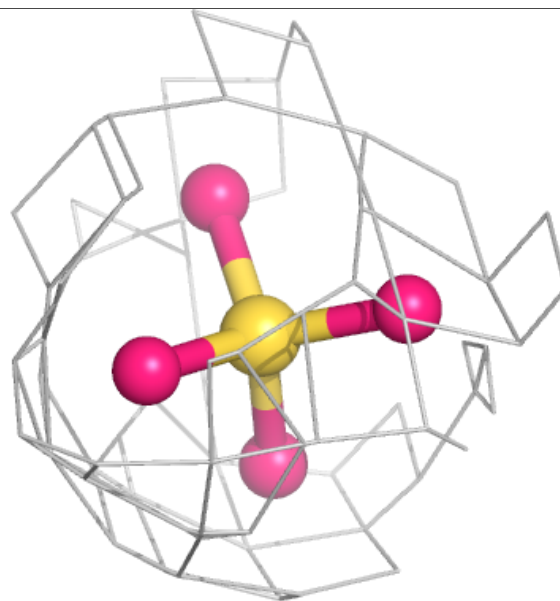
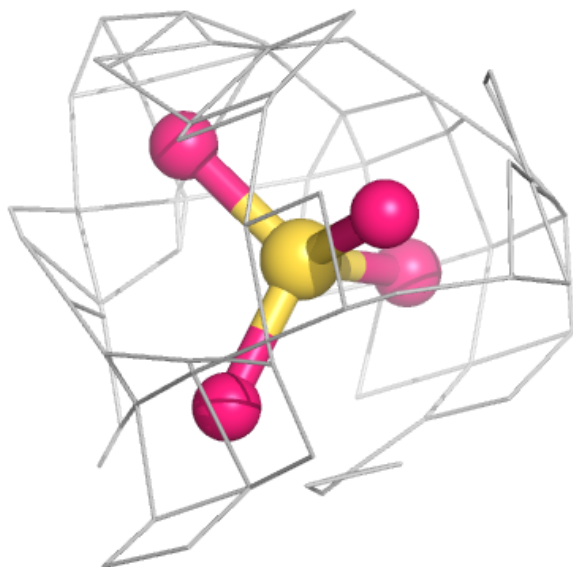
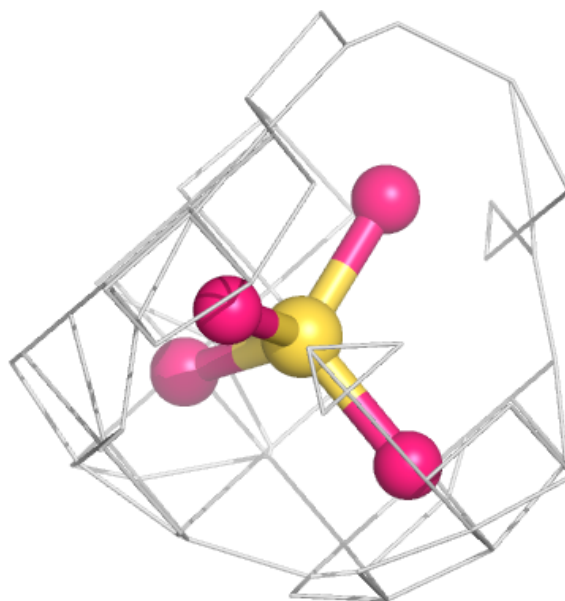
Electron density around SO4 F 505:

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



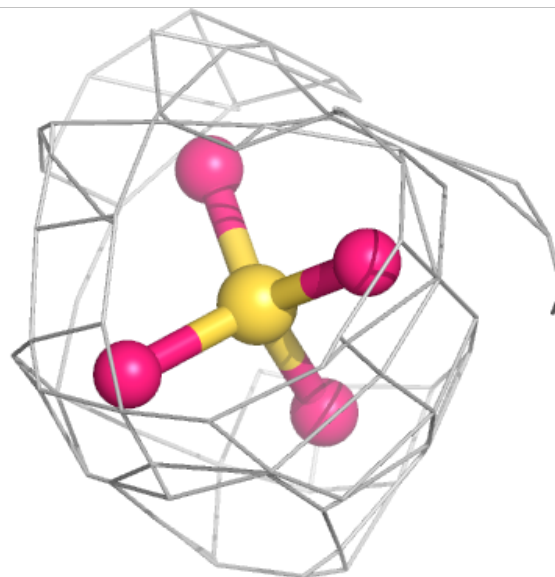
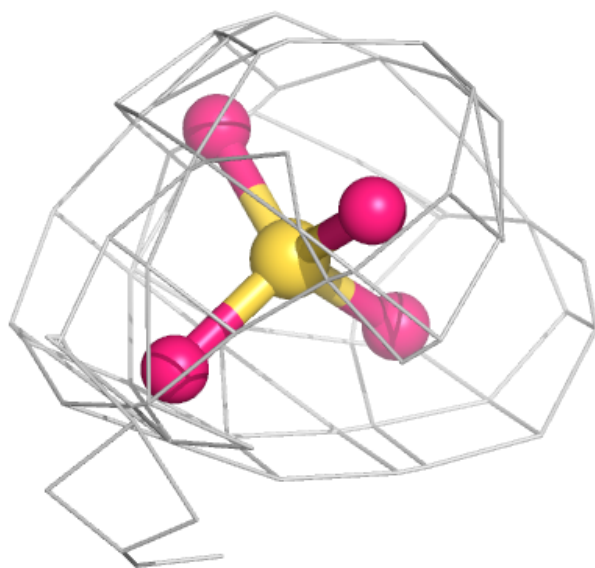
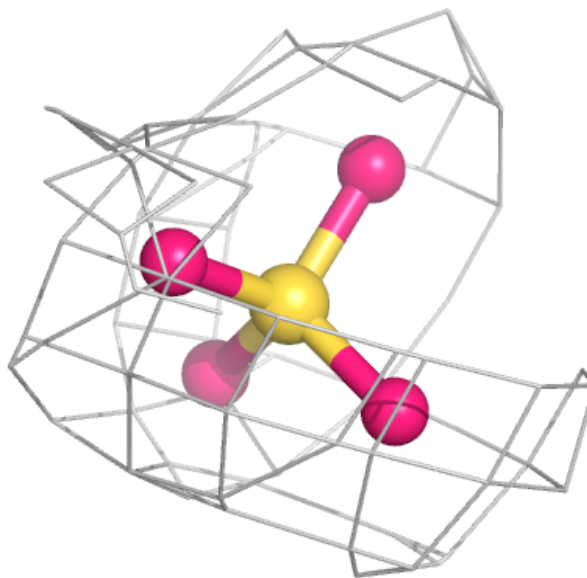
Electron density around SO4 C 1202:

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



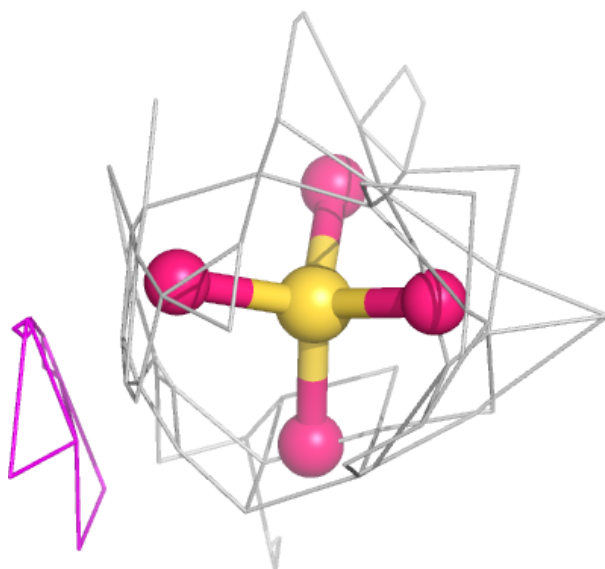
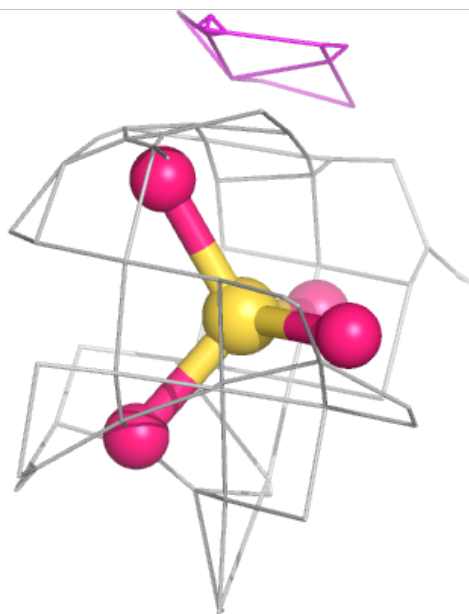
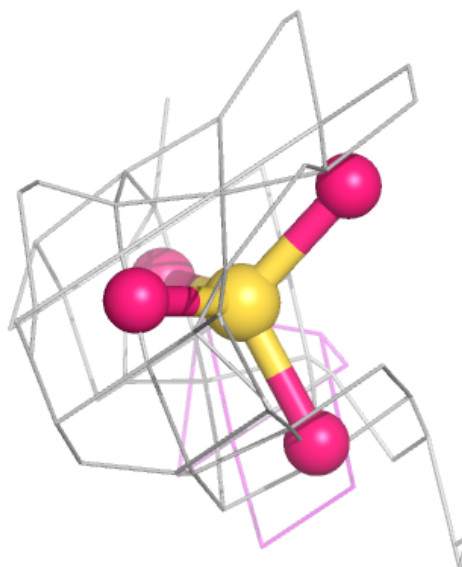
Electron density around SO4 D 2006:

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



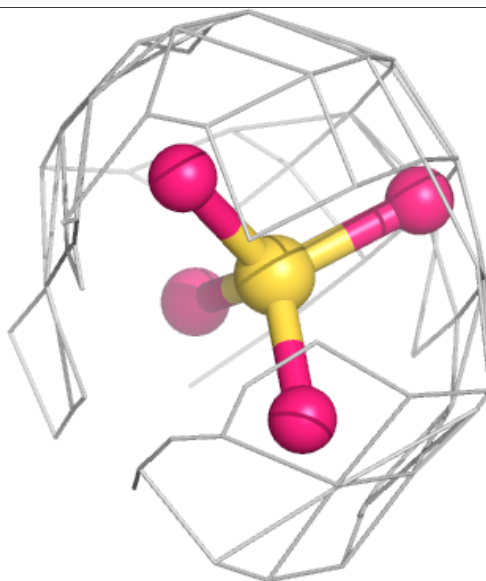
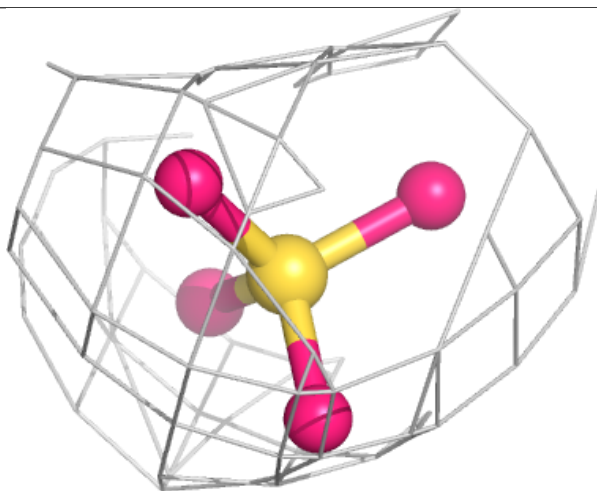
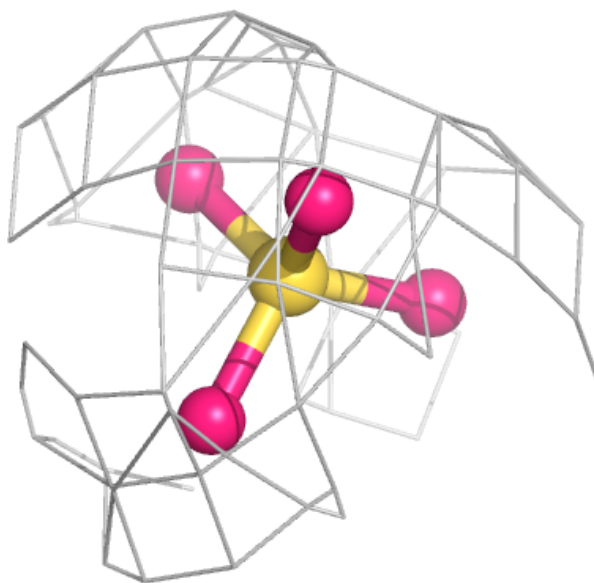
Electron density around SO4 C 1206:

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



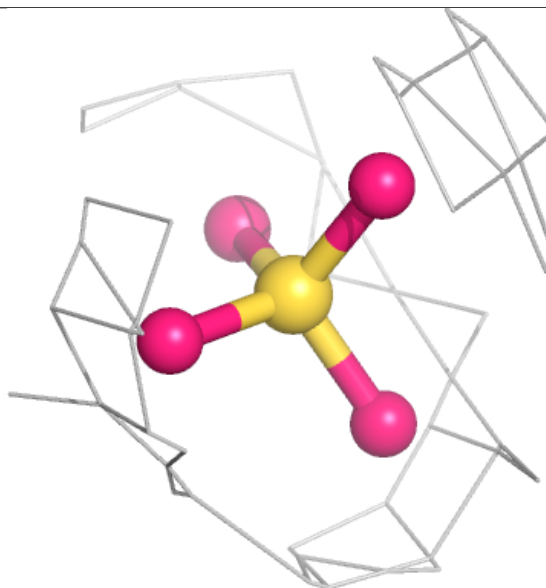
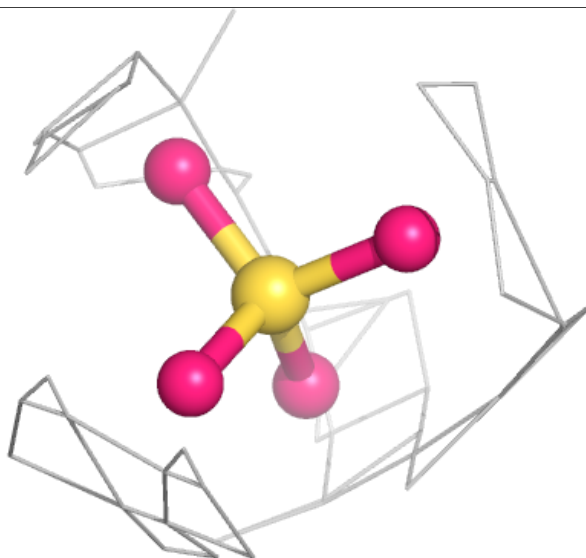
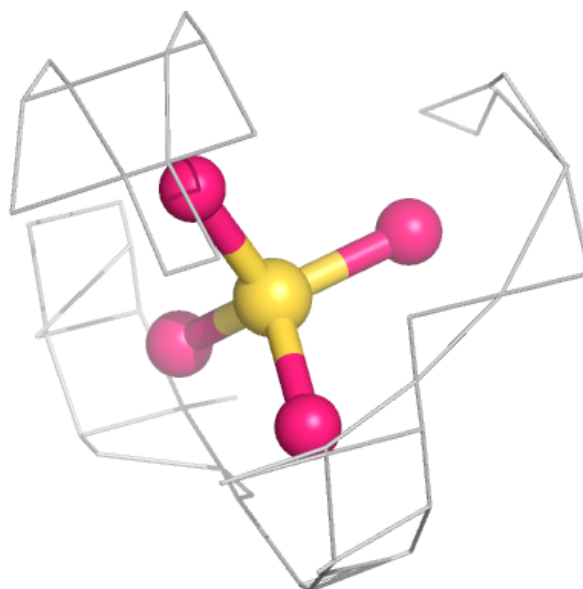
Electron density around SO4 F 503:

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



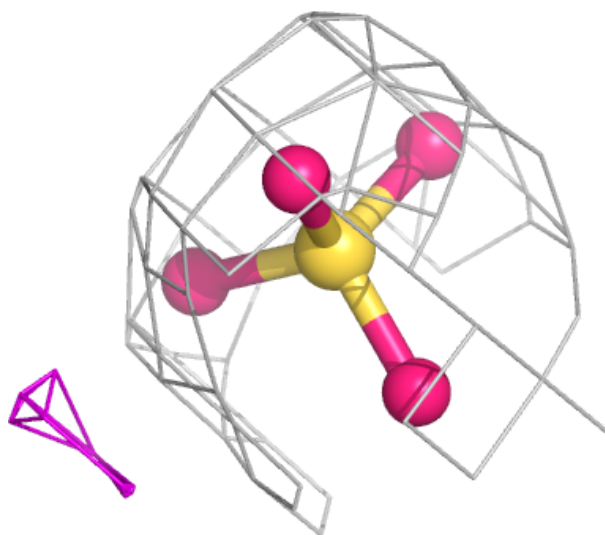
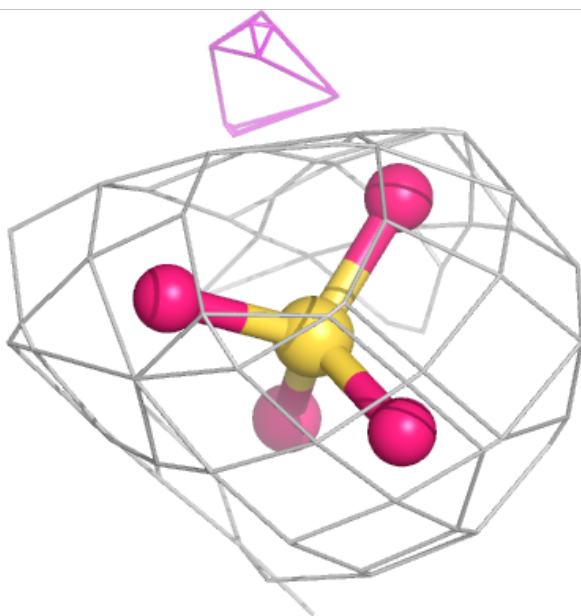
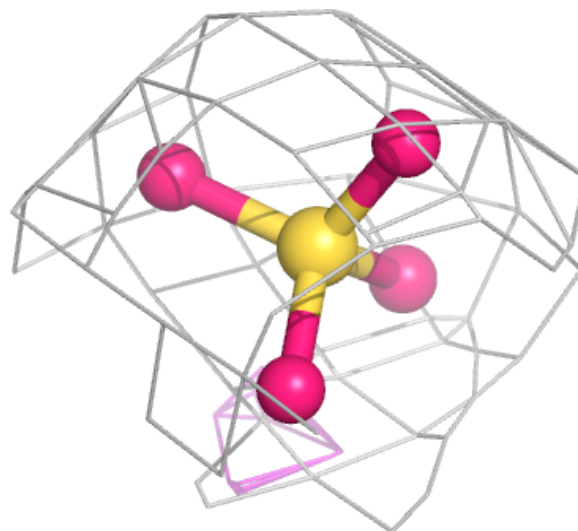
Electron density around SO4 D 2005:

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



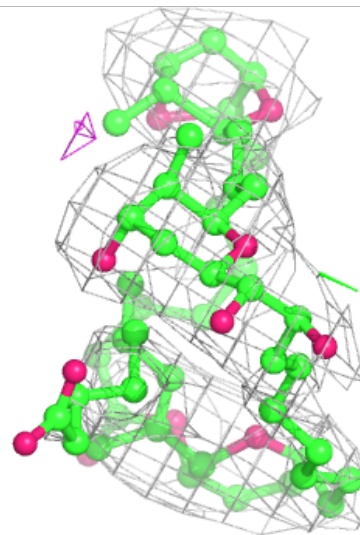
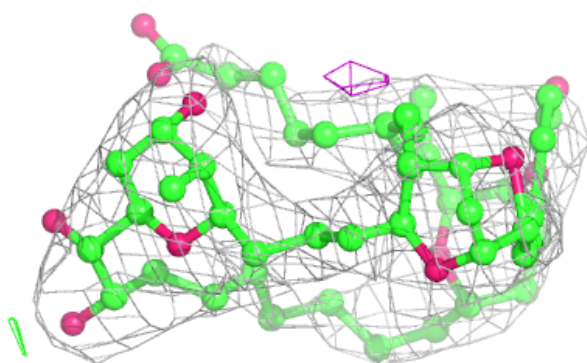
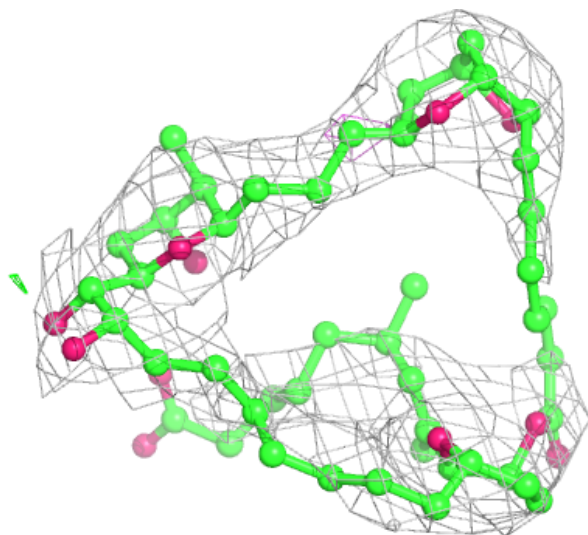
Electron density around SO4 D 2010:

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



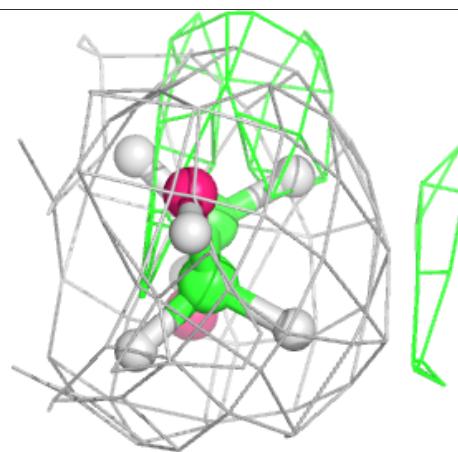
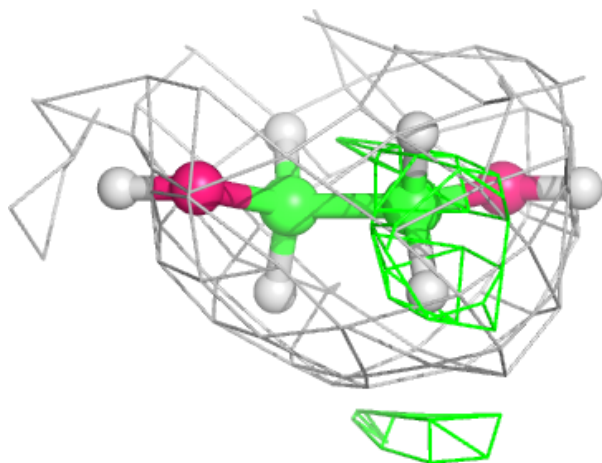
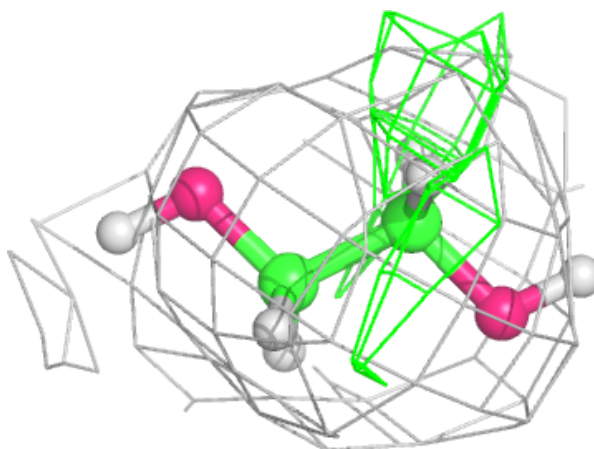
Electron density around SRN C 1205:

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



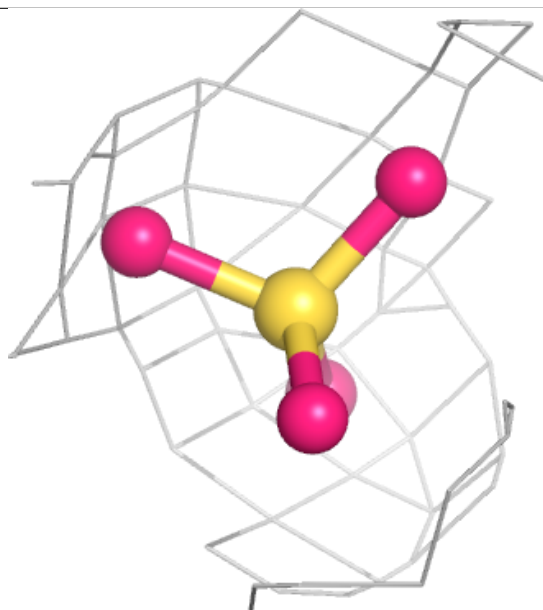
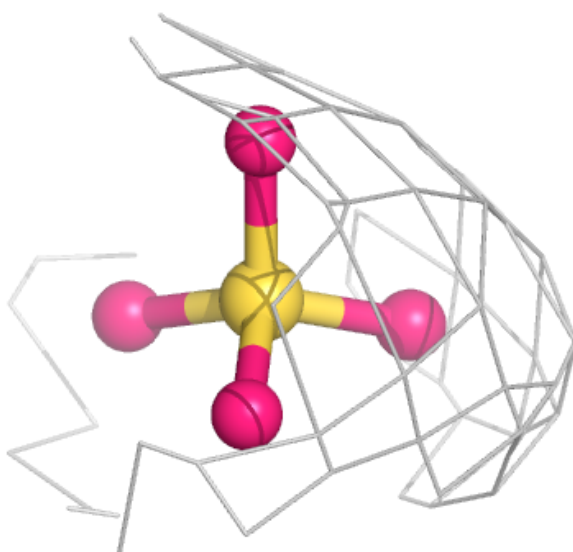
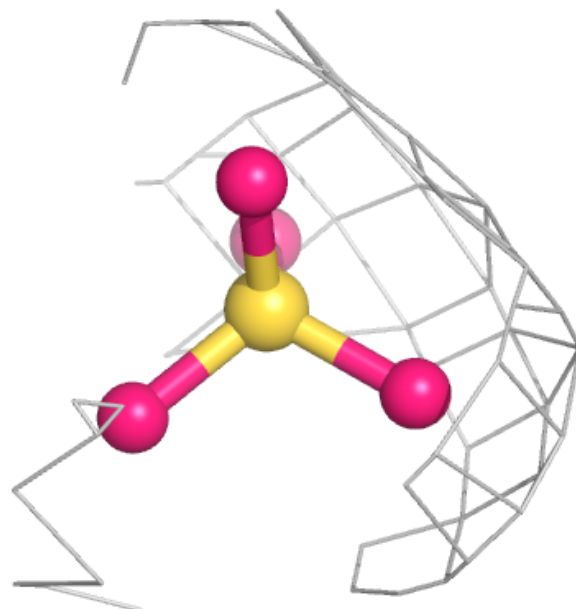
Electron density around EDO C 1204:

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



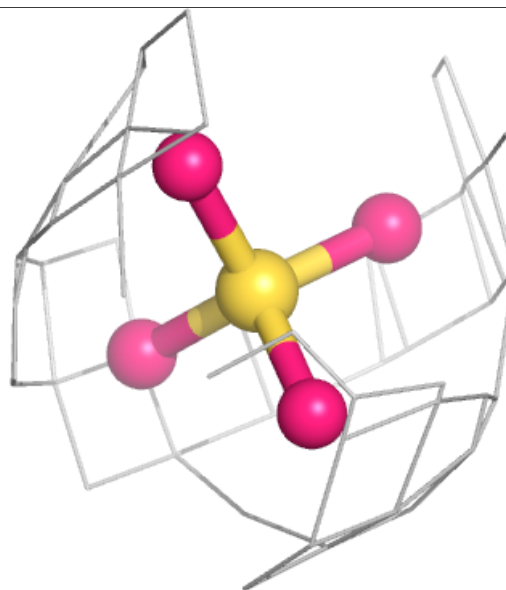
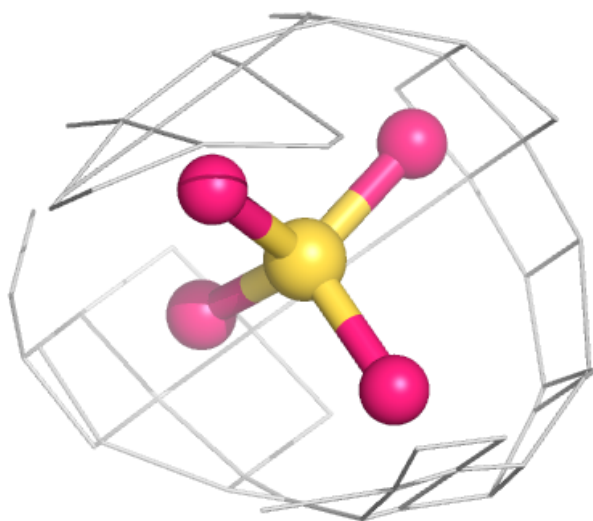
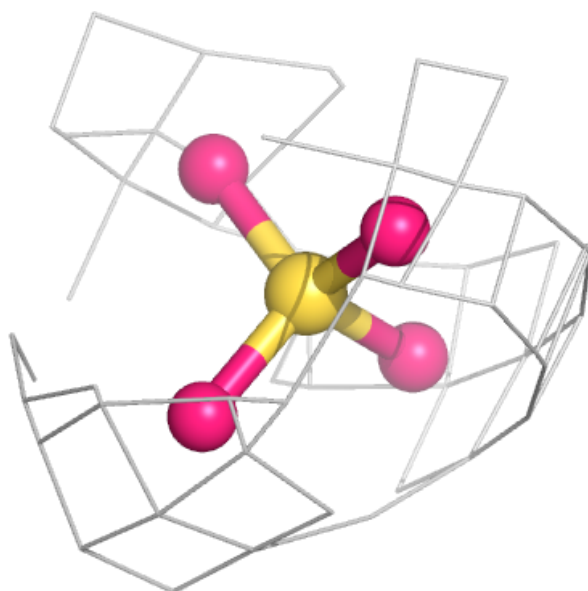
Electron density around SO4 D 2004:

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



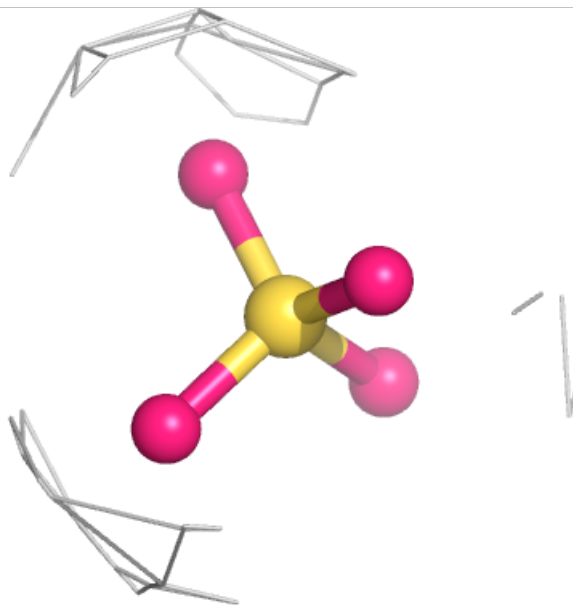
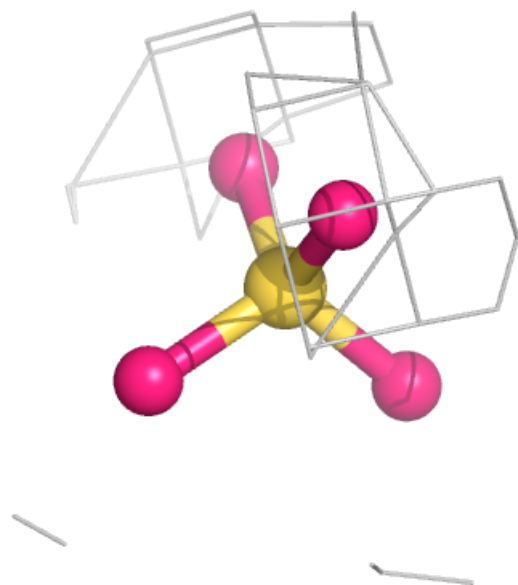
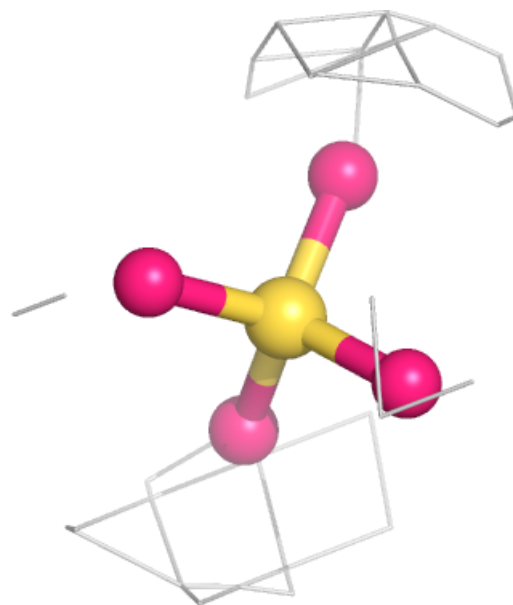
Electron density around SO4 C 1201:

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



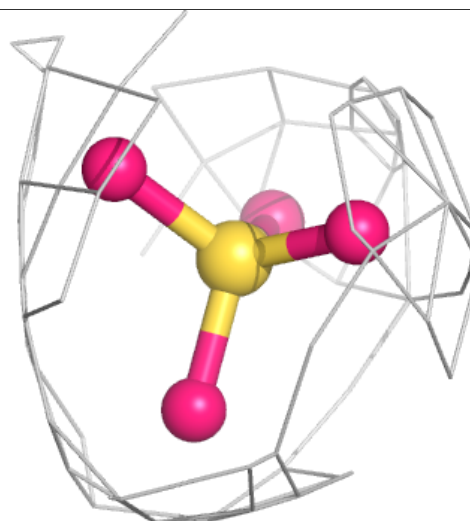
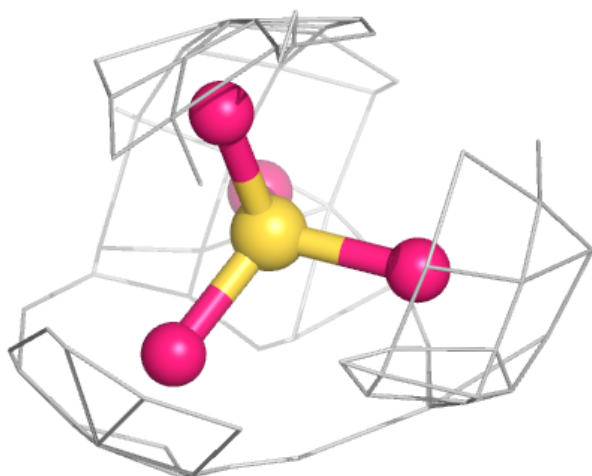
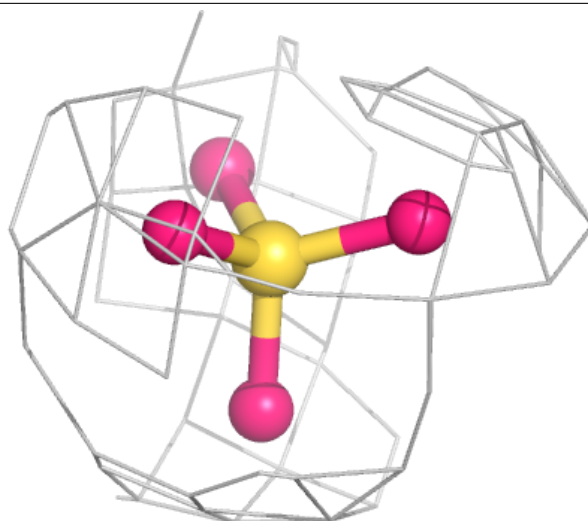
Electron density around SO4 F 501:

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



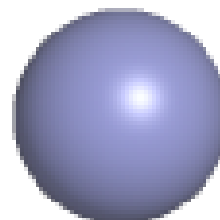
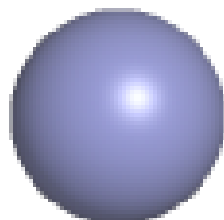
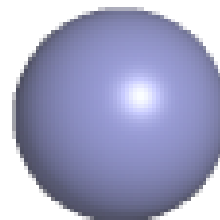
Electron density around SO4 D 2003:

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



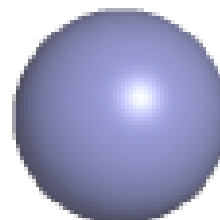
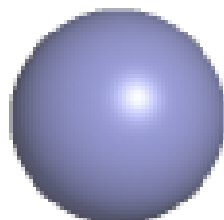
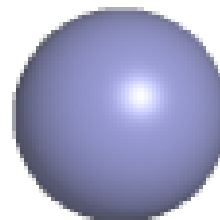
Electron density around ZN D 2002:

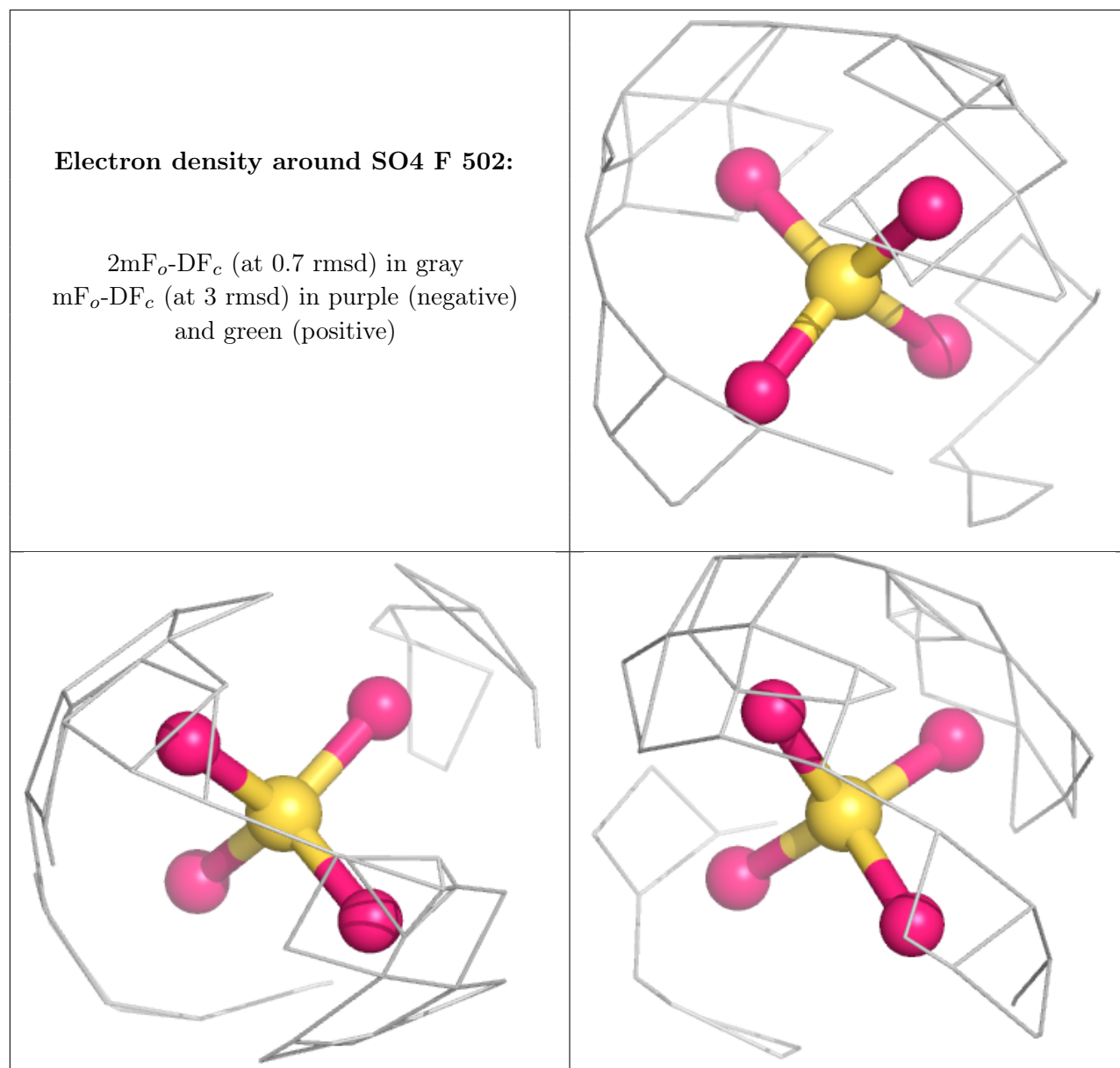
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.