



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:08 PM UTC

PDB ID : 6VVS / pdb_00006vvs
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

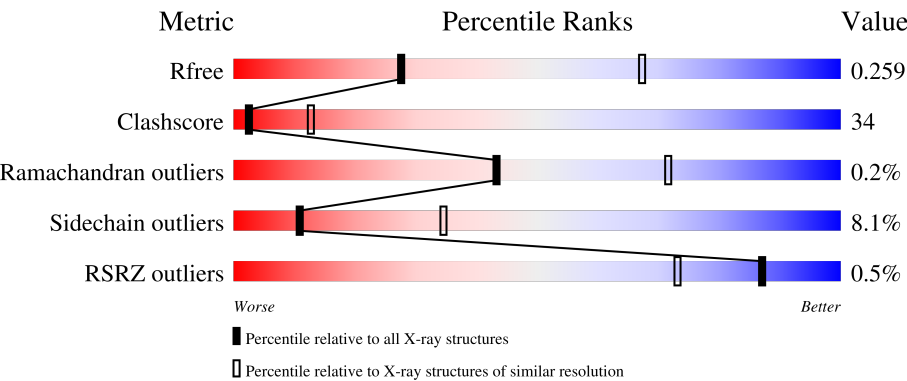
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	350	29% 31% • 38%
1	B	350	% 26% 35% 5% 33%
1	T	350	12% • 85%
2	C	1169	% 43% 47% 5% 6%
3	D	1317	49% 42% • 5%

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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	-

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			

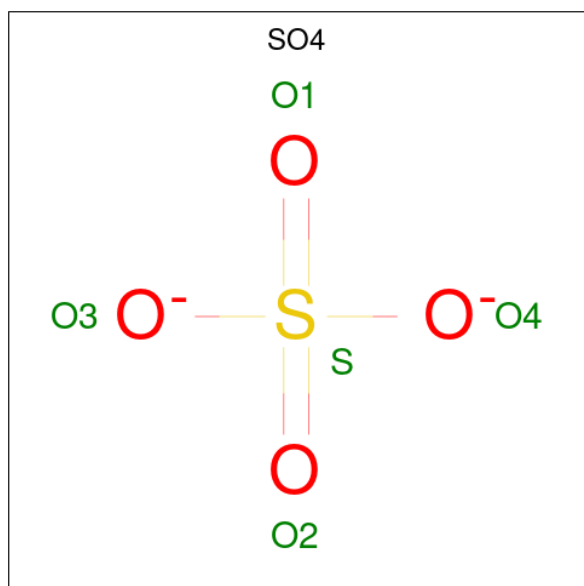
- Molecule 8 is a DNA chain called DNA (31-MER).

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 (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

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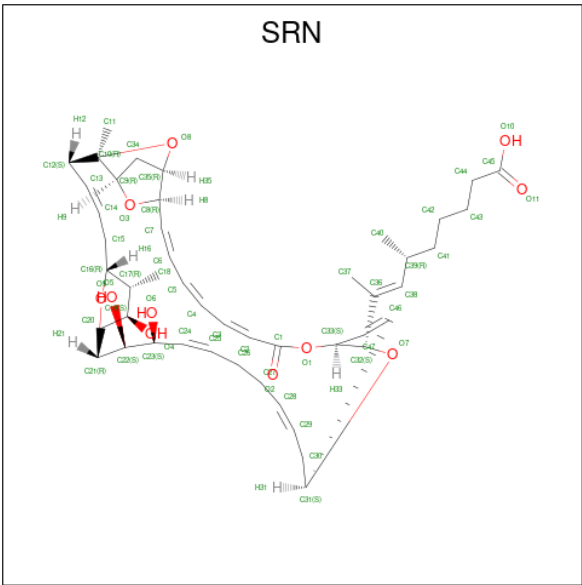
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	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 (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: SRN) (formula: C₄₇H₆₆O₁₁) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

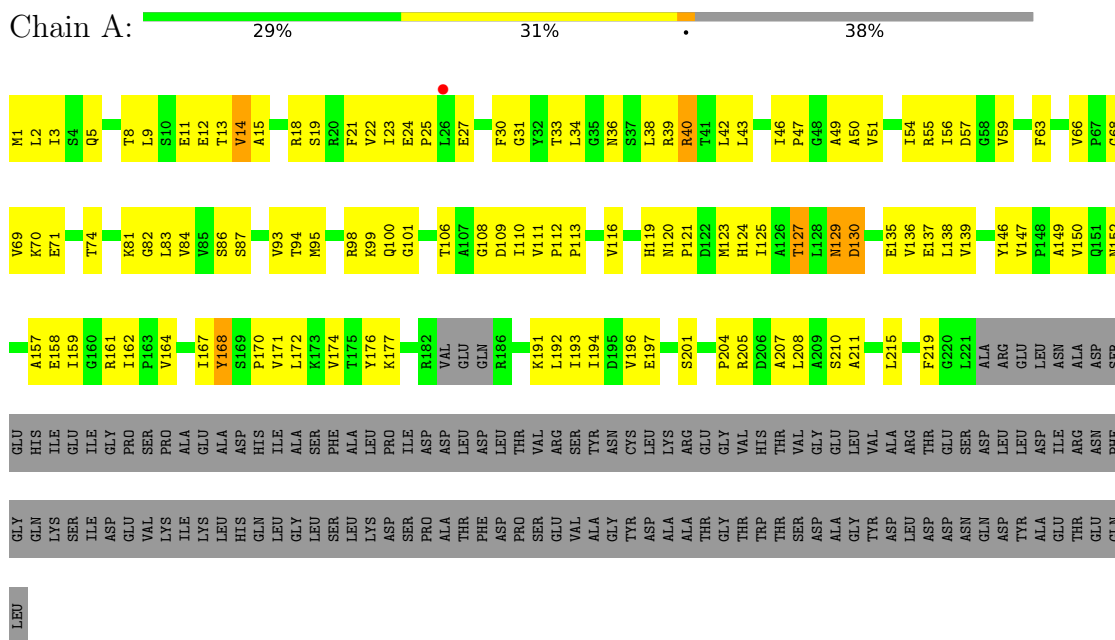
- Molecule 14 is water.

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			

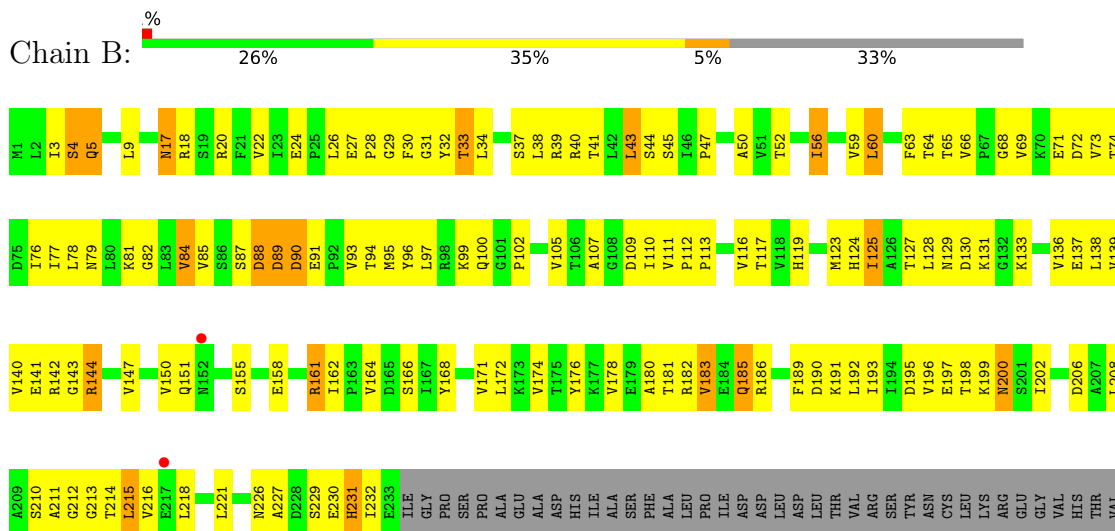
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



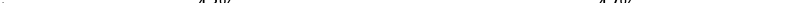
[illegible]

- Molecule 1: DNA-directed RNA polymerase subunit alpha

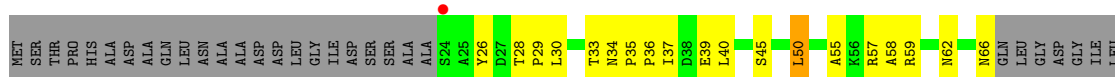
Chain T: 12% . 85%

THR	ALA	THR	PRO	MET
SER	ASP	ARG	ASP	LEU
ASP	HIS	VAL	MET	PHE
ALA	ILE	GLU	HIS	THR
GLY	ALA	GLN	ILE	THR
TYR	SER	ARG	ALA	ARG
ASP	PHE	THR	THR	PRO
ALA	ALA	ASP	LEU	THR
LEU	LEU	PHE	ASN	LEU
ASP	PRO	ASP	ASP	SER
ASN	1251	LYS	LYS	GLY
GLN	D262	LEU	GLY	ASP
ASP		ILE	LYS	THR
TYR	V258	ILE	LEU	VAL
ALA	R259	ASP	GLU	ASP
GLU	V260	VAL	VAL	ALA
THR	V261	GLU	GLU	ILE
GLU		THR	LEU	ASN
GLN	L264	LYS	VAL	ARG
LEU		ASN	VAL	SER
	V269	SER	GLU	ARG
		ILE	ARG	PHE
	V272	SER	GLY	VAL
		PRO	ARG	LEU
	T279	ARG	GLY	GLU
		ASP	TYR	PRO
	D282	ALA	VAL	SER
	L283	LEU	PRO	GLU
	L284	ALA	ALA	ASP
		SER	VAL	PHE
	G290	ALA	GLN	GLY
		GLY	ASN	TYR
	L303	LEU	ASP	ASN
		LEU	ALA	SER
		SER	LEU	LEU
		LYS	ILE	ARG
		ASP	GLY	ARG
		SER	ARG	THR
		PRO	ILE	LEU
		ALA	PRO	LEU
		THR	VAL	SER
		PHE	ASP	THR
		ASP	ASN	ILE
		PRO	ILE	ALA
		SER	TYR	PRO
		GLU	SER	GLY
		VAL	PRO	ASP
		ALA	VAL	ALA
		ALA	VAL	VAL
		GLY	LEU	THR
		TYR	LYS	SER
		ASP	VAL	ILE
		ALA	THR	ARG
		ALA	TYR	VAL
		THR	LYS	THR
		GLY	VAL	GLY
		THR	GLU	VAL
		THR	ALA	THR

- Molecule 2: DNA-directed RNA polymerase subunit beta

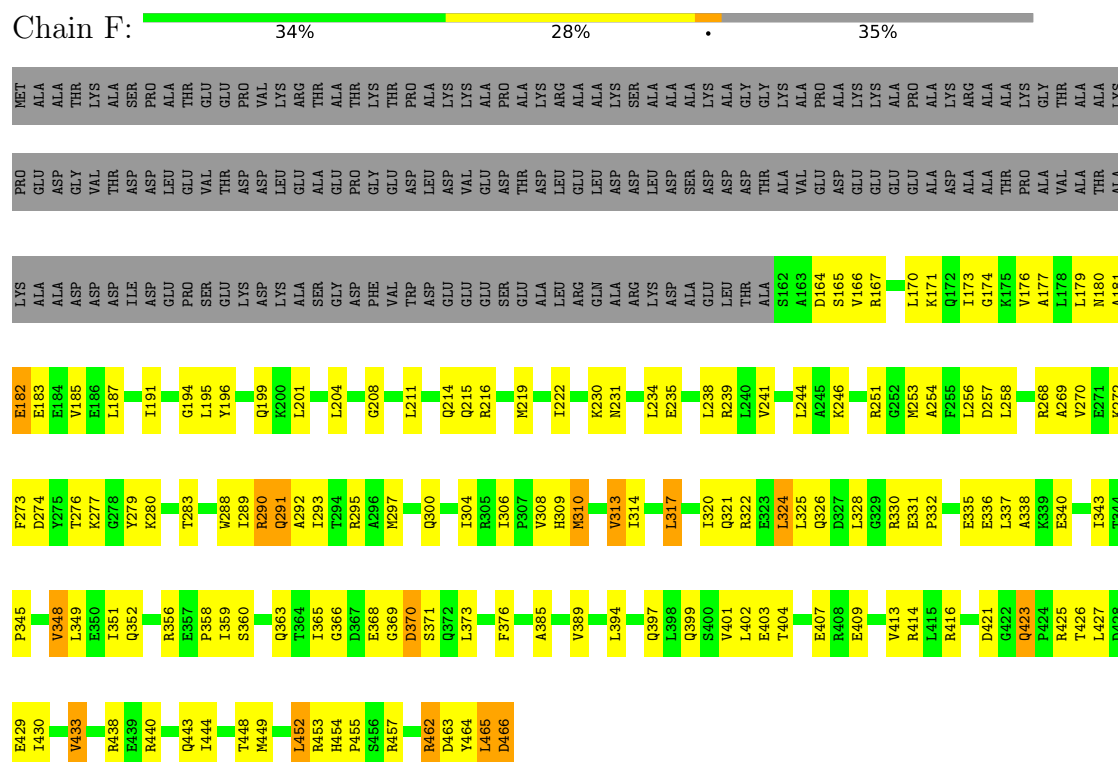
Chain C:  43% 47% 5% 6%

R412	D328	M249	V171	S85	LEU	MET
I418	V329	M250	R172	P86	GLU	
F421	T332	L253	S173	I87	GLY	
S425	I333	E254	G175	E88	CYS	
Q426	E334	L253	V176	G92	ILE	
Q427	I335	E254	V177	S93	LEU	
S428	L336	T261	F178	M94	ALA	
Q429	L337	D262	I179	S95	VAL	
F430	R338	L265	E180	L96	SER	
M431	Q343	L265	T186	D100	SER	
D432	T344	T268	E187	F101	SER	
Q433	S345	Y269	K188	R102	LYS	
M434	T347	L272	V193	F103	SER	
M435	V348	R273	K194	D104	ASN	
P436	P349	P274	V195	E105	ALA	
L437			V196	V106	ILE	
L440	P355	P278	I197	M118	THR	
L441	V356	T279	G198	T119	ASN	
H442	E357	K280	R199	Y120		
K443	V358	Q284	G200	L124		
R444	I361	T285	W202	F125		
R445	F364	L286	L203	I216		
S447		L287	E204	T127		
L448	R367	F291	F205	A128		
L449	R368	E294	ASP	E129		
G450	L369	K295	VAL	M132		
P451	R370	L296	ASP	M133		
G452	T371	R296	LYS	T135		
G453	V372	Y297	ARG	G136		
L454	G373	D298	ASP			
	E374	L299	THR			
A459	L375	A300	VAL			
G460	I376	R301	GLY	K139		
L461	Q379	V302	W215	S140		
E462	G379	R302	R216	Q141		
G463	I380	G303	I217	T142		
R464				V413		
				F144		
	E388	F306	R221	M145		
H467	R389	V307	R222			
P468	V390	K310	Q223	E33		
S469		L311	P224	F148		
	R394	GLY	V225	L55		
Q472	M395	LEU	T226	M150		
		ASN	V227	V56		
			L228	G57		
C475	Q398	ASN	R229	K154		
P476	D399	GLY	L230			
I477	V400	ALA	R230	I158		
E478	E401	LYS	A231	I159		
T479	A402	PRO	L232	A65		
P480	I403	ILE	G233	R164		
E481	T404	THR	W234	V165		
G482	P405	SER	T235	V166		
P483	Q406	TER	N236	V167		
H484	T407	S323		S168		
		L324		Q169		
			T239	I470		

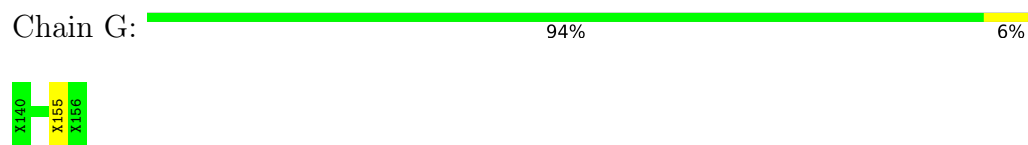




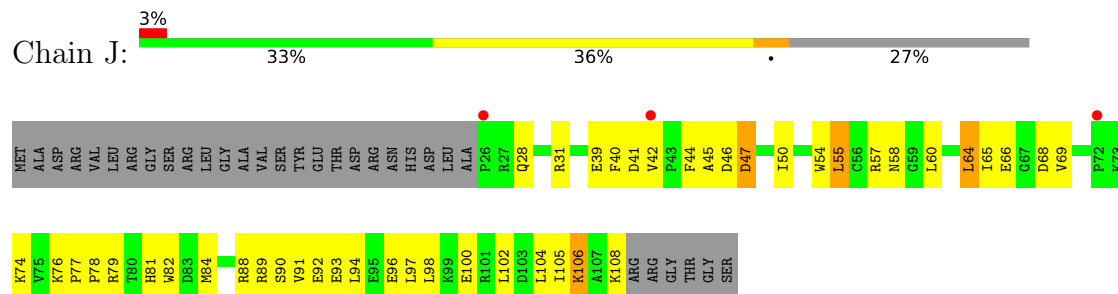
- Molecule 5: RNA polymerase sigma factor SigA



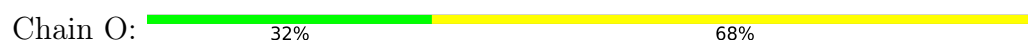
- Molecule 6: unknown

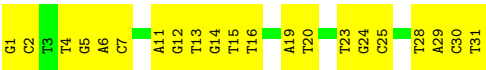


- Molecule 7: RNA polymerase-binding protein RbpA

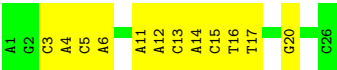


- Molecule 8: DNA (31-MER)





● Molecule 9: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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 0.218 , 0.259	Depositor DCC
R_{free} test set	1997 reflections (1.97%)	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)	0.30 , 72.5	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, SO4, SRN, 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	0.13	0/1629	0.32	0/2220
1	B	0.13	0/1698	0.34	0/2322
1	T	0.10	0/343	0.26	0/468
2	C	0.14	0/8421	0.35	0/11444
3	D	0.16	0/9706	0.35	0/13140
4	E	0.17	0/604	0.38	0/822
5	F	0.14	0/2438	0.33	0/3291
7	J	0.16	0/685	0.40	0/927
8	O	0.23	0/710	0.41	0/1095
9	P	0.27	0/589	0.43	0/906
All	All	0.15	0/26823	0.35	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	146	0
1	B	1672	0	1643	182	0
1	T	342	0	275	14	0
2	C	8275	0	8025	696	1
3	D	9555	0	9509	604	1
4	E	592	0	583	42	0
5	F	2407	0	2428	158	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	13	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	1793	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 34.

All (1793) 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:C12	12:C:1205:SRN:C10	1.77	1.57
12:C:1205:SRN:C8	12:C:1205:SRN:O3	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
3:D:622:MET:HE3	3:D:667:LEU:HD13	1.37	1.06
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:HE2	7:J:106:LYS:HA	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
1:A:152:ASN:HB2	1:A:157:ALA:HB3	1.43	1.00
2:C:176:VAL:HG12	2:C:195:VAL:HG22	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
2:C:1128:VAL:HG11	2:C:1138:MET:HE3	1.42	0.98
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
5:F:253:MET:HE2	5:F:300:GLN:HB2	1.48	0.95
3:D:656:LYS:HE3	3:D:656:LYS:H	1.29	0.94
3:D:819:MET:HE2	3:D:821:GLY:HA2	1.48	0.94
3:D:527:LEU:HD21	3:D:581:MET:HE1	1.47	0.94
3:D:106:TYR:HB3	3:D:312:MET:HE3	1.47	0.93
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
5:F:253:MET:HE3	5:F:297:MET:HA	1.49	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:622:MET:HE2	3:D:629:VAL:HG22	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
2:C:602:MET:HE1	2:C:883:LYS:HB3	1.51	0.90
3:D:892:THR:OG1	3:D:894:ARG:NH1	2.04	0.90
3:D:1009:LEU:HD12	3:D:1146:GLN:HG3	1.54	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
1:A:82:GLY:HA3	1:A:123:MET:HE1	1.55	0.89
5:F:219:MET:HA	5:F:219:MET:HE2	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
3:D:590:THR:HG21	3:D:630:ARG:HH21	1.37	0.88
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:1048:LEU:HD23	2:C:1048:LEU:H	1.37	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
3:D:1165:ARG:HD2	3:D:1209:MET:HE1	1.59	0.84
2:C:150:MET:HA	2:C:150:MET:HE2	1.59	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
5:F:320:ILE:HG23	5:F:340:GLU:HG2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:324:LEU:HD23	5:F:328:LEU:HD13	1.59	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
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:21:ARG:NE	3:D:96:GLU:OE2	2.14	0.80
3:D:84:ARG:NH1	14:D:2101:HOH:O	2.14	0.80
3:D:327:MET:HG3	3:D:337:THR:HB	1.60	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:H	3:D:365:ILE:HD12	1.46	0.78
3:D:641:ARG:HA	3:D:656:LYS:NZ	1.98	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
1:B:100:GLN:HA	1:B:133:LYS:HA	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:581:MET:HE3	3:D:716:LYS:HA	1.66	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:1071:ASP:HB2	3:D:1072:GLY:C	2.11	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
2:C:895:MET:SD	14:C:1303:HOH:O	2.42	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
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
7:J:74:LYS:O	7:J:74:LYS:NZ	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:899:PRO:HD2	2:C:992:MET:HE1	1.72	0.72
2:C:590:HIS:HB3	2:C:919:ILE:HD13	1.71	0.72
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
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
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
5:F:253:MET:CE	5:F:300:GLN:HB2	2.19	0.71
1:A:11:GLU:CD	1:A:205:ARG:HD3	2.16	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
3:D:641:ARG:HA	3:D:656:LYS:HZ3	1.54	0.70
5:F:176:VAL:HG12	5:F:177:ALA:H	1.56	0.70
2:C:338:ARG:HH11	2:C:343:GLN:HE22	1.38	0.70
2:C:710:LEU:HD13	2:C:1021:ILE:HG12	1.73	0.70
5:F:462:ARG:NH1	5:F:465:LEU:HB2	2.07	0.70
3:D:114:LEU:HG	3:D:312:MET:HE2	1.74	0.70
1:B:74:THR:HG21	3:D:611:VAL:HG11	1.72	0.70
2:C:613:GLU:O	2:C:705:ALA:HB1	1.92	0.70
3:D:622:MET:CE	3:D:667:LEU:HD13	2.20	0.70
2:C:894:ASP:HA	2:C:1004:GLY:HA3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1087:LEU:HD23	3:D:1113:MET:HE2	1.74	0.69
1:B:64:THR:O	1:B:65:THR:OG1	2.06	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:74:THR:CG2	3:D:611:VAL:HG11	2.22	0.69
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.58	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:56:ILE:HB	1:A:59:VAL:HG22	1.75	0.69
1:A:158:GLU:H	1:A:161:ARG:HH11	1.40	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
3:D:262:LYS:HG3	3:D:310:MET:HE1	1.73	0.68
2:C:872:ASP:OD1	2:C:872:ASP:N	2.20	0.68
2:C:344:THR:O	2:C:355:PRO:HA	1.92	0.68
3:D:131:PHE:HA	3:D:256:MET:HE2	1.75	0.68
3:D:721:TYR:O	3:D:725:ARG:HG2	1.92	0.68
1:B:88:ASP:OD2	1:B:88:ASP:N	2.26	0.68
1:B:107:ALA:O	1:B:110:ILE:HG22	1.93	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
9:P:15:DC:H2'	9:P:16:DT:H71	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:953:GLU:OE1	2:C:953:GLU:N	2.27	0.68
3:D:430:ILE:HD13	3:D:541:MET:HG3	1.76	0.68
3:D:656:LYS:H	3:D:656:LYS:CE	2.03	0.68
3:D:614:SER:HB2	3:D:615:PRO:HD2	1.76	0.68
2:C:215:VAL:O	2:C:223:GLN:HB2	1.94	0.68
2:C:437:LEU:HB2	2:C:704:MET:HE2	1.75	0.68
3:D:500:ARG:HB2	3:D:541:MET:HE3	1.76	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
2:C:96:LEU:HA	2:C:129:GLU:O	1.95	0.67
3:D:330:LEU:HD22	3:D:330:LEU:H	1.58	0.67
3:D:1165:ARG:CD	3:D:1209:MET:HE1	2.25	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:642:PRO:CD	3:D:656:LYS:HD2	2.24	0.67
3:D:1168:ILE:O	3:D:1178:PRO:HA	1.95	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
3:D:1087:LEU:CD2	3:D:1113:MET:HE2	2.25	0.67
1:A:82:GLY:CA	1:A:123:MET:HE1	2.25	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:899:PRO:CD	2:C:992:MET:HE1	2.24	0.66
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HB3	1:A:127:THR:HG23	1.77	0.66
3:D:527:LEU:HD22	3:D:575:ALA:O	1.96	0.66
3:D:1247:ASN:O	3:D:1260:PRO:HG3	1.96	0.66
5:F:204:LEU:O	5:F:208:GLY:N	2.29	0.66
3:D:76:GLU:HA	7:J:44:PHE:HE2	1.59	0.66
3:D:599:TYR:HB2	3:D:610:GLY:HA3	1.78	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
3:D:137:THR:HG22	3:D:253:THR:C	2.21	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:1275:PRO:HB3	4:E:79:LEU:HD11	1.76	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
12:C:1205:SRN:O1	12:C:1205:SRN:H4	1.97	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
2:C:346:MET:HE2	2:C:348:VAL:HG13	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:90:ASP:O	1:B:91:GLU:HG3	1.97	0.65
1:B:95:MET:HG2	1:B:113:PRO:CD	2.25	0.65
3:D:1249:LEU:HD12	3:D:1250:LYS:N	2.12	0.65
1:B:24:GLU:OE2	1:B:181:THR:HG21	1.97	0.65
1:B:144:ARG:NH1	1:B:144:ARG:HB2	2.12	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
3:D:622:MET:CE	3:D:629:VAL:HG22	2.27	0.65
2:C:652:MET:HE2	2:C:658:ARG:HD2	1.79	0.65
1:A:95:MET:HE2	1:A:110:ILE:HG22	1.79	0.64
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:OD1	7:J:47:ASP:N	2.22	0.64
9:P:11:DA:H4'	9:P:12:DA:OP1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:HG23	3:D:607:PRO:HG2	1.79	0.64
2:C:765:PRO:HD2	2:C:825:ASP:HB2	1.78	0.64
2:C:898:LEU:HB3	2:C:992:MET:HE2	1.78	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
2:C:1014:VAL:HG13	3:D:729:THR:HG21	1.80	0.64
3:D:278:ARG:O	3:D:281:ILE:HD12	1.96	0.64
3:D:585:LEU:HD12	3:D:692:GLN:NE2	2.12	0.64
3:D:668:GLY:HA2	3:D:671:MET:CE	2.27	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
1:A:95:MET:HE2	1:A:110:ILE:CG2	2.28	0.64
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:31:PRO:HB2	3:D:345:ARG:HG2	1.79	0.64
3:D:177:LEU:HD23	3:D:177:LEU:O	1.96	0.64
3:D:1266:SER:HA	3:D:1269:ARG:NH1	2.13	0.64
7:J:28:GLN:HG2	7:J:46:ASP:HA	1.80	0.64
1:B:93:VAL:HG11	1:B:116:VAL:HG11	1.80	0.64
2:C:578:VAL:HG13	2:C:582:THR:CB	2.27	0.64
2:C:1003:ASP:OD1	2:C:1006:SER:N	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:52:PHE:O	3:D:91:ARG:HD2	1.97	0.64
3:D:144:ARG:NH2	3:D:229:LEU:O	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:288:LYS:HD2	3:D:291:ARG:NH2	2.08	0.63
3:D:1122:VAL:HG23	3:D:1126:GLN:HE21	1.64	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
3:D:956:ILE:HD12	3:D:956:ILE:O	1.97	0.63
1:B:144:ARG:HB2	1:B:144:ARG:HH11	1.61	0.63
2:C:132:ASN:CB	2:C:135:THR:HG22	2.27	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:538:PRO:O	2:C:546:THR:HG23	1.99	0.63
2:C:540:ASP:CB	2:C:546:THR:HG22	2.25	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
1:B:82:GLY:CA	1:B:123:MET:HE1	2.29	0.62
2:C:87:ILE:HD12	2:C:388:GLU:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:523:THR:HG23	2:C:526:GLU:CD	2.23	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:HE3	3:D:656:LYS:N	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
2:C:33:ALA:HB2	2:C:966:PRO:HG3	1.80	0.62
2:C:328:ASP:O	2:C:332:THR:HG23	2.00	0.62
12:C:1205:SRN:C3	12:C:1205:SRN:H401	2.29	0.62
3:D:573:PRO:HG2	3:D:576:MET:HE3	1.80	0.62
3:D:648:ALA:O	3:D:652:GLU:HB2	1.99	0.62
5:F:253:MET:HE2	5:F:300:GLN:CB	2.28	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
3:D:1036:PHE:HA	3:D:1162:MET:HE1	1.82	0.62
1:A:33:THR:CG2	1:B:37:SER:HA	2.30	0.62
12:C:1205:SRN:C12	12:C:1205:SRN:C9	2.61	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
2:C:1098:VAL:HG11	3:D:469:ILE:HD12	1.81	0.62
5:F:204:LEU:HD11	5:F:211:LEU:HD21	1.81	0.62
2:C:973:GLU:O	3:D:732:MET:HE1	1.99	0.61
2:C:967:VAL:HG23	2:C:968:PHE:H	1.64	0.61
2:C:1128:VAL:HG13	2:C:1136:ILE:HB	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:272:LYS:HE2	7:J:84:MET:HE3	1.81	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
3:D:245:GLN:O	3:D:249:GLY:HA3	2.00	0.61
3:D:1132:GLN:NE2	3:D:1163:LEU:HD12	2.16	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
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: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
3:D:1220:SER:OG	3:D:1244:ASP:OD2	2.15	0.60
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:OD1	2:C:636:ASP:N	2.32	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
3:D:1168:ILE:HD13	3:D:1176:PHE:CB	2.31	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
2:C:992:MET:HA	2:C:992:MET:HE3	1.83	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
1:B:79:ASN:O	1:B:123:MET:HE2	2.02	0.60
1:B:82:GLY:HA3	1:B:123:MET:HE1	1.82	0.60
5:F:201:LEU:HD11	5:F:219:MET:CB	2.32	0.60
2:C:65:ALA:HB1	2:C:70:GLU:OE1	2.02	0.59
2:C:560:GLU:HG3	2:C:561:PHE:H	1.67	0.59
3:D:67:ARG:HG3	3:D:69:ARG:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:143:MET:HE1	3:D:250:GLU:O	2.02	0.59
3:D:951:LEU:C	3:D:956:ILE:HD11	2.26	0.59
2:C:965:THR:O	2:C:965:THR:OG1	2.19	0.59
1:A:24:GLU:CD	1:A:191:LYS:HD3	2.27	0.59
2:C:590:HIS:O	2:C:919:ILE:HD11	2.02	0.59
2:C:882:ASN:HD21	2:C:1019:MET:HE1	1.66	0.59
2:C:873:GLY:HA3	2:C:1028:VAL:HG11	1.84	0.59
2:C:899:PRO:CG	2:C:992:MET:HE1	2.32	0.59
2:C:1043:ILE:HG23	2:C:1044:THR:H	1.68	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:HE21	3:D:740:GLN:H	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:581:MET:HE3	3:D:716:LYS:CA	2.32	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:H	4:E:85:GLN:NE2	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
2:C:510:VAL:HG23	2:C:514:VAL:C	2.28	0.59
3:D:666:THR:OG1	3:D:669:ARG:HG3	2.03	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
2:C:1011:PRO:HB2	2:C:1012:TYR:HD2	1.68	0.59
3:D:155:MET:HE1	3:D:219:LEU:CD2	2.33	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:29:ARG:CD	2:C:964:ALA:HB2	2.33	0.58
2:C:436:PRO:HD2	2:C:698:CYS:HB2	1.84	0.58
2:C:1039:PRO:HB2	2:C:1048:LEU:HD21	1.84	0.58
3:D:957:THR:O	3:D:958:THR:HG23	2.03	0.58
3:D:1100:LEU:HD23	3:D:1101:SER:N	2.18	0.58
4:E:80:VAL:HG12	4:E:81:GLU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:479:THR:HG22	2:C:597:LEU:HD11	1.85	0.58
2:C:1130:SER:HB3	2:C:1133:GLY:HA3	1.84	0.58
3:D:634:LYS:HA	3:D:664:GLU:HA	1.86	0.58
3:D:668:GLY:HA2	3:D:671:MET:HE2	1.85	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
1:B:172:LEU:HD12	3:D:620:MET:SD	2.43	0.58
2:C:556:GLY:N	2:C:557:GLY:HA2	2.18	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
2:C:1059:PHE:HZ	2:C:1067:MET:HE3	1.67	0.58
3:D:581:MET:HE3	3:D:716:LYS:CB	2.34	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
2:C:508:ARG:CD	2:C:570:MET:HE2	2.33	0.58
3:D:1191:ASN:OD1	3:D:1202:ALA:HB3	2.03	0.58
2:C:45:LEU:CD2	2:C:443:LYS:HD2	2.34	0.58
2:C:240:VAL:HA	2:C:250:MET:HE1	1.85	0.58
2:C:1130:SER:HB3	2:C:1133:GLY:CA	2.34	0.58
3:D:880:SER:O	3:D:995:GLY:HA3	2.03	0.58
3:D:1086:ARG:O	3:D:1087:LEU:HD23	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:251:ARG:HB2	5:F:297:MET:HE1	1.85	0.58
5:F:276:THR:HG23	7:J:89:ARG:NH2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:498:ASN:OD1	2:C:499:PRO:HD2	2.03	0.58
2:C:622:GLU:OE1	2:C:622:GLU:N	2.37	0.58
2:C:809:GLU:O	2:C:813:ARG:HG2	2.04	0.58
2:C:1011:PRO:HB2	2:C:1012:TYR:CD2	2.39	0.58
1:A:24:GLU:OE1	1:A:191:LYS:HD3	2.03	0.57
1:A:68:GLY:HA3	1:A:129:ASN:HD21	1.69	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:50:ALA:HB3	1:B:168:TYR:HD2	1.68	0.57
1:B:95:MET:HB2	1:B:110:ILE:HD11	1.85	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
2:C:1059:PHE:CZ	2:C:1067:MET:HE3	2.39	0.57
3:D:327:MET:CE	5:F:304:ILE:HD11	2.34	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:740:GLN:O	3:D:744:ILE:HG13	2.05	0.57
3:D:1069:PRO:HB2	3:D:1073:GLY:H	1.69	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
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
3:D:1089:VAL:HG13	3:D:1098:GLY:C	2.30	0.57
3:D:1276:THR:CG2	4:E:102:GLU:HG3	2.34	0.57
2:C:432:ASP:HB2	12:C:1205:SRN:H182	1.85	0.57
3:D:951:LEU:CB	3:D:956:ILE:HD11	2.24	0.57
3:D:1088:ARG:HD2	3:D:1111:GLN:HB3	1.86	0.57
1:A:137:GLU:C	1:A:138:LEU:HD12	2.30	0.57
2:C:51:SER:HB2	2:C:371:THR:OG1	2.04	0.57
2:C:1026:HIS:HB3	2:C:1031:LYS:HE3	1.87	0.57
2:C:1029:ASP:OD1	3:D:520:LYS:HD2	2.04	0.57
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
3:D:661:TRP:CZ3	3:D:663:ALA:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:510:VAL:HG12	2:C:568:ASP:C	2.29	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:637:LYS:HD2	2:C:659:GLN:HE22	1.70	0.56
2:C:641:ILE:HG21	2:C:644:VAL:HG13	1.85	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
3:D:1071:ASP:OD2	3:D:1071:ASP:N	2.38	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
1:B:85:VAL:HG23	1:B:117:THR:C	2.30	0.56
2:C:269:TYR:CE2	2:C:278:PRO:HB3	2.39	0.56
3:D:25:TYR:C	7:J:57:ARG:HG3	2.29	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:A:30:PHE:CE1	1:B:40:ARG:HG3	2.40	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: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
1:B:95:MET:HE3	1:B:110:ILE:CD1	2.35	0.56
2:C:1041:SER:HB3	2:C:1044:THR:O	2.05	0.56
3:D:108:LYS:O	3:D:108:LYS:HG3	2.06	0.56
3:D:488:GLU:HG3	3:D:516:LEU:HD12	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
3:D:1166:VAL:HA	3:D:1207:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:J:68:ASP:HA	7:J:69:VAL:CB	2.31	0.56
2:C:602:MET:HE2	2:C:1024:LEU:HD21	1.86	0.56
2:C:875:LYS:C	2:C:876:LEU:HD12	2.30	0.56
3:D:435:GLN:OE1	3:D:435:GLN:N	2.34	0.56
3:D:656:LYS:O	3:D:656:LYS:HG2	2.05	0.56
3:D:676:LEU:HD12	3:D:676:LEU:N	2.21	0.56
5:F:462:ARG:O	5:F:462:ARG:HD3	2.05	0.56
1:A:21:PHE:HB2	1:A:194:ILE:HG12	1.86	0.56
1:B:32:TYR:CE2	1:B:178:VAL:HG21	2.41	0.56
1:B:102:PRO:HG3	1:B:131:LYS:H	1.70	0.56
2:C:508:ARG:HD3	2:C:570:MET:HE2	1.86	0.56
2:C:771:VAL:HG23	2:C:792:ILE:CD1	2.36	0.56
2:C:1048:LEU:H	2:C:1048:LEU:CD2	2.14	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
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:437:LEU:HB2	2:C:704:MET:CE	2.36	0.56
2:C:609:LEU:HD12	2:C:708:LYS:HE3	1.87	0.56
2:C:622:GLU:HB3	2:C:703:GLU:HB2	1.88	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
1:A:82:GLY:HA3	1:A:123:MET:CE	2.34	0.55
2:C:102:ARG:CG	2:C:125:PHE:HB2	2.36	0.55
2:C:1015:THR:OG1	3:D:731:SER:OG	2.24	0.55
3:D:735:VAL:HG22	3:D:798:ILE:HD11	1.88	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
2:C:852:LEU:HD23	2:C:856:VAL:HG12	1.87	0.55
2:C:1068:GLN:NE2	3:D:1249:LEU:HD13	2.22	0.55
3:D:468:ASN:OD1	3:D:470:LYS:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:PHE:HE1	2:C:380:ILE:HD11	1.71	0.55
2:C:233:GLY:HA2	2:C:261:THR:CB	2.37	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:76:GLU:CD	3:D:76:GLU:H	2.14	0.55
3:D:527:LEU:CD2	3:D:581:MET:HE1	2.29	0.55
3:D:599:TYR:CB	3:D:610:GLY:HA3	2.35	0.55
3:D:1054:VAL:CG2	3:D:1065:ILE:HG23	2.37	0.55
5:F:234:LEU:HD23	5:F:270:VAL:HG21	1.88	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:614:ALA:HB1	2:C:615:PRO:HD2	1.88	0.55
2:C:896:PRO:HB2	2:C:1001:LEU:HD13	1.87	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:O	2:C:440:LEU:HD12	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:370:ARG:HH22	2:C:452:GLY:HA3	1.72	0.55
2:C:398:GLN:HB3	2:C:403:ILE:CG2	2.37	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:693:ALA:O	3:D:697:ASN:HB2	2.05	0.55
3:D:1037:GLU:HG2	3:D:1039:ARG:NH1	2.22	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:O	2:C:714:ILE:HG22	2.07	0.55
2:C:525:ASP:OD1	2:C:525:ASP:N	2.39	0.55
2:C:931:ALA:HB1	2:C:961:SER:O	2.07	0.55
3:D:878:ASP:OD1	3:D:1215:SER:HB2	2.07	0.55
3:D:1009:LEU:CD1	3:D:1146:GLN:HG3	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1119:PRO:HA	3:D:1122:VAL:HG12	1.89	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:169:GLN:O	2:C:369:LEU:HD12	2.06	0.54
2:C:203:LEU:HD11	2:C:217:ILE:HB	1.89	0.54
2:C:390:VAL:O	2:C:394:ARG:HB2	2.07	0.54
3:D:327:MET:HE2	5:F:304:ILE:HD11	1.88	0.54
3:D:555:ALA:HA	3:D:559:MET:HE3	1.89	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
1:A:192:LEU:C	1:A:192:LEU:HD12	2.32	0.54
2:C:70:GLU:CD	2:C:70:GLU:H	2.15	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:74:ILE:HD12	7:J:42:VAL:HG13	1.89	0.54
3:D:1056:LEU:HD21	3:D:1063:PHE:CD1	2.42	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:30:VAL:HG11	2:C:954:LEU:HG	1.89	0.54
2:C:52:PHE:HZ	2:C:150:MET:HE2	1.72	0.54
2:C:346:MET:HE2	2:C:348:VAL:CG1	2.37	0.54
2:C:1129:LEU:HA	2:C:1134:ALA:O	2.07	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:448:ALA:HB1	3:D:491:ILE:HD11	1.90	0.54
3:D:1118:ASP:HB3	3:D:1121:GLU:HB2	1.88	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:H	2:C:919:ILE:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:ALA:HB2	14:D:2104:HOH:O	2.07	0.54
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:OD2	5:F:370:ASP:N	2.29	0.54
1:B:137:GLU:C	1:B:138:LEU:HD12	2.33	0.54
11:C:1207:EDO:O2	5:F:322:ARG:HD2	2.07	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
3:D:578:ARG:HB2	11:D:2007:EDO:C2	2.38	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
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
1:B:183:VAL:HG13	3:D:488:GLU:OE2	2.08	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
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:736:LEU:H	3:D:792:TYR:HH	1.54	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: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
3:D:1009:LEU:HB3	3:D:1029:LEU:HD13	1.90	0.53
2:C:32:PHE:O	2:C:34:LYS:HD2	2.09	0.53
2:C:240:VAL:HA	2:C:250:MET:SD	2.49	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:272:LEU:C	2:C:274:PRO:HD3	2.34	0.53
2:C:280:LYS:NZ	2:C:280:LYS:HB3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:938:GLU:OE1	3:D:938:GLU:N	2.33	0.53
3:D:1181:LEU:CD1	3:D:1213:LYS:HE2	2.38	0.53
1:A:193:ILE:HD12	1:A:193:ILE:O	2.09	0.53
2:C:602:MET:HE1	2:C:883:LYS:CB	2.31	0.53
2:C:946:TRP:CE2	2:C:978:GLY:HA3	2.44	0.53
2:C:1127:GLU:OE1	3:D:11:ARG:NH2	2.35	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:299:LEU:CB	2:C:323:THR:HB	2.36	0.53
2:C:1103:ILE:N	10:C:1206:SO4:O3	2.41	0.53
3:D:58:TRP:HZ3	3:D:71:LYS:HB2	1.74	0.53
3:D:1119:PRO:HA	3:D:1122:VAL:CG1	2.38	0.53
4:E:26:TYR:CE1	4:E:29:PRO:HD3	2.44	0.53
5:F:423:GLN:HG3	5:F:423:GLN:O	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:910:ILE:HG23	3:D:910:ILE:O	2.08	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
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:510:VAL:HG11	2:C:567:VAL:HG12	1.91	0.52
2:C:935:TRP:C	2:C:983:THR:HG23	2.34	0.52
2:C:1103:ILE:HD12	3:D:548:SER:HA	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:THR:HA	1:A:125:ILE:HD13	1.91	0.52
1:B:56:ILE:O	1:B:56:ILE:HD12	2.09	0.52
2:C:720:HIS:CE1	2:C:888:LYS:HD3	2.43	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
3:D:1168:ILE:HD11	3:D:1182:THR:HG21	1.90	0.52
5:F:274:ASP:CG	7:J:89:ARG:HH22	2.15	0.52
1:B:151:GLN:OE1	1:B:151:GLN:N	2.37	0.52
2:C:652:MET:CE	2:C:658:ARG:HD2	2.40	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
5:F:251:ARG:CB	5:F:297:MET:HE1	2.39	0.52
2:C:224:PRO:HG2	2:C:227:VAL:HG11	1.91	0.52
3:D:981:SER:HB3	3:D:984:THR:HG1	1.75	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:545:PHE:HD2	2:C:564:ALA:HB1	1.70	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:HA	2:C:534:GLN:NE2	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:162:ILE:CG2	3:D:607:PRO:HG2	2.40	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:593:ALA:HB2	3:D:852:THR:HG22	1.92	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
3:D:875:ARG:HH22	3:D:1033:GLN:CD	2.18	0.52
1:A:54:ILE:C	1:A:54:ILE:HD12	2.35	0.52
2:C:792:ILE:HD12	2:C:792:ILE:N	2.25	0.52

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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:130:TYR:O	3:D:372:ARG:HD3	2.09	0.51
3:D:155:MET:HE1	3:D:219:LEU:HD22	1.92	0.51
3:D:578:ARG:HB2	11:D:2007:EDO:H21	1.92	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: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
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: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:1112:PHE:CE2	3:D:1255:ILE:HG22	2.46	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: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
2:C:1078:GLU:HG3	2:C:1082:ILE:HD11	1.91	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
2:C:851:GLU:C	2:C:852:LEU:HD12	2.35	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
3:D:736:LEU:HB2	3:D:792:TYR:CE2	2.45	0.51
3:D:1054:VAL:HG12	3:D:1104:ASP:O	2.11	0.51
5:F:462:ARG:HH12	5:F:465:LEU:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:745:LEU:O	3:D:749:GLU:HG2	2.11	0.51
3:D:1034:GLU:OE2	3:D:1041:PRO:HA	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:150:THR:O	3:D:154:GLU:HG3	2.10	0.51
3:D:327:MET:HE1	5:F:304:ILE:CG1	2.41	0.51
3:D:915:VAL:O	3:D:920:PHE:HD2	1.94	0.51
3:D:1088:ARG:HG2	3:D:1089:VAL:N	2.22	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
2:C:777:GLU:CD	2:C:777:GLU:H	2.18	0.50
3:D:432:VAL:CG2	3:D:434:PRO:HD3	2.32	0.50
3:D:444:PRO:HD2	3:D:447:MET:HE2	1.92	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:882:ASN:ND2	2:C:1019:MET:HE1	2.26	0.50
2:C:892:VAL:HG22	2:C:903:PRO:HG2	1.94	0.50
2:C:992:MET:HE3	2:C:992:MET:CA	2.40	0.50
3:D:119:ASP:C	3:D:120:LEU:HD12	2.36	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:2:LEU:HD12	1:B:143:GLY:CA	2.41	0.50
1:A:177:LYS:HG2	1:A:193:ILE:HD11	1.93	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:43:LYS:O	3:D:44:ASP:HB2	2.11	0.50
3:D:281:ILE:HG22	3:D:289:LYS:HG3	1.93	0.50
1:B:74:THR:HG21	3:D:608:GLU:OE1	2.12	0.50
2:C:132:ASN:CG	2:C:135:THR:HG22	2.37	0.50
2:C:442:HIS:O	2:C:445:ARG:HB2	2.11	0.50
2:C:446:LEU:N	2:C:446:LEU:HD23	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:449:LEU:HD12	2:C:449:LEU:N	2.27	0.50
2:C:1026:HIS:HB3	2:C:1031:LYS:CE	2.41	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
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:66:LYS:HG2	3:D:66:LYS:O	2.11	0.50
3:D:1136:VAL:HG22	3:D:1155:ILE:HG22	1.93	0.50
2:C:176:VAL:O	2:C:176:VAL:HG23	2.11	0.50
2:C:709:ASN:C	2:C:710:LEU:HD12	2.36	0.50
7:J:97:LEU:HD23	7:J:97:LEU:O	2.10	0.50
1:A:84:VAL:HG12	1:A:120:ASN:CG	2.37	0.50
2:C:202:TRP:H	2:C:202:TRP:CD1	2.29	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:O	4:E:57:ARG:HD3	2.11	0.50
8:O:15:DT:OP2	8:O:15:DT:H6	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:336:LEU:O	2:C:336:LEU:HD23	2.11	0.50
2:C:627:ILE:HD12	2:C:628:ASP:N	2.27	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
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
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: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
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.93	0.49
3:D:1044:LYS:HE3	3:D:1118:ASP:HB2	1.93	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
2:C:477:ILE:HD11	3:D:852:THR:HG21	1.94	0.49
3:D:20:ILE:HG23	3:D:318:PRO:HB3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:54:TRP:HD1	2:C:61:TRP:CZ2	2.31	0.49
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: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:1081:LEU:HB3	3:D:1113:MET:HE1	1.94	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
3:D:460:LEU:C	3:D:460:LEU:HD12	2.38	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:299:LEU:C	2:C:299:LEU:HD12	2.37	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:287:GLN:CG	3:D:288:LYS:HZ2	2.26	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
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: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
3:D:1153:LYS:O	3:D:1157:VAL:HG23	2.13	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
2:C:1045:GLN:HG2	2:C:1087:THR:CG2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:873:THR:O	3:D:877:VAL:HG23	2.13	0.49
1:A:63:PHE:CE1	2:C:741:ILE:HD13	2.47	0.49
2:C:102:ARG:O	2:C:124:LEU:HD23	2.13	0.49
2:C:510:VAL:HG12	2:C:568:ASP:O	2.13	0.49
2:C:916:ARG:NH2	10:C:1201:SO4:O1	2.45	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:A:149:ALA:HB2	1:A:164:VAL:C	2.38	0.49
1:B:105:VAL:HG12	1:B:125:ILE:HG21	1.94	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:911:ARG:NH1	3:D:949:ASP:OD1	2.32	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
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: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
2:C:1084:SER:OG	2:C:1085:ASP:N	2.46	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:32:TYR:CE1	2:C:1005:ARG:HD3	2.48	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
2:C:477:ILE:CD1	3:D:852:THR:HG21	2.43	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
8:O:31:DT:H5'	8:O:31:DT:C6	2.48	0.48
2:C:174:PRO:O	2:C:303:GLY:HA2	2.13	0.48
2:C:665:LYS:NZ	2:C:677:GLN:O	2.41	0.48
2:C:751:ARG:HG2	2:C:856:VAL:HG22	1.93	0.48
2:C:788:ARG:O	2:C:830:VAL:HG11	2.13	0.48
1:B:87:SER:HB3	1:B:116:VAL:HG12	1.96	0.48
3:D:452:PHE:CE1	3:D:491:ILE:HG12	2.48	0.48
3:D:622:MET:HE3	3:D:667:LEU:CD1	2.25	0.48
5:F:170:LEU:HA	5:F:173:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:277:LYS:HB3	5:F:279:TYR:CD2	2.48	0.48
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:641:ARG:O	3:D:682:PHE:HB2	2.13	0.48
3:D:972:GLY:HA2	10:D:2004:SO4:O2	2.14	0.48
1:A:146:TYR:CG	2:C:734:GLU:HG2	2.48	0.48
2:C:148:PHE:HD2	2:C:150:MET:HE3	1.79	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:OE1	2:C:70:GLU:N	2.46	0.48
2:C:712:VAL:CG1	2:C:925:THR:HG23	2.44	0.48
3:D:231:PRO:O	3:D:232:LYS:HB2	2.12	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
5:F:219:MET:HA	5:F:219:MET:CE	2.36	0.48
7:J:74:LYS:O	7:J:74:LYS:HG3	2.14	0.48
1:B:113:PRO:HD2	1:B:116:VAL:HG21	1.96	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:1070:TYR:CD1	3:D:559:MET:HG2	2.48	0.48
3:D:480:ARG:HB3	3:D:482:GLN:OE1	2.13	0.48
1:A:9:LEU:HD23	1:B:221:LEU:C	2.38	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:58:TRP:CZ3	3:D:71:LYS:HE3	2.49	0.48
3:D:1123:LEU:HD22	3:D:1208:LEU:HB2	1.95	0.48
5:F:306:ILE:CG2	5:F:310:MET:HB3	2.44	0.48
1:B:111:VAL:O	1:B:111:VAL:HG13	2.14	0.47
2:C:572:VAL:O	2:C:573:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:614:ALA:HA	2:C:705:ALA:CB	2.44	0.47
2:C:876:LEU:HD12	2:C:876:LEU:N	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
3:D:664:GLU:HG3	3:D:664:GLU:O	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:39:ARG:O	1:A:43:LEU:HD13	2.14	0.47
1:A:210:SER:HB3	1:B:229:SER:HB2	1.96	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: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
2:C:431:MET:HE3	2:C:443:LYS:HZ3	1.79	0.47
1:B:32:TYR:CZ	2:C:1005:ARG:HD3	2.49	0.47
2:C:236:ASN:HA	2:C:239:ILE:CD1	2.44	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
3:D:651:PHE:C	3:D:653:ASN:H	2.22	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
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:B:22:VAL:CG1	1:B:193:ILE:HD12	2.44	0.47
2:C:148:PHE:CE1	2:C:380:ILE:HD11	2.50	0.47
2:C:224:PRO:HB2	2:C:227:VAL:CG1	2.32	0.47
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
2:C:732:LEU:HA	2:C:737:VAL:HG12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:997:GLY:O	2:C:1015:THR:HG23	2.14	0.47
2:C:1028:VAL:HG12	3:D:429:VAL:HG12	1.95	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
3:D:694:ARG:CZ	3:D:694:ARG:HB3	2.45	0.47
3:D:1081:LEU:HB3	3:D:1113:MET:CE	2.45	0.47
5:F:234:LEU:CD2	5:F:270:VAL:HG21	2.44	0.47
8:O:28:DT:H2'	8:O:29:DA:C8	2.49	0.47
1:A:111:VAL:O	1:A:111:VAL:CG2	2.62	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
2:C:1137:GLU:OE1	2:C:1137:GLU:N	2.44	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
5:F:462:ARG:HD3	5:F:462:ARG:C	2.38	0.47
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.50	0.47
1:B:213:GLY:HA2	1:B:216:VAL:HG12	1.97	0.47
2:C:85:SER:HA	2:C:86:PRO:HA	1.70	0.47
2:C:412:ARG:HD2	5:F:322:ARG:NE	2.30	0.47
2:C:708:LYS:NZ	2:C:737:VAL:O	2.42	0.47
2:C:712:VAL:HA	2:C:906:ILE:HG13	1.96	0.47
3:D:22:ASN:HA	7:J:57:ARG:HH12	1.79	0.47
3:D:822:LEU:HD23	3:D:834:PRO:CA	2.42	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
5:F:366:GLY:C	5:F:369:GLY:H	2.23	0.47
1:A:40:ARG:CD	1:B:33:THR:HG22	2.40	0.46
1:A:152:ASN:HD21	2:C:837:LYS:HZ3	1.63	0.46
1:B:52:THR:HG21	1:B:141:GLU:OE2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:727:ILE:HA	2:C:888:LYS:O	2.15	0.46
3:D:28:VAL:O	3:D:28:VAL:HG22	2.15	0.46
3:D:278:ARG:HH11	3:D:278:ARG:HG3	1.80	0.46
3:D:642:PRO:HD3	3:D:656:LYS:CE	2.45	0.46
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:36:ASN:CB	2:C:1007:GLY:HA3	2.44	0.46
1:A:43:LEU:HD11	1:A:174:VAL:HB	1.96	0.46
1:A:172:LEU:C	1:A:172:LEU:HD23	2.41	0.46
1:B:147:VAL:HG13	1:B:147:VAL:O	2.16	0.46
1:B:226:ASN:O	1:B:227:ALA:HB3	2.15	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:650:LEU:HD13	3:D:651:PHE:CE2	2.49	0.46
3:D:825:ASN:CB	3:D:826:PRO:HD2	2.46	0.46
4:E:45:SER:OG	4:E:105:GLU:OE2	2.31	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:35:LEU:HD13	2:C:969:ASP:OD2	2.15	0.46
2:C:41:VAL:HG13	2:C:493:VAL:CG1	2.45	0.46
2:C:572:VAL:HG22	2:C:576:GLN:CD	2.41	0.46
3:D:961:VAL:HG22	3:D:962:ARG:N	2.30	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:508:ARG:HD2	2:C:570:MET:HE2	1.98	0.46
2:C:565:ASP:OD1	2:C:566:GLN:N	2.48	0.46
2:C:801:GLY:O	2:C:802:GLU:C	2.58	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: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:HD23	2:C:623:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:HG13	3:D:488:GLU:CD	2.41	0.46
2:C:52:PHE:CZ	2:C:150:MET:HE2	2.51	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:589:GLU:HB3	2:C:968:PHE:CD1	2.51	0.46
2:C:805:LEU:HD22	2:C:805:LEU:N	2.31	0.46
2:C:822:GLU:CD	2:C:822:GLU:H	2.24	0.46
2:C:882:ASN:HD21	2:C:1019:MET:CE	2.29	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:O	2:C:344:THR:HG22	2.16	0.46
2:C:454:LEU:HD23	2:C:454:LEU:O	2.16	0.46
3:D:262:LYS:CG	3:D:310:MET:HE1	2.42	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:215:VAL:HG22	2:C:225:VAL:N	2.29	0.46
2:C:898:LEU:HD23	2:C:1001:LEU:CD2	2.46	0.46
2:C:1126:VAL:HG23	2:C:1126:VAL:O	2.16	0.46
3:D:900:LEU:O	3:D:901:ALA:HB2	2.15	0.46
3:D:1132:GLN:CD	3:D:1163:LEU:HD12	2.41	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
2:C:859:LEU:C	2:C:859:LEU:HD13	2.40	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:55:LEU:HD22	2:C:376:ILE:HB	1.98	0.45
2:C:217:ILE:O	2:C:217:ILE:HG13	2.14	0.45
2:C:708:LYS:HG3	2:C:737:VAL:HG23	1.98	0.45
2:C:716:PRO:HB3	2:C:909:ASN:OD1	2.16	0.45
2:C:1043:ILE:HD13	3:D:412:ARG:HH22	1.81	0.45
3:D:91:ARG:O	3:D:321:PRO:HG3	2.16	0.45
3:D:633:ILE:C	3:D:633:ILE:HD12	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:614:ALA:H	2:C:700:GLN:NE2	2.14	0.45
2:C:1138:MET:C	2:C:1139:ARG:HG3	2.41	0.45
3:D:31:PRO:HB3	3:D:348:ILE:HG23	1.99	0.45
3:D:285:LYS:HA	3:D:289:LYS:HB2	1.99	0.45
3:D:929:VAL:HG23	3:D:929:VAL:O	2.16	0.45
3:D:1062:PHE:CE1	3:D:1080:LYS:HB3	2.51	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
5:F:231:ASN:O	5:F:235:GLU:HG3	2.16	0.45
1:T:269:VAL:O	1:T:269:VAL:HG23	2.16	0.45
2:C:754:LYS:HD3	3:D:39:LEU:CD1	2.46	0.45
2:C:967:VAL:HG23	2:C:968:PHE:N	2.31	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
3:D:1140:GLN:NE2	3:D:1155:ILE:HD12	2.32	0.45
5:F:325:LEU:O	5:F:325:LEU:HD23	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:708:LYS:HG3	2:C:737:VAL:CG2	2.46	0.45
3:D:568:PRO:HB3	3:D:983:ALA:HB2	1.98	0.45
3:D:582:VAL:HB	3:D:806:ALA:HB2	1.99	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
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: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:HD12	1:B:138:LEU:N	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:622:MET:HE1	3:D:629:VAL:HG13	1.99	0.45
3:D:711:THR:O	3:D:715:LEU:HG	2.17	0.45
7:J:106:LYS:HA	7:J:106:LYS:CE	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
2:C:895:MET:HE2	2:C:895:MET:HB2	1.78	0.45
3:D:320:ILE:CG1	3:D:321:PRO:HD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:PHE:HE1	1:B:44:SER:HB3	1.81	0.45
1:A:54:ILE:HD12	1:A:54:ILE:O	2.17	0.45
1:A:125:ILE:N	1:A:125:ILE:HD12	2.31	0.45
1:B:34:LEU:C	1:B:34:LEU:HD12	2.42	0.45
1:B:174:VAL:HA	1:B:195:ASP:O	2.16	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:OD1	2:C:945:ASP:N	2.48	0.45
2:C:1128:VAL:HG11	2:C:1138:MET:CE	2.30	0.45
3:D:47:PHE:CD1	3:D:322:PRO:HB3	2.52	0.45
3:D:1132:GLN:CG	3:D:1163:LEU:HD12	2.46	0.45
5:F:440:ARG:O	5:F:444:ILE:HG13	2.16	0.45
7:J:106:LYS:HE2	7:J:106:LYS:CA	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
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:44:LEU:HD13	2:C:440:LEU:HD21	1.98	0.45
2:C:197:PRO:HG3	2:C:297:TYR:CE1	2.51	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:602:ALA:CB	3:D:607:PRO:O	2.65	0.45
5:F:348:VAL:O	5:F:352:GLN:HG3	2.17	0.45
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.87	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:HG2	2:C:949:LYS:O	2.17	0.44
2:C:1048:LEU:HD23	2:C:1048:LEU:N	2.19	0.44
3:D:191:SER:O	3:D:195:ARG:HG2	2.17	0.44
3:D:203:ARG:NE	3:D:203:ARG:HA	2.31	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:295:ARG:NH2	8:O:24:DG:O6	2.50	0.44
5:F:465:LEU:O	5:F:466:ASP:HB2	2.16	0.44
1:A:54:ILE:CD1	1:A:162:ILE:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLY:HA2	1:B:216:VAL:CG1	2.48	0.44
2:C:51:SER:OG	2:C:371:THR:HG23	2.17	0.44
2:C:231:ALA:HB1	2:C:287:LEU:HD11	1.99	0.44
2:C:575:ARG:HE	2:C:967:VAL:CG2	2.24	0.44
2:C:627:ILE:HD12	2:C:627:ILE:C	2.43	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:O	5:F:317:LEU:HD23	2.17	0.44
2:C:203:LEU:C	2:C:204:GLU:HG3	2.41	0.44
2:C:885:VAL:CG1	3:D:538:GLY:HA2	2.47	0.44
2:C:1015:THR:HG1	3:D:731:SER:HG	1.66	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:CZ	2:C:199:ARG:HB3	2.47	0.44
2:C:335:TYR:O	2:C:335:TYR:HD1	2.00	0.44
2:C:744:GLU:HG3	2:C:834:GLU:OE2	2.18	0.44
3:D:106:TYR:HB3	3:D:312:MET:CE	2.34	0.44
3:D:177:LEU:HD23	3:D:177:LEU:C	2.42	0.44
3:D:240:LEU:HD23	3:D:240:LEU:C	2.43	0.44
3:D:525:HIS:O	3:D:528:VAL:HG22	2.18	0.44
3:D:1056:LEU:HD23	3:D:1057:GLU:H	1.82	0.44
1:B:77:ILE:O	1:B:81:LYS:HG3	2.17	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
2:C:1031:LYS:NZ	10:C:1203:SO4:S	2.90	0.44
3:D:79:GLY:HA2	7:J:54:TRP:CH2	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:HA	5:F:214:GLN:NE2	2.33	0.44
1:A:93:VAL:HG22	1:A:113:PRO:HG2	2.00	0.44
1:B:29:GLY:HA2	1:B:190:ASP:OD2	2.17	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
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:293:LEU:HD23	3:D:293:LEU:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:141:GLN:CD	2:C:406:GLN:HG2	2.42	0.44
3:D:622:MET:CE	3:D:629:VAL:HG13	2.48	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
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
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
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
1:A:124:HIS:C	1:A:125:ILE:HD12	2.43	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: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:706:ILE:CD1	4:E:36:PRO:HB3	2.47	0.44
3:D:737:VAL:HG13	3:D:738:PRO:HD2	2.00	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
1:A:147:VAL:HG13	1:A:147:VAL:O	2.18	0.43
2:C:47:VAL:HG23	2:C:497:VAL:HG21	2.00	0.43
2:C:77:LEU:HD23	2:C:77:LEU:HA	1.85	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:664:ARG:HB2	2:C:677:GLN:OE1	2.18	0.43
2:C:726:ILE:HG23	2:C:908:LEU:HD23	2.00	0.43
2:C:753:THR:HG23	2:C:756:GLY:C	2.43	0.43
2:C:1138:MET:O	2:C:1139:ARG:HG3	2.18	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:HG12	7:J:69:VAL:O	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:96:LEU:C	2:C:96:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:ILE:O	5:F:304:ILE:HG23	2.18	0.43
3:D:46:LEU:O	3:D:47:PHE:HB2	2.18	0.43
3:D:106:TYR:CB	3:D:312:MET:HE3	2.35	0.43
3:D:354:LEU:O	3:D:358:ILE:HG12	2.19	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
2:C:228:LEU:HD23	2:C:228:LEU:HA	1.89	0.43
2:C:445:ARG:NE	12:C:1205:SRN:O6	2.31	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
3:D:668:GLY:HA2	3:D:671:MET:HE3	1.99	0.43
3:D:885:VAL:O	3:D:990:ILE:O	2.36	0.43
7:J:65:ILE:O	7:J:65:ILE:HG22	2.19	0.43
2:C:53:GLU:O	2:C:57:GLY:N	2.52	0.43
2:C:476:PRO:HG3	2:C:577:MET:HE3	2.01	0.43
2:C:917:MET:HE2	3:D:839:PHE:CD2	2.52	0.43
3:D:612:TYR:HB2	3:D:635:VAL:CG1	2.48	0.43
3:D:813:THR:O	3:D:813:THR:HG22	2.17	0.43
3:D:1009:LEU:HD12	3:D:1146:GLN:CG	2.38	0.43
1:B:139:VAL:HG21	1:B:161:ARG:HH21	1.83	0.43
2:C:361:ILE:HD12	2:C:361:ILE:N	2.28	0.43
2:C:891:PRO:CB	2:C:893:GLU:HG2	2.37	0.43
3:D:591:LEU:HD22	3:D:592:VAL:N	2.33	0.43
3:D:1004:GLU:N	3:D:1005:PRO:HD2	2.34	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:398:GLN:HB3	2:C:398:GLN:HE21	1.57	0.43
2:C:563:SER:O	2:C:564:ALA:HB3	2.18	0.43
2:C:780:ILE:O	2:C:780:ILE:HG13	2.19	0.43
2:C:797:VAL:HG13	2:C:824:ARG:O	2.18	0.43
2:C:1043:ILE:HG23	2:C:1044:THR:N	2.31	0.43
3:D:536:PHE:C	3:D:538:GLY:H	2.27	0.43
3:D:581:MET:CE	3:D:716:LYS:HA	2.45	0.43
3:D:641:ARG:HA	3:D:656:LYS:HZ1	1.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:800:LYS:HG3	2:C:801:GLY:N	2.34	0.43
2:C:879:ARG:NH2	2:C:1020:TYR:HB3	2.34	0.43
12:C:1205:SRN:H181	12:C:1205:SRN:H152	1.70	0.43
3:D:869:SER:HB2	3:D:1029:LEU:HD21	2.00	0.43
3:D:1161:GLN:HA	3:D:1164:ARG:HD3	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:718:GLU:H	3:D:724:THR:CG2	2.32	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
3:D:884:ILE:HD12	3:D:885:VAL:C	2.44	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:94:MET:HE3	2:C:395:MET:HB3	2.00	0.43
2:C:728:LEU:HB2	2:C:889:ILE:HG12	2.00	0.43
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:602:ALA:HB3	3:D:607:PRO:C	2.44	0.42
3:D:921:ALA:HB3	3:D:1151:HIS:NE2	2.34	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
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
2:C:1012:TYR:CG	3:D:727:GLY:HA3	2.54	0.42
3:D:331:ASP:OD1	3:D:331:ASP:N	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
5:F:246:LYS:HE2	5:F:246:LYS:HB3	1.80	0.42
1:A:36:ASN:HB3	2:C:1007:GLY:HA3	2.00	0.42
1:A:50:ALA:HB3	1:A:168:TYR:CE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:772:LEU:HD12	2:C:772:LEU:N	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
3:D:590:THR:HG23	3:D:630:ARG:HE	1.84	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:155:MET:HE2	3:D:219:LEU:O	2.20	0.42
3:D:880:SER:HB3	3:D:1158:ILE:HD13	2.02	0.42
1:A:2:LEU:HD13	1:B:142:ARG:CB	2.50	0.42
1:A:193:ILE:HD12	1:A:193:ILE:C	2.44	0.42
1:B:96:TYR:O	1:B:110:ILE:HG13	2.19	0.42
1:B:150:VAL:HG13	1:B:150:VAL:O	2.19	0.42
2:C:193:VAL:CG1	2:C:336:LEU:HD12	2.49	0.42
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:327:MET:HE1	5:F:304:ILE:HD11	2.01	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:180:GLU:HG3	2:C:180:GLU:O	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:HD23	2:C:976:LEU:HA	1.83	0.42
2:C:1036:SER:HB3	3:D:450:GLU:O	2.20	0.42
3:D:92:MET:HG2	3:D:321:PRO:HD3	2.01	0.42
3:D:706:ILE:CD1	4:E:36:PRO:HA	2.50	0.42
3:D:899:THR:HA	3:D:958:THR:HG22	2.00	0.42
8:O:16:DT:H5'	8:O:16:DT:H6	1.84	0.42
1:B:56:ILE:HG23	1:B:136:VAL:HG23	2.01	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
2:C:1037:THR:HG22	2:C:1038:GLY:N	2.35	0.42
3:D:269:ASP:HB3	3:D:272:ALA:CB	2.42	0.42
3:D:656:LYS:H	3:D:656:LYS:CD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:1035:ARG:HD3	2:C:1056:GLY:CA	2.50	0.42
2:C:1108:ILE:HD12	2:C:1108:ILE:N	2.28	0.42
3:D:927:ASP:OD1	3:D:938:GLU:HA	2.19	0.42
5:F:416:ARG:HA	5:F:430:ILE:HD11	2.02	0.42
1:B:41:THR:HG22	1:B:211:ALA:HB1	2.00	0.42
1:B:143:GLY:HA3	1:B:168:TYR:CE1	2.55	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
2:C:723:GLU:HB3	3:D:536:PHE:HD1	1.85	0.42
3:D:417:LEU:HD12	3:D:417:LEU:HA	1.75	0.42
3:D:581:MET:HE3	3:D:716:LYS:HB2	2.02	0.42
3:D:890:CYS:O	3:D:891:GLU:HB2	2.19	0.42
5:F:283:THR:OG1	8:O:29:DA:H8	2.03	0.42
1:A:8:THR:OG1	1:A:24:GLU:O	2.35	0.41
1:B:147:VAL:HG11	1:B:168:TYR:CZ	2.55	0.41
2:C:481:GLU:HG2	2:C:597:LEU:CD2	2.50	0.41
2:C:541:GLU:C	2:C:543:GLY:H	2.26	0.41
2:C:1093:VAL:O	2:C:1097:ILE:HG13	2.20	0.41
12:C:1205:SRN:O1	12:C:1205:SRN:C4	2.66	0.41
3:D:58:TRP:HA	3:D:82:VAL:HG23	2.01	0.41
3:D:397:ARG:HH21	5:F:360:SER:CB	2.33	0.41
3:D:417:LEU:CG	3:D:1254:ILE:HG23	2.42	0.41
3:D:1035:LEU:HD11	3:D:1138:GLU:HB3	2.02	0.41
5:F:313:VAL:CG2	5:F:351:ILE:HD13	2.50	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
1:B:183:VAL:HG22	3:D:488:GLU:CD	2.45	0.41
2:C:170:LEU:N	2:C:447:SER:O	2.43	0.41
2:C:294:GLU:OE1	2:C:295:LYS:N	2.53	0.41
2:C:691:GLN:HG2	2:C:692:VAL:N	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:367:ARG:NH2	2:C:448:ALA:HB2	2.35	0.41
2:C:911:HIS:CE1	3:D:580:ASP:HA	2.55	0.41
3:D:413:PHE:CD2	3:D:1226:SER:HB3	2.54	0.41
3:D:646:LEU:HD23	3:D:646:LEU:C	2.45	0.41
3:D:650:LEU:HB3	3:D:651:PHE:CD2	2.55	0.41
3:D:687:MET:HE2	3:D:695:ILE:CD1	2.50	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
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:95:MET:HE3	1:B:110:ILE:HD11	2.01	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
3:D:133:ALA:C	3:D:256:MET:HE3	2.44	0.41
3:D:320:ILE:HG12	3:D:321:PRO:CD	2.49	0.41
3:D:613:SER:N	3:D:617:GLU:OE1	2.50	0.41
3:D:1132:GLN:HG3	3:D:1163:LEU:CD1	2.50	0.41
3:D:1271:ILE:HG12	4:E:105:GLU:HA	2.02	0.41
5:F:272:LYS:HB2	7:J:84:MET:CE	2.50	0.41
5:F:321:GLN:NE2	5:F:331:GLU:OE2	2.54	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:441:THR:CB	2:C:604:ARG:HD3	2.51	0.41
2:C:601:ASN:O	2:C:605:GLN:HG3	2.21	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
3:D:884:ILE:HD12	3:D:884:ILE:C	2.45	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:118:MET:HE2	2:C:118:MET:HB3	1.93	0.41
2:C:199:ARG:HB3	2:C:199:ARG:NH1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:41:VAL:HG13	2:C:493:VAL:HG12	2.02	0.41
2:C:150:MET:HA	2:C:150:MET:CE	2.42	0.41
2:C:1122:LEU:HD12	2:C:1122:LEU:HA	1.80	0.41
3:D:676:LEU:HD12	3:D:676:LEU:H	1.83	0.41
3:D:1045:ALA:HA	3:D:1046:PRO:HD3	1.92	0.41
3:D:1100:LEU:HD23	3:D:1100:LEU:C	2.46	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:51:SER:CB	2:C:371:THR:OG1	2.69	0.41
2:C:433:GLN:HE21	2:C:670:ASN:H	1.68	0.41
2:C:597:LEU:HD23	2:C:597:LEU:C	2.45	0.41
2:C:641:ILE:CG2	2:C:644:VAL:HG13	2.50	0.41
2:C:1117:LYS:HA	2:C:1117:LYS:HD2	1.71	0.41
3:D:28:VAL:HG21	3:D:46:LEU:CD2	2.46	0.41
3:D:236:VAL:HG12	3:D:236:VAL:O	2.20	0.41
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:A:33:THR:HG22	1:B:37:SER:HA	2.03	0.41
1:B:34:LEU:CD1	1:B:192:LEU:HD22	2.51	0.41
1:B:47:PRO:HB3	1:B:144:ARG:HD2	2.03	0.41
1:B:63:PHE:CE1	3:D:604:LYS:HA	2.56	0.41
1:B:210:SER:O	1:B:214:THR:HG23	2.20	0.41
2:C:446:LEU:HD21	2:C:491:LEU:N	2.36	0.41
2:C:464:ARG:HG2	2:C:485:ILE:O	2.21	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:54:PRO:HG3	3:D:81:GLU:O	2.20	0.41
3:D:143:MET:HG2	3:D:251:TYR:CD1	2.55	0.41
3:D:183:GLU:O	3:D:187:GLU:HG2	2.21	0.41
3:D:237:ASP:OD2	3:D:240:LEU:HB2	2.21	0.41
3:D:285:LYS:HG3	3:D:289:LYS:CD	2.51	0.41
3:D:321:PRO:HD2	3:D:324:LEU:HD12	2.02	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
3:D:796:ASN:ND2	3:D:798:ILE:H	2.19	0.41
3:D:920:PHE:CZ	3:D:948:ILE:HG13	2.56	0.41
3:D:1208:LEU:HD23	3:D:1208:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:67:ARG:NH1	5:F:423:GLN:HA	2.36	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:O	3:D:939:ARG:HG3	2.21	0.41
3:D:1162:MET:HE2	3:D:1211:ILE:HG23	2.03	0.41
5:F:230:LYS:O	5:F:234:LEU:HG	2.21	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
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:59:GLU:HG2	3:D:66:LYS:HG3	2.03	0.40
3:D:541:MET:HE2	3:D:541:MET:HB3	1.99	0.40
3:D:1009:LEU:CD2	3:D:1029:LEU:HD12	2.51	0.40
4:E:76:VAL:HG13	4:E:77:GLY:N	2.36	0.40
8:O:16:DT:H5'	8:O:16:DT:C6	2.56	0.40
1:B:202:ILE:HG12	1:B:206:ASP:HB2	2.03	0.40
2:C:852:LEU:HD22	2:C:856:VAL:O	2.21	0.40
2:C:1034:ALA:O	2:C:1054:PHE:HE2	2.04	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: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: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:650:LEU:HD11	3:D:661:TRP:HB2	2.02	0.40
3:D:1010:THR:O	3:D:1011:MET:CB	2.70	0.40
3:D:1081:LEU:HD22	3:D:1081:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:31:SER:HA	2:C:964:ALA:O	2.20	0.40
2:C:171:VAL:HG12	2:C:172:ARG:N	2.36	0.40
2:C:481:GLU:HG2	2:C:597:LEU:HD21	2.03	0.40
2:C:512:ASN:O	2:C:512:ASN:ND2	2.55	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:1012:TYR:HB3	2:C:1013:PRO:HD2	2.03	0.40
3:D:34:ILE:HG22	3:D:41:PRO:HA	2.02	0.40
3:D:302:PHE:CE2	3:D:309:PRO:HA	2.57	0.40
3:D:505:HIS:HD2	3:D:1004:GLU:HG3	1.87	0.40
3:D:704:PRO:HD2	3:D:707:VAL:CG2	2.51	0.40
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:A:95:MET:HE2	1:A:110:ILE:HG21	2.00	0.40
1:A:100:GLN:HG3	1:A:101:GLY:N	2.36	0.40
1:A:174:VAL:O	2:C:901:GLY:HA3	2.22	0.40
1:B:202:ILE:HD11	1:B:206:ASP:C	2.47	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
2:C:728:LEU:HD23	2:C:906:ILE:HG22	2.02	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
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.87	0.40
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.93	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
4:E:75:TYR:O	4:E:76:VAL:HB	2.22	0.40
5:F:219:MET:HE2	5:F:219:MET:CA	2.39	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/350 (61%)	202 (94%)	12 (6%)	0	100	100
1	B	231/350 (66%)	211 (91%)	19 (8%)	1 (0%)	30	60
1	T	51/350 (15%)	51 (100%)	0	0	100	100
2	C	1093/1169 (94%)	1040 (95%)	52 (5%)	1 (0%)	48	77
3	D	1234/1317 (94%)	1181 (96%)	51 (4%)	2 (0%)	43	71
4	E	72/107 (67%)	66 (92%)	4 (6%)	2 (3%)	4	19
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%)	43	71

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%)	162 (93%)	12 (7%)	14	40
1	B	173/297 (58%)	154 (89%)	19 (11%)	6	23
1	T	26/297 (9%)	25 (96%)	1 (4%)	29	58
2	C	862/984 (88%)	798 (93%)	64 (7%)	13	38
3	D	989/1095 (90%)	905 (92%)	84 (8%)	10	33
4	E	62/86 (72%)	56 (90%)	6 (10%)	8	28
5	F	251/379 (66%)	233 (93%)	18 (7%)	13	39
7	J	72/98 (74%)	65 (90%)	7 (10%)	8	28
All	All	2609/3533 (74%)	2398 (92%)	211 (8%)	11	34

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	14	VAL
1	A	40	ARG
1	A	51	VAL
1	A	74	THR
1	A	81	LYS
1	A	127	THR
1	A	129	ASN
1	A	130	ASP
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	56	ILE
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

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Mol	Chain	Res	Type
1	B	185	GLN
1	B	200	ASN
1	B	215	LEU
1	B	231	HIS
2	C	44	LEU
2	C	70	GLU
2	C	81	LEU
2	C	102	ARG
2	C	119	THR
2	C	124	LEU
2	C	193	VAL
2	C	215	VAL
2	C	236	ASN
2	C	280	LYS
2	C	294	GLU
2	C	299	LEU
2	C	301	ARG
2	C	323	THR
2	C	364	PHE
2	C	390	VAL
2	C	398	GLN
2	C	437	LEU
2	C	441	THR
2	C	443	LYS
2	C	445	ARG
2	C	446	LEU
2	C	454	LEU
2	C	461	LEU
2	C	520	ASP
2	C	523	THR
2	C	525	ASP
2	C	531	VAL
2	C	546	THR
2	C	568	ASP
2	C	607	VAL
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

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Mol	Chain	Res	Type
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	876	LEU
2	C	919	ILE
2	C	927	LEU
2	C	936	ASN
2	C	953	GLU
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	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	101	VAL
3	D	144	ARG
3	D	148	LEU
3	D	150	THR
3	D	165	GLN
3	D	187	GLU
3	D	234	LEU
3	D	238	GLU
3	D	239	VAL
3	D	243	GLU
3	D	246	ASP

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Mol	Chain	Res	Type
3	D	259	GLU
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
3	D	485	ASP
3	D	498	LEU
3	D	504	LEU
3	D	507	LEU
3	D	518	GLU
3	D	558	LEU
3	D	566	LEU
3	D	574	LEU
3	D	576	MET
3	D	588	LEU
3	D	591	LEU
3	D	599	TYR
3	D	627	LEU
3	D	629	VAL
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	741	LYS
3	D	767	THR
3	D	784	VAL
3	D	799	ILE
3	D	830	PHE

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Mol	Chain	Res	Type
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	956	ILE
3	D	1049	ASP
3	D	1056	LEU
3	D	1071	ASP
3	D	1079	ASP
3	D	1086	ARG
3	D	1112	LEU
3	D	1183	GLU
3	D	1186	GLU
3	D	1190	GLU
3	D	1208	LEU
3	D	1234	LEU
3	D	1243	SER
3	D	1258	LEU
3	D	1278	GLU
4	E	37	ILE
4	E	50	LEU
4	E	76	VAL
4	E	85	GLN
4	E	101	LEU
4	E	102	GLU
5	F	182	GLU
5	F	290	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

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Mol	Chain	Res	Type
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	66	GLU
7	J	104	LEU
7	J	105	ILE
7	J	106	LYS
1	T	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) 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	185	GLN
2	C	48	GLN
2	C	160	ASN
2	C	191	HIS
2	C	308	ASN
2	C	343	GLN
2	C	398	GLN
2	C	433	GLN
2	C	467	HIS
2	C	484	ASN
2	C	512	ASN
2	C	576	GLN
2	C	590	HIS
2	C	691	GLN
2	C	700	GLN
2	C	720	HIS
2	C	911	HIS
2	C	921	GLN

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Mol	Chain	Res	Type
2	C	926	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	540	GLN
3	D	564	ASN
3	D	600	GLN
3	D	653	ASN
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	853	HIS
3	D	881	GLN
3	D	888	HIS
3	D	932	ASN
3	D	1085	GLN
3	D	1126	GLN
3	D	1132	GLN
4	E	85	GLN
4	E	103	HIS
5	F	172	GLN
5	F	214	GLN
5	F	309	HIS
5	F	397	GLN
5	F	454	HIS
7	J	58	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	C	1201	-	4,4,4	0.23	0	6,6,6	0.11	0
10	SO4	F	504	-	4,4,4	0.25	0	6,6,6	0.08	0
10	SO4	F	502	-	4,4,4	0.25	0	6,6,6	0.13	0
10	SO4	F	505	-	4,4,4	0.24	0	6,6,6	0.12	0
10	SO4	C	1202	-	4,4,4	0.24	0	6,6,6	0.07	0
10	SO4	D	2006	-	4,4,4	0.25	0	6,6,6	0.11	0
11	EDO	F	506	-	3,3,3	0.45	0	2,2,2	0.31	0
10	SO4	D	2005	-	4,4,4	0.23	0	6,6,6	0.13	0
10	SO4	C	1203	-	4,4,4	0.23	0	6,6,6	0.08	0
10	SO4	D	2010	-	4,4,4	0.24	0	6,6,6	0.12	0
11	EDO	C	1204	-	3,3,3	0.38	0	2,2,2	0.44	0
11	EDO	C	1207	-	3,3,3	0.46	0	2,2,2	0.31	0
10	SO4	C	1206	-	4,4,4	0.23	0	6,6,6	0.07	0
10	SO4	D	2004	-	4,4,4	0.22	0	6,6,6	0.11	0
10	SO4	F	501	-	4,4,4	0.24	0	6,6,6	0.08	0
10	SO4	F	503	-	4,4,4	0.23	0	6,6,6	0.11	0
11	EDO	D	2009	-	3,3,3	0.45	0	2,2,2	0.30	0
10	SO4	D	2003	-	4,4,4	0.23	0	6,6,6	0.17	0
12	SRN	C	1205	-	60,62,62	5.19	31 (51%)	61,84,84	1.72	14 (22%)
11	EDO	D	2008	-	3,3,3	0.40	0	2,2,2	0.40	0
11	EDO	D	2007	-	3,3,3	0.44	0	2,2,2	0.33	0
11	EDO	D	2011	-	3,3,3	0.42	0	2,2,2	0.32	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	C	1204	-	-	1/1/1/1	-
11	EDO	C	1207	-	-	0/1/1/1	-
11	EDO	F	506	-	-	0/1/1/1	-
12	SRN	C	1205	-	-	5/52/105/105	0/4/5/5
11	EDO	D	2008	-	-	0/1/1/1	-
11	EDO	D	2007	-	-	0/1/1/1	-
11	EDO	D	2011	-	-	0/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1205	SRN	O3-C8	20.71	1.80	1.44
12	C	1205	SRN	O3-C9	16.16	1.80	1.45
12	C	1205	SRN	C34-C9	-11.71	1.28	1.52
12	C	1205	SRN	C3-C2	9.58	1.59	1.34
12	C	1205	SRN	C34-C35	-9.32	1.33	1.52
12	C	1205	SRN	C4-C5	7.87	1.57	1.36
12	C	1205	SRN	C13-C14	7.09	1.60	1.31
12	C	1205	SRN	C6-C7	6.45	1.57	1.33
12	C	1205	SRN	C24-C25	6.44	1.57	1.31
12	C	1205	SRN	C8-C7	-6.08	1.30	1.50
12	C	1205	SRN	C12-C13	-5.67	1.31	1.50
12	C	1205	SRN	C10-C9	-5.47	1.43	1.53
12	C	1205	SRN	C28-C29	5.21	1.61	1.31
12	C	1205	SRN	O7-C32	5.00	1.53	1.43
12	C	1205	SRN	C11-C10	-4.52	1.44	1.53
12	C	1205	SRN	C3-C4	4.51	1.58	1.44
12	C	1205	SRN	C5-C6	4.36	1.58	1.44
12	C	1205	SRN	O8-C12	4.30	1.50	1.43
12	C	1205	SRN	C35-C8	-4.14	1.46	1.53
12	C	1205	SRN	O1-C33	3.91	1.52	1.46
12	C	1205	SRN	C46-C47	3.82	1.45	1.33
12	C	1205	SRN	C2-C1	3.80	1.56	1.48
12	C	1205	SRN	C30-C29	3.71	1.60	1.50
12	C	1205	SRN	O1-C1	3.65	1.42	1.34
12	C	1205	SRN	C33-C47	-3.61	1.44	1.49
12	C	1205	SRN	O7-C31	3.48	1.53	1.44
12	C	1205	SRN	C23-C24	3.43	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1205	SRN	C15-C14	2.79	1.58	1.50
12	C	1205	SRN	C31-C46	2.26	1.53	1.50
12	C	1205	SRN	O8-C35	2.08	1.49	1.44
12	C	1205	SRN	O6-C23	-2.05	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1205	SRN	O9-C21-C20	4.90	115.31	109.78
12	C	1205	SRN	C8-C7-C6	-4.21	117.35	125.88
12	C	1205	SRN	C6-C5-C4	-3.48	116.66	124.72
12	C	1205	SRN	C9-C34-C35	3.37	113.21	103.67
12	C	1205	SRN	C37-C36-C32	3.08	122.03	115.96
12	C	1205	SRN	C30-C31-C46	-2.55	108.52	113.00
12	C	1205	SRN	C18-C17-C19	-2.49	108.43	111.35
12	C	1205	SRN	O3-C9-C34	2.38	109.66	104.76
12	C	1205	SRN	C30-C29-C28	-2.33	117.64	126.21
12	C	1205	SRN	C15-C16-C17	-2.31	108.56	113.68
12	C	1205	SRN	O3-C8-C35	2.14	107.40	104.26
12	C	1205	SRN	C39-C38-C36	-2.10	119.90	127.23
12	C	1205	SRN	C43-C44-C45	-2.10	109.03	114.51
12	C	1205	SRN	O9-C16-C17	2.09	113.10	110.60

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

11 monomers are involved in 25 short contacts:

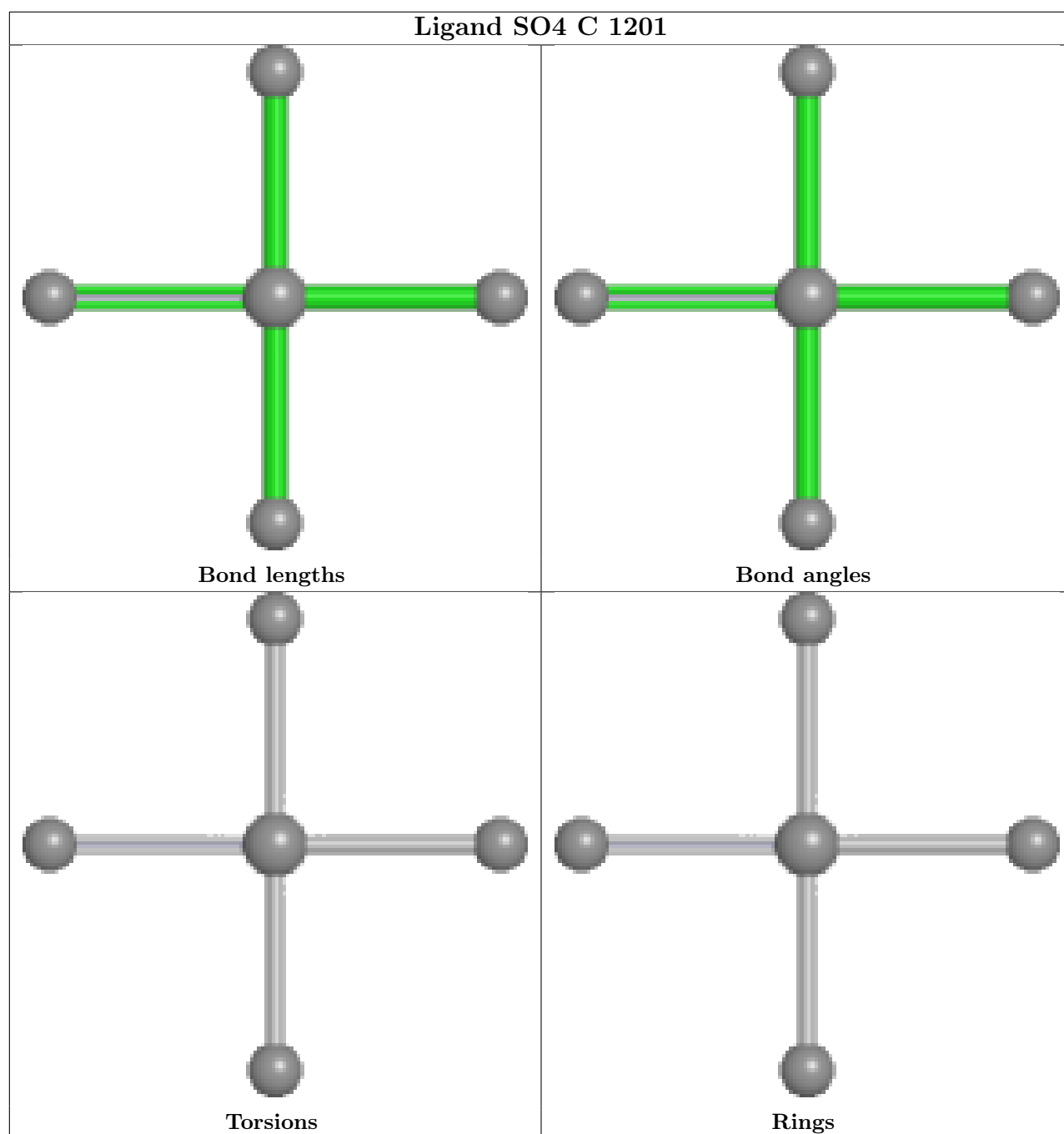
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	SO4	1	0
10	F	502	SO4	1	0
10	F	505	SO4	1	0

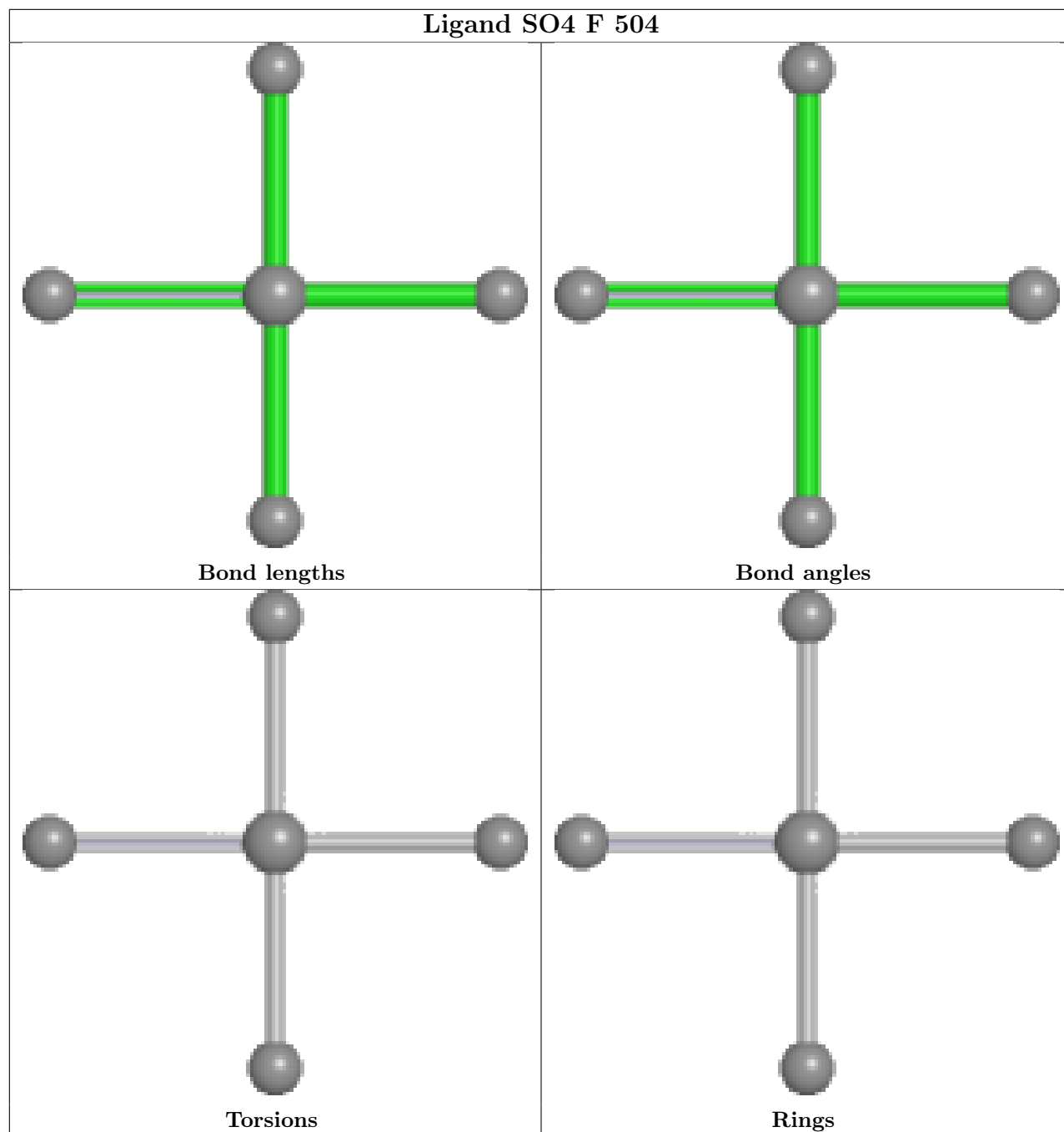
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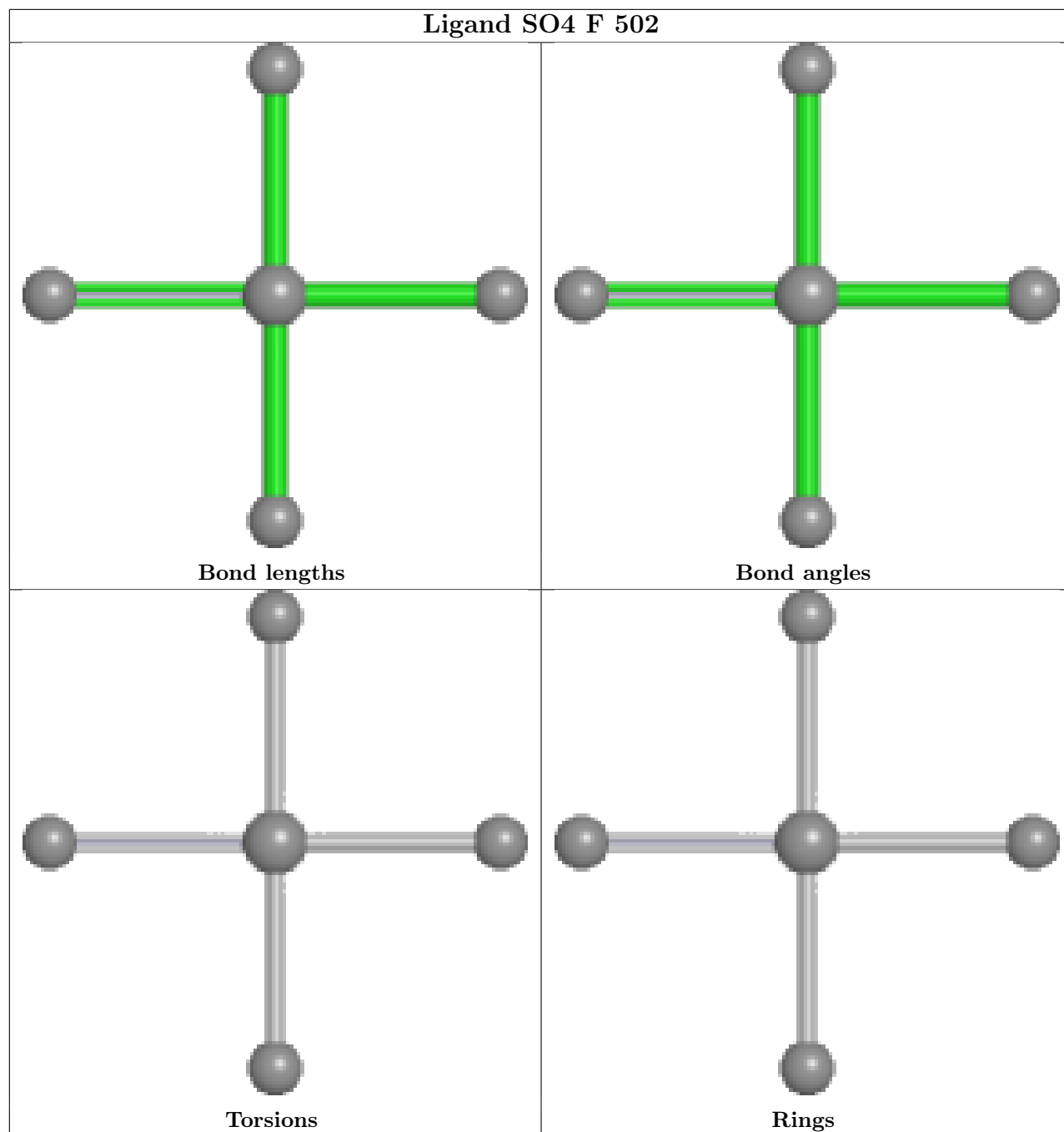
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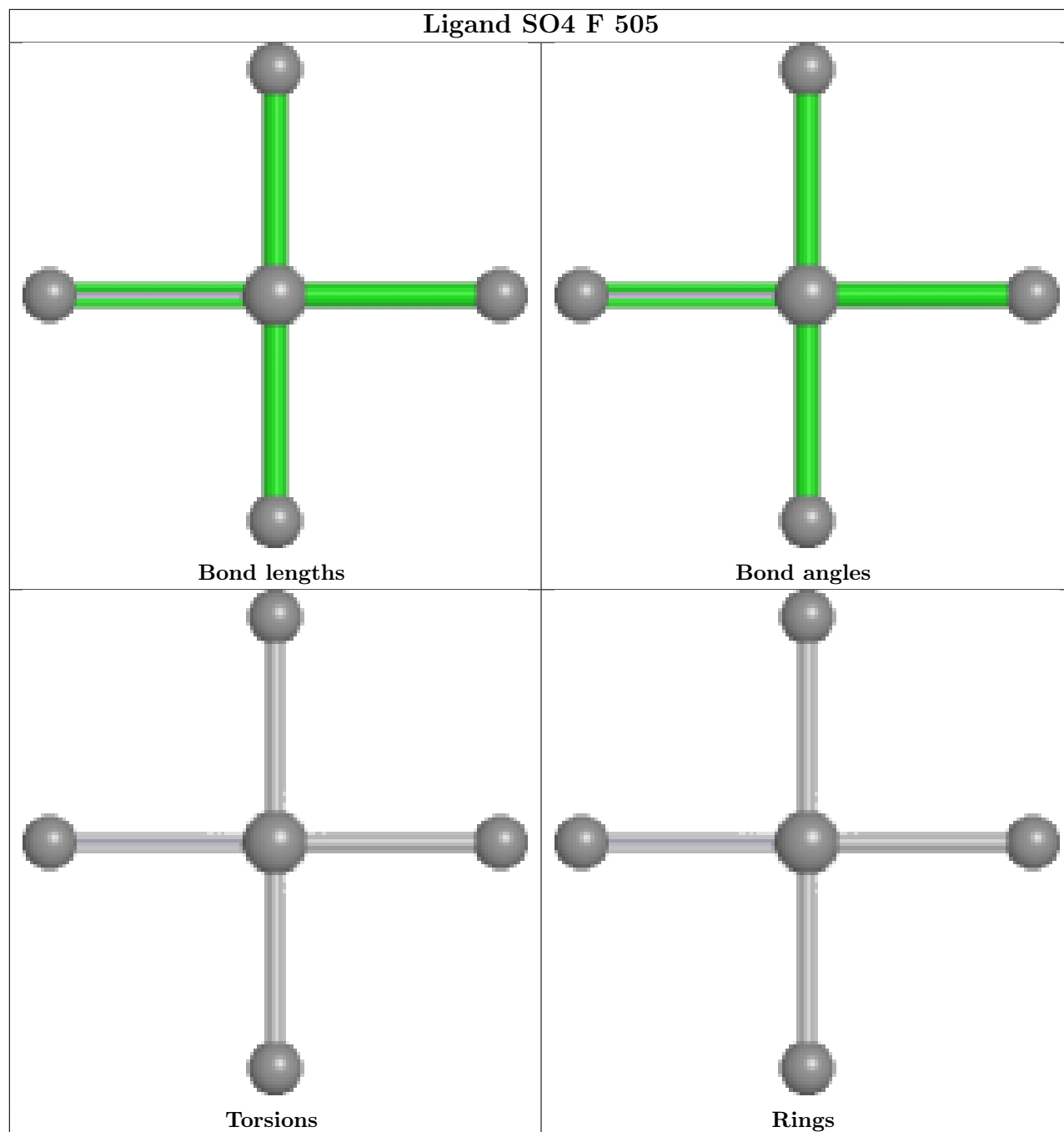
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	506	EDO	1	0
10	C	1203	SO4	1	0
11	C	1207	EDO	1	0
10	C	1206	SO4	1	0
10	D	2004	SO4	2	0
12	C	1205	SRN	13	0
11	D	2007	EDO	2	0
11	D	2011	EDO	1	0

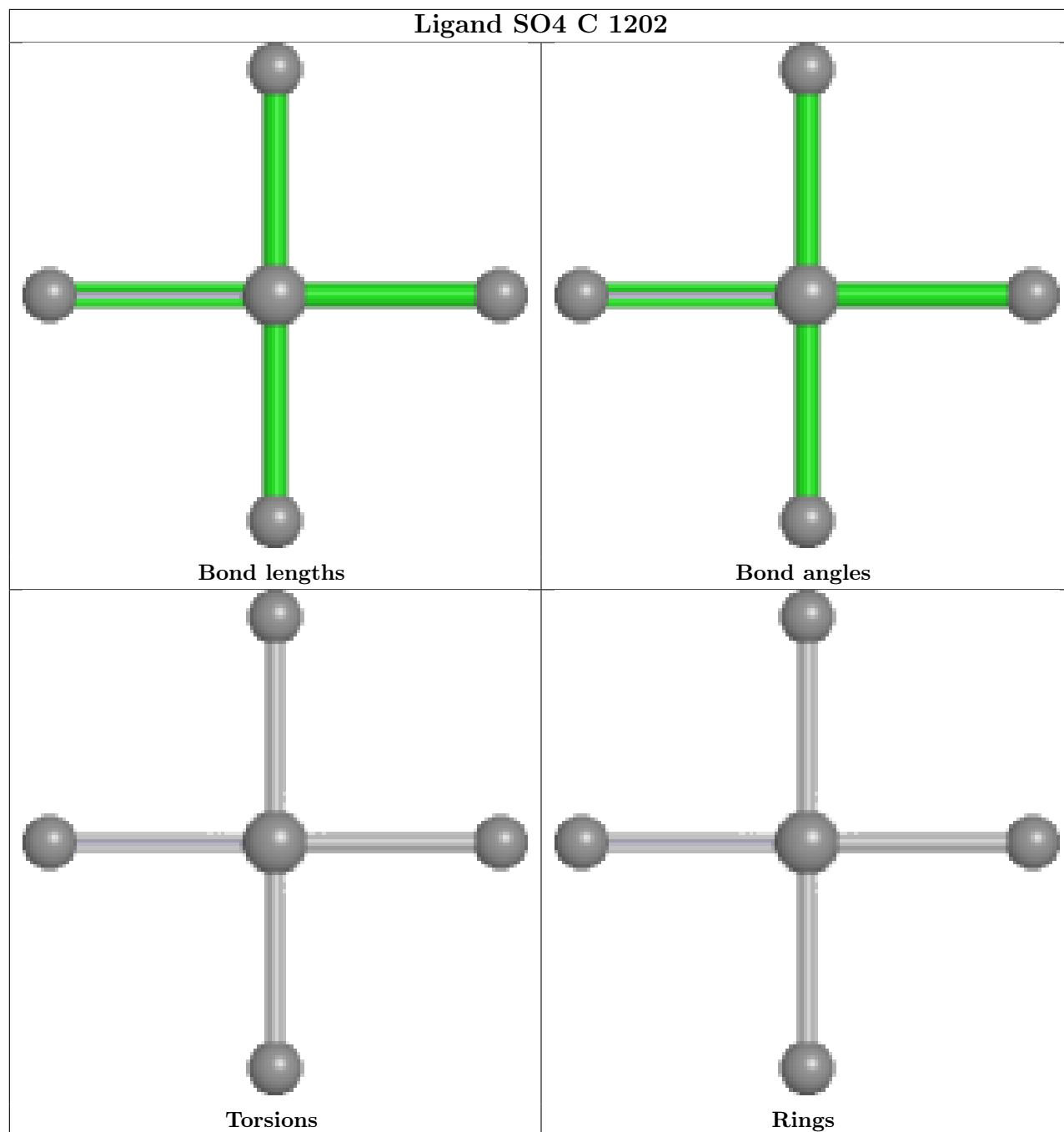
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

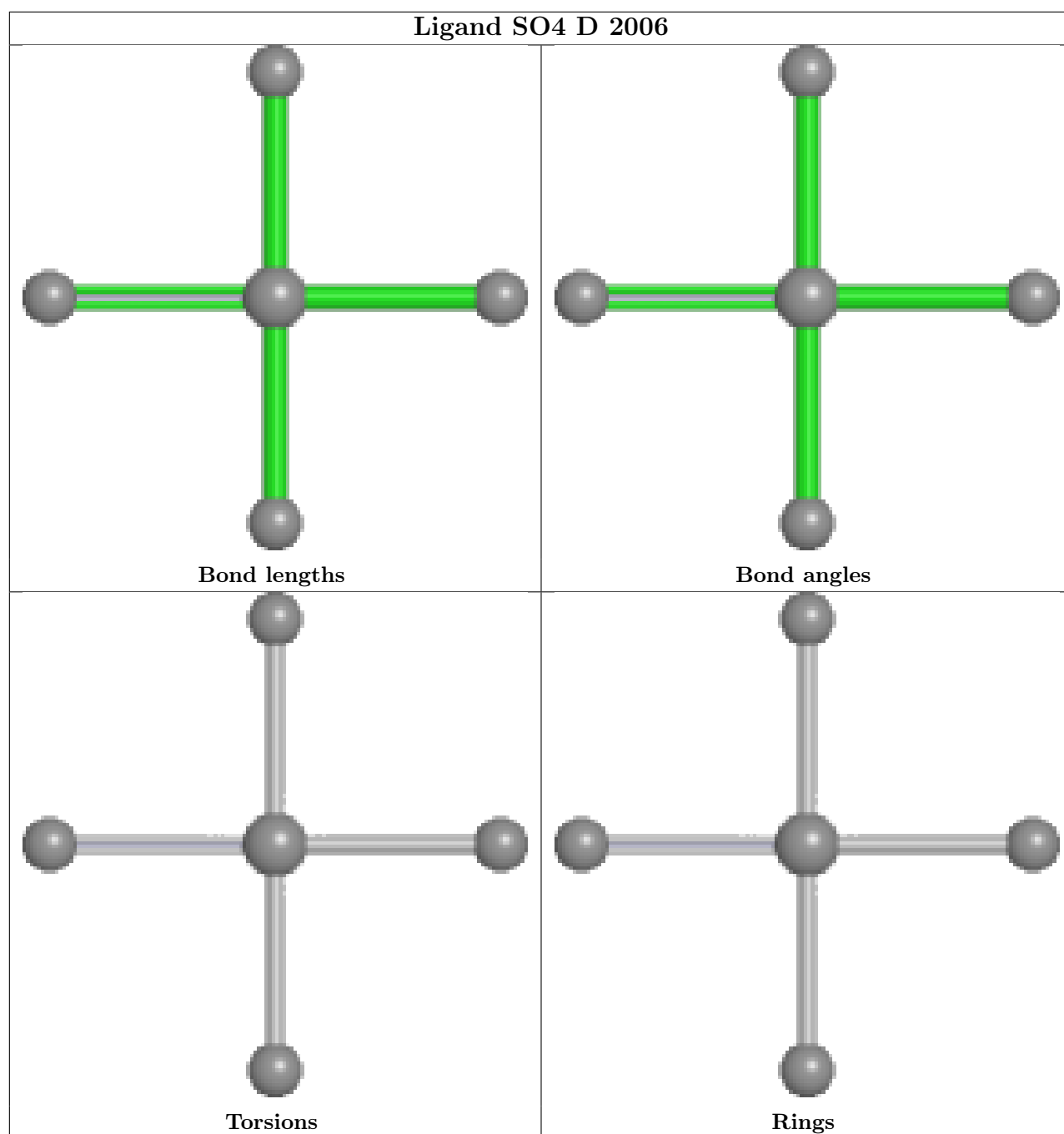


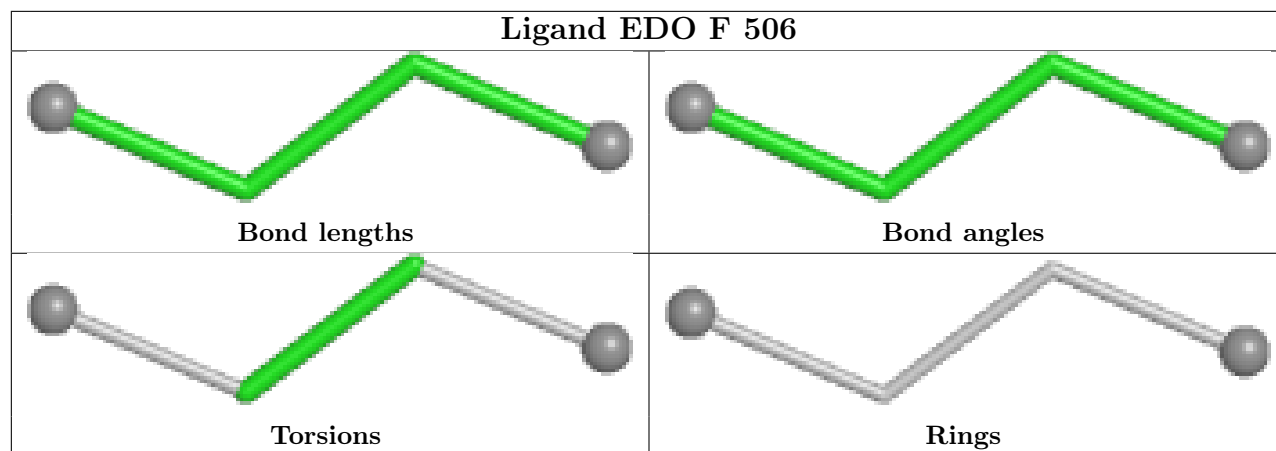


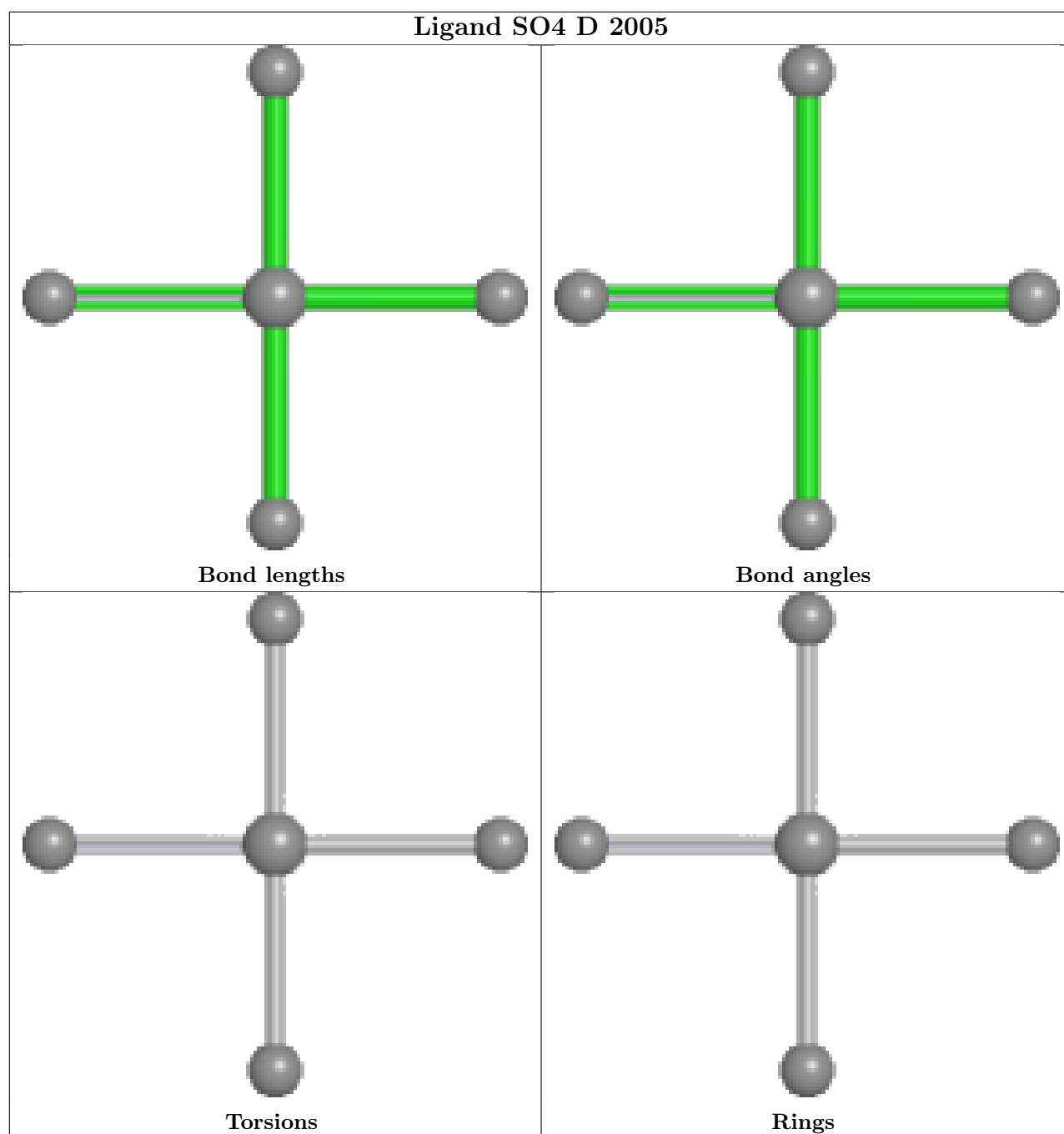


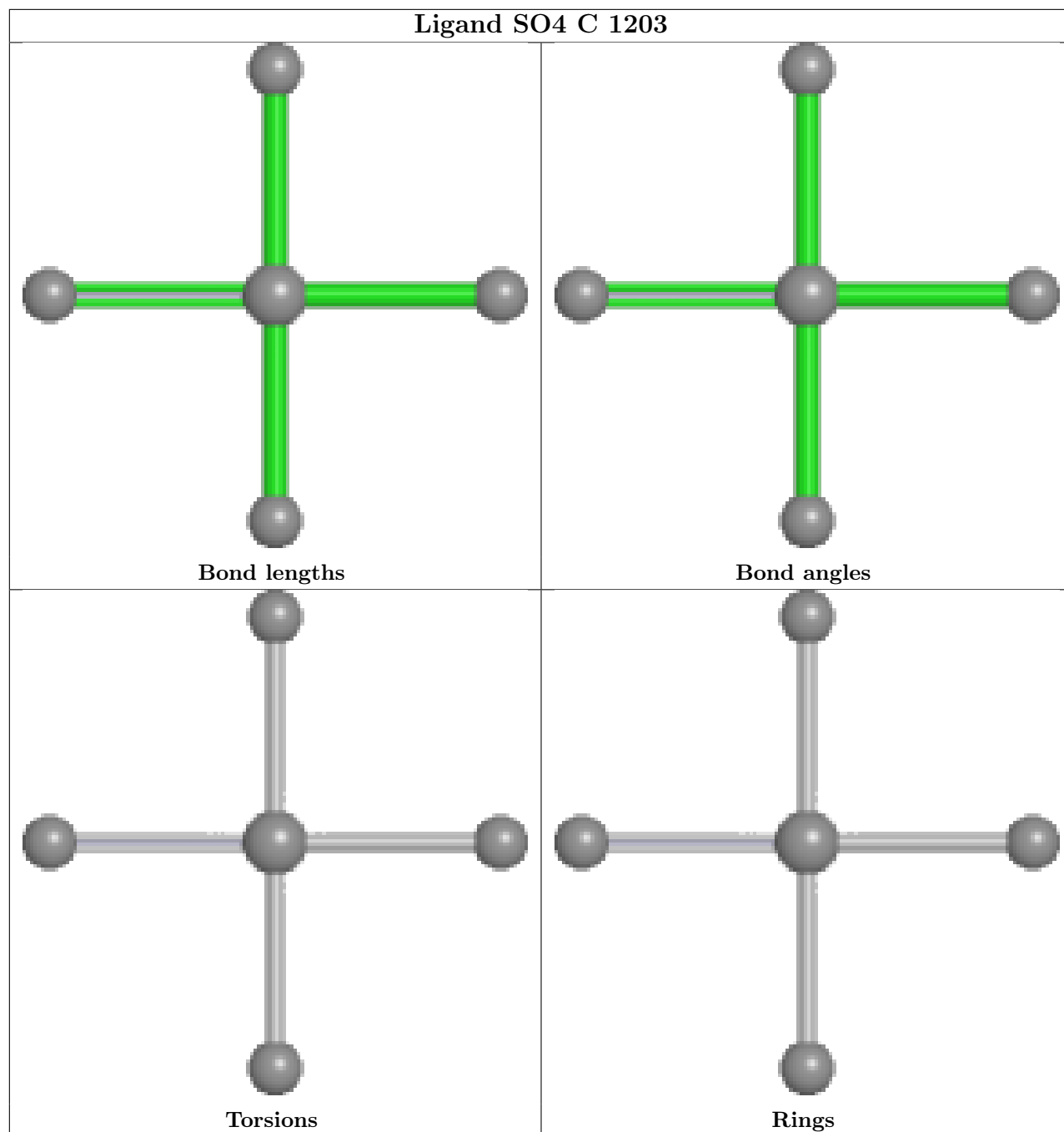


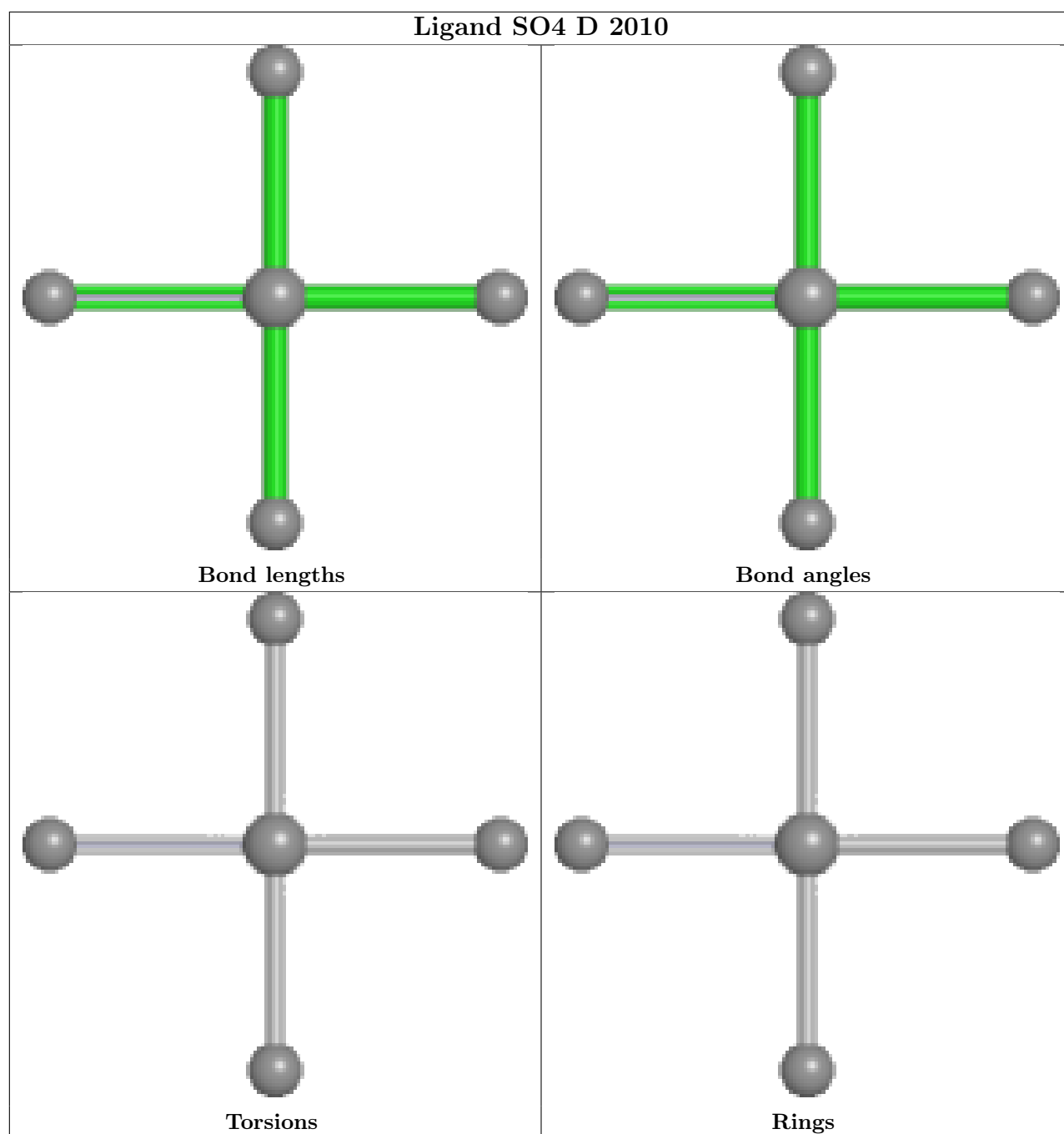


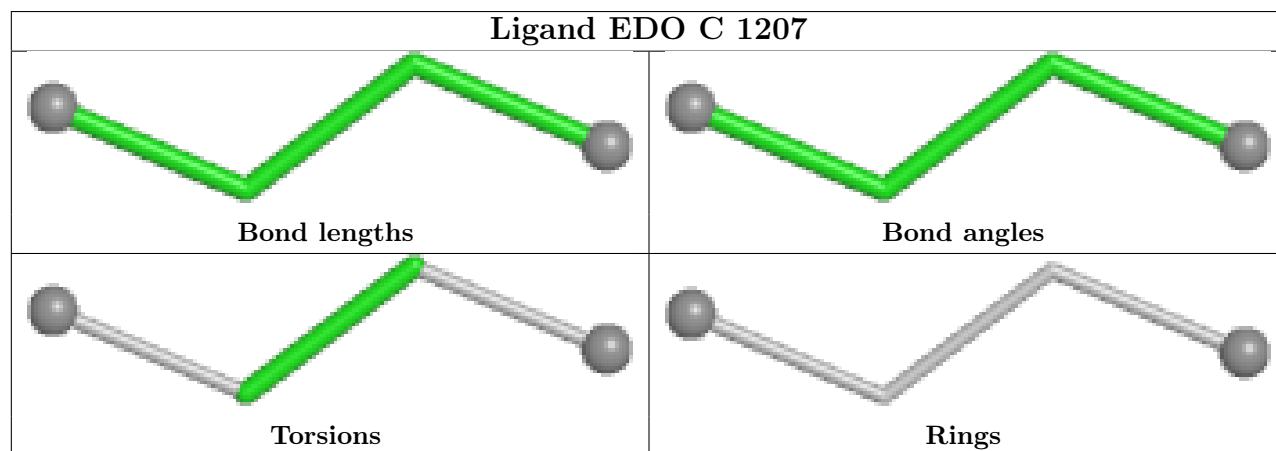
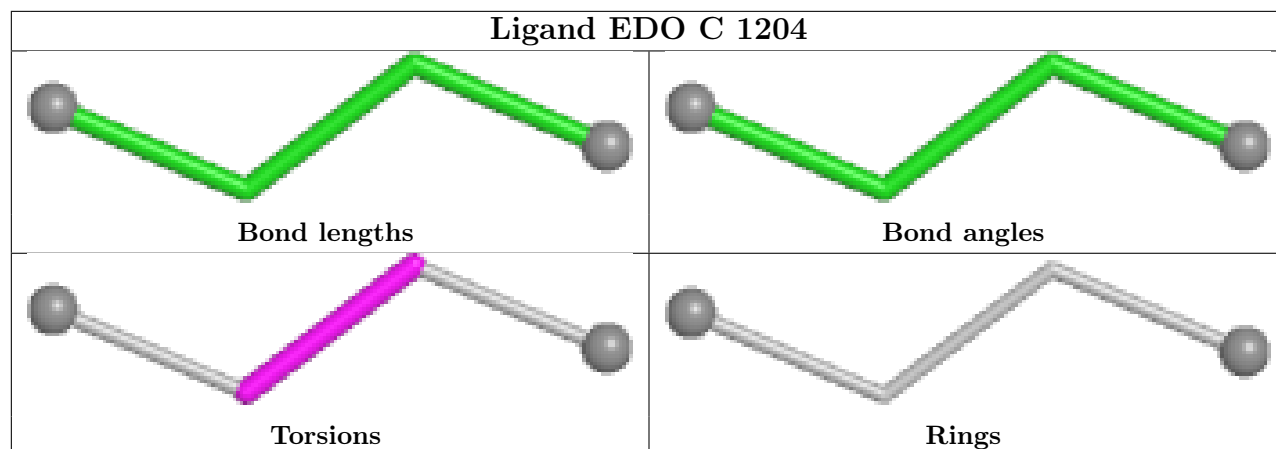


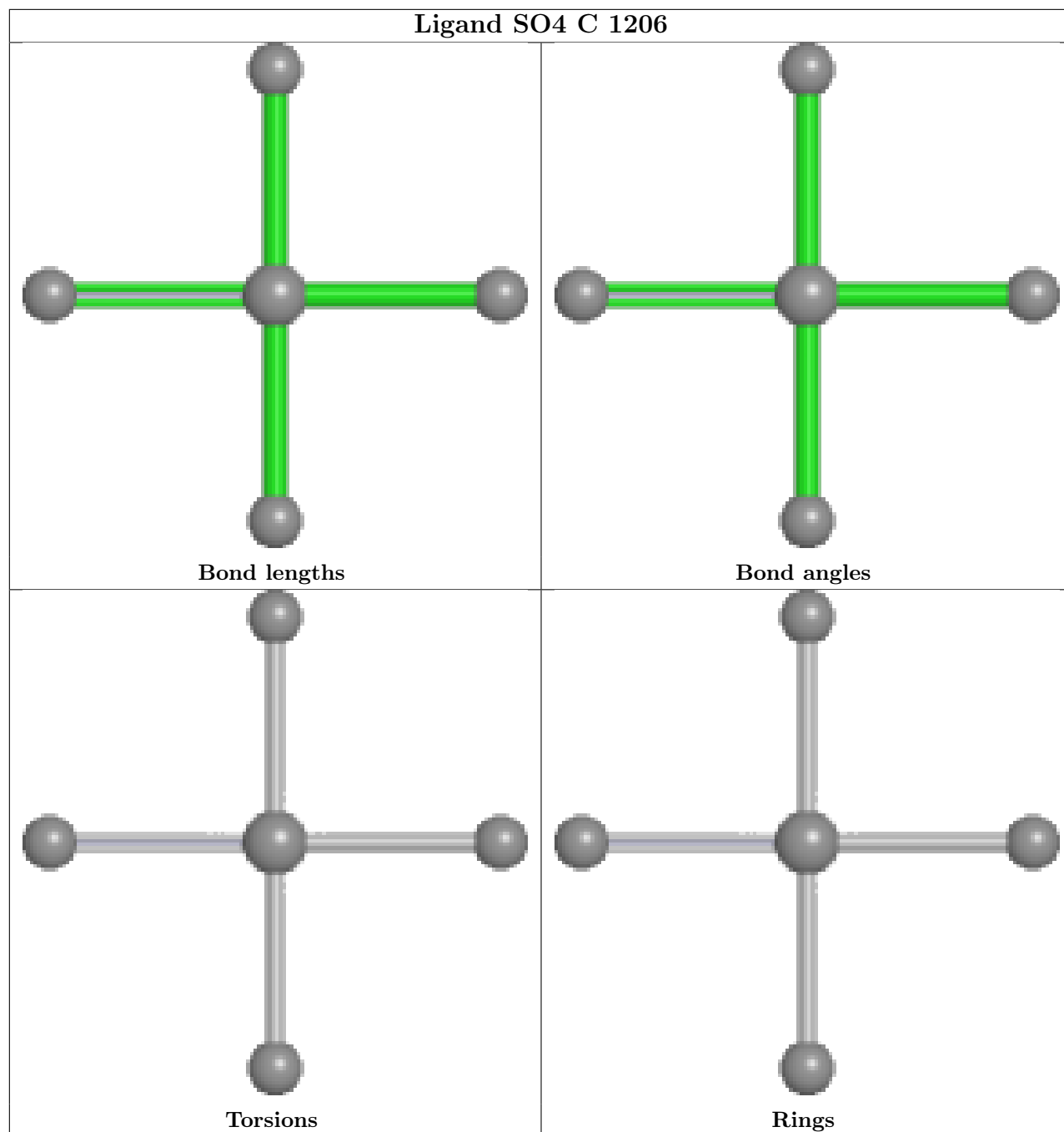


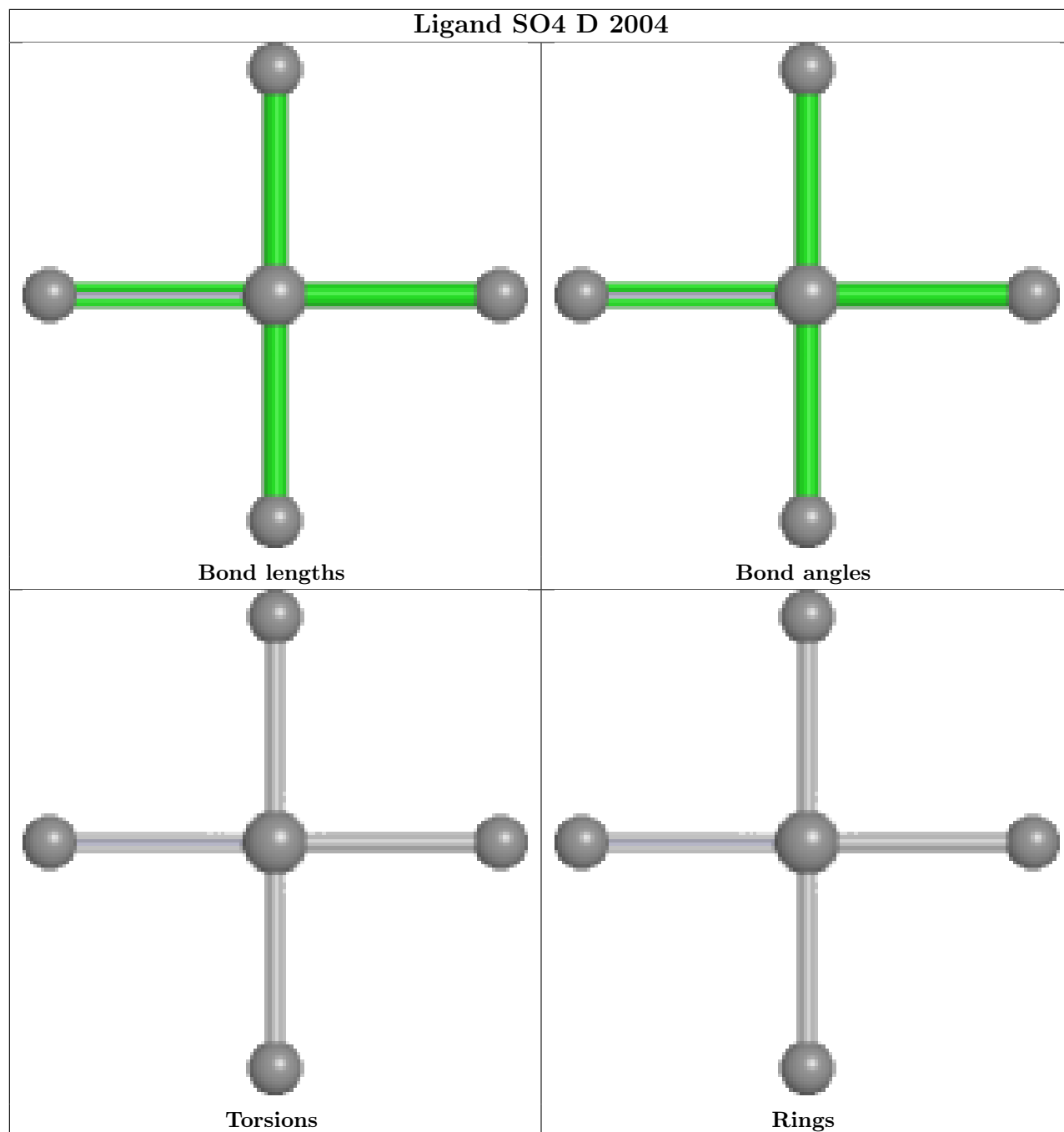


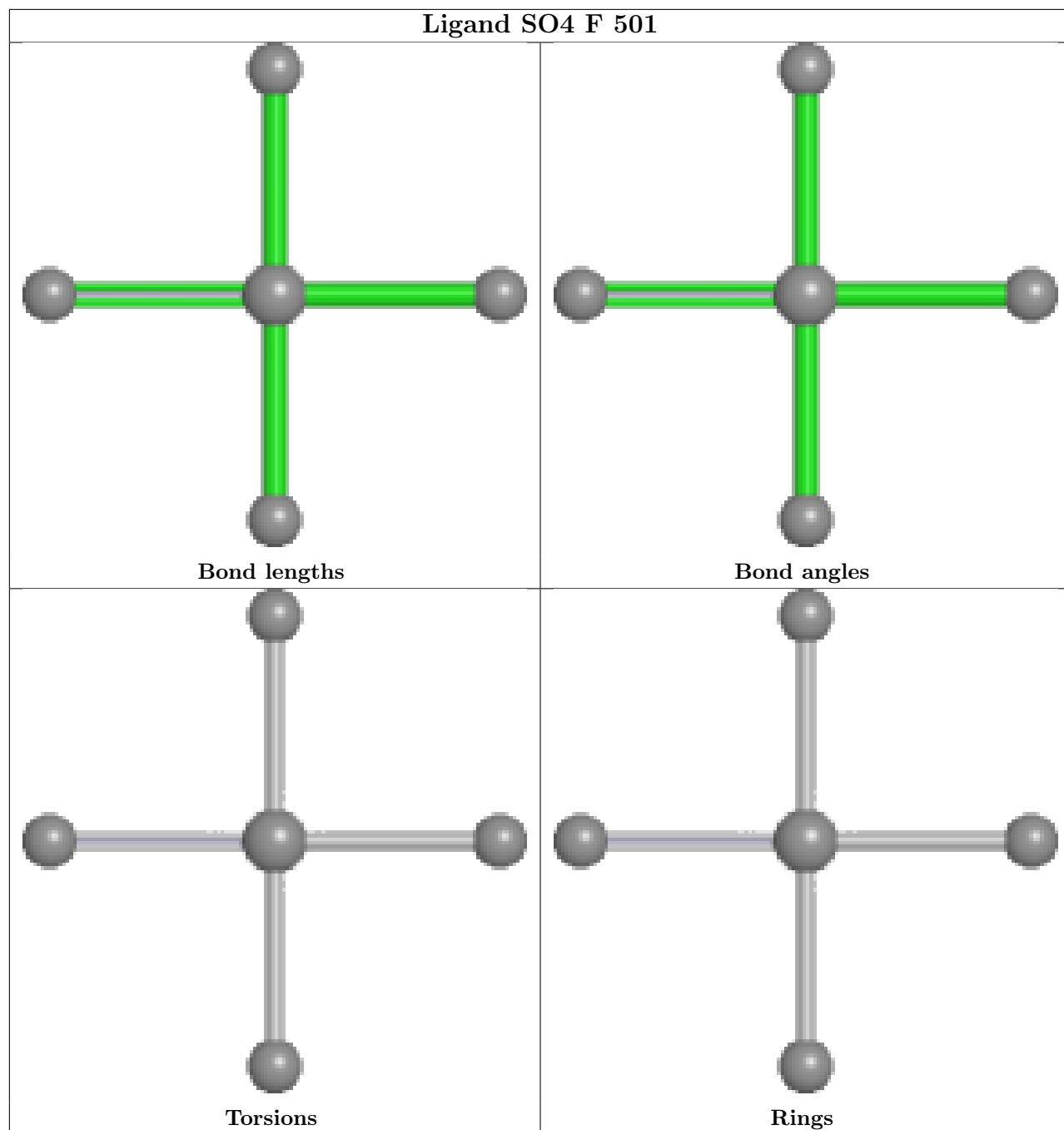


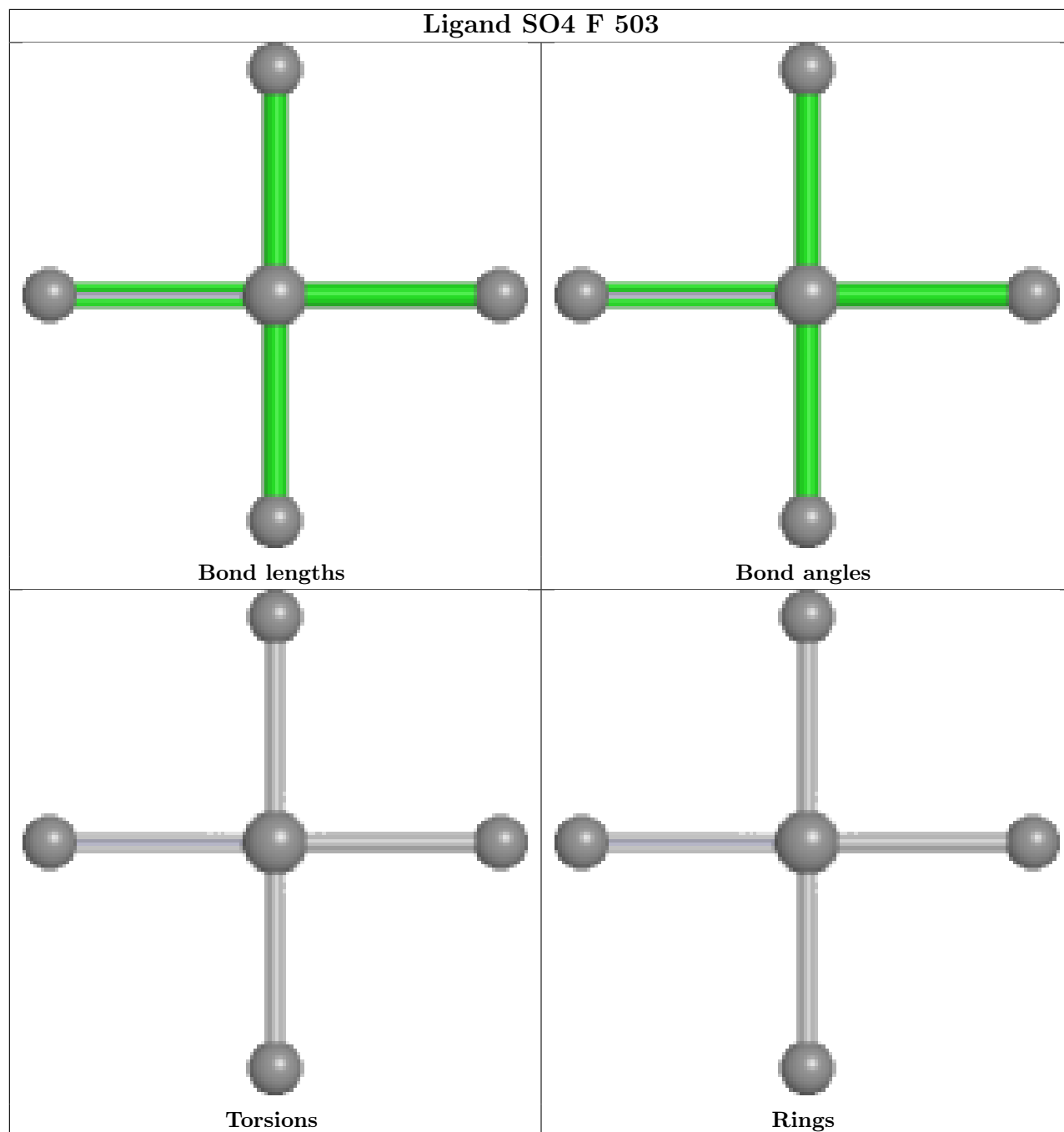


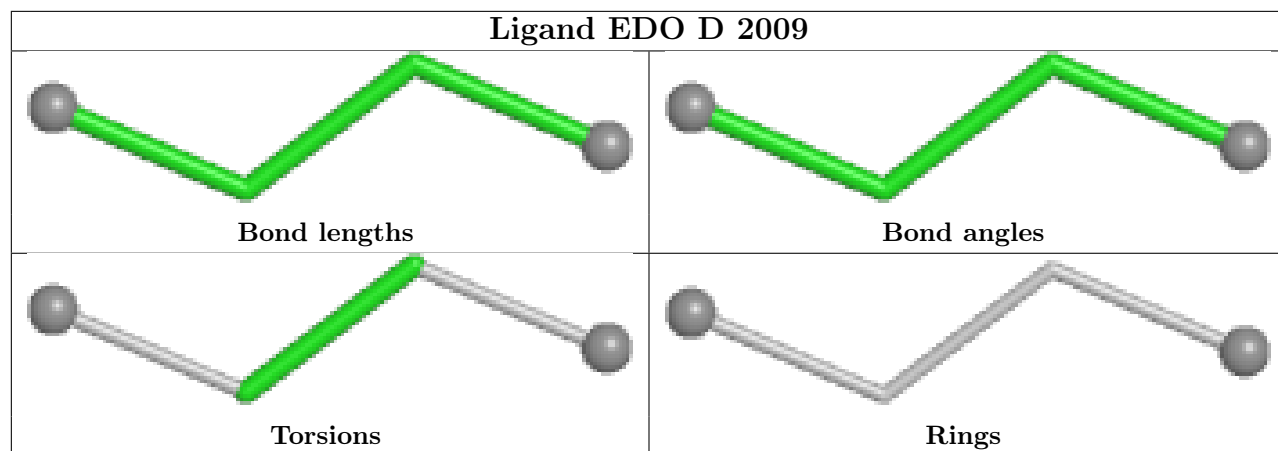


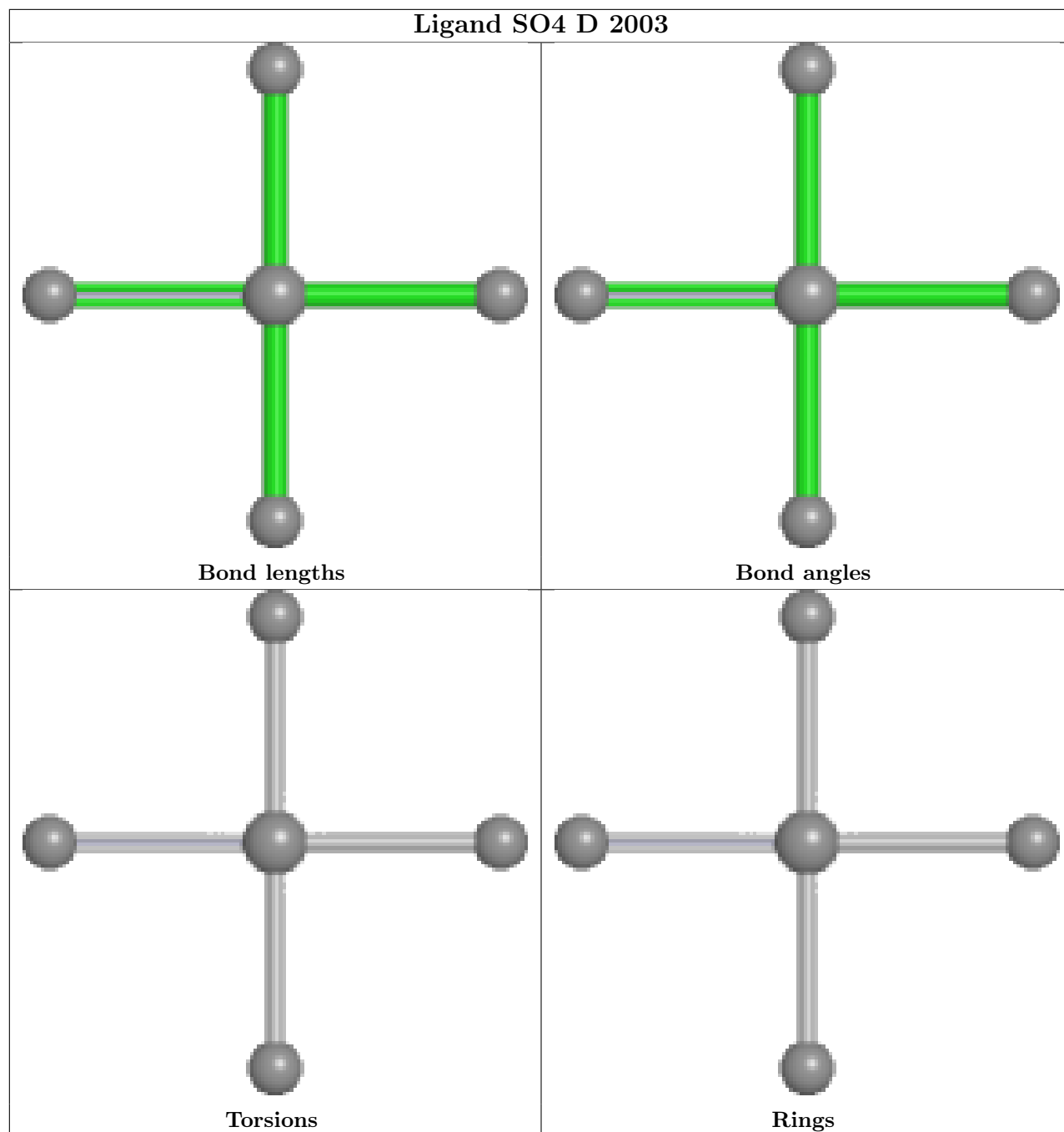


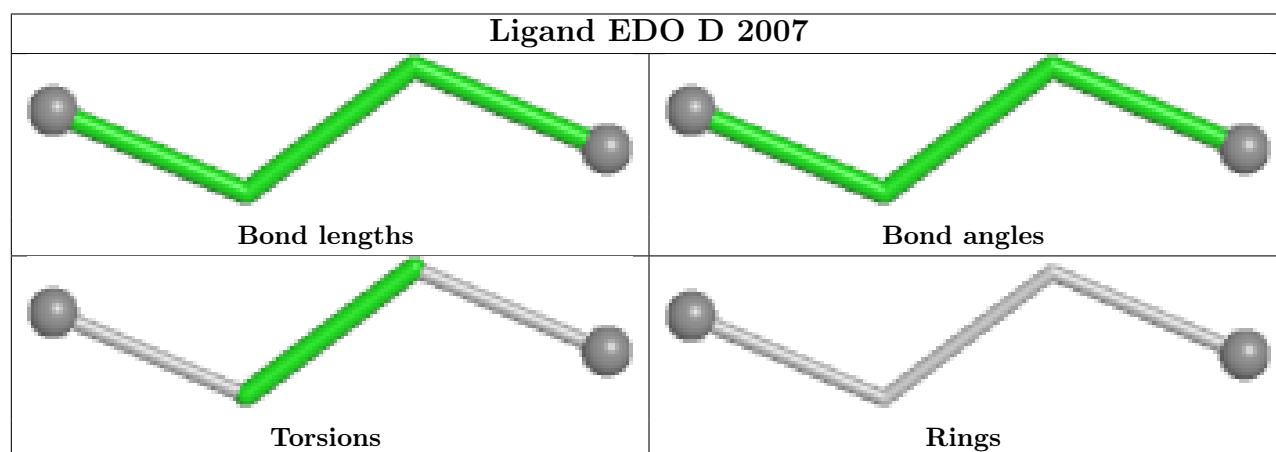
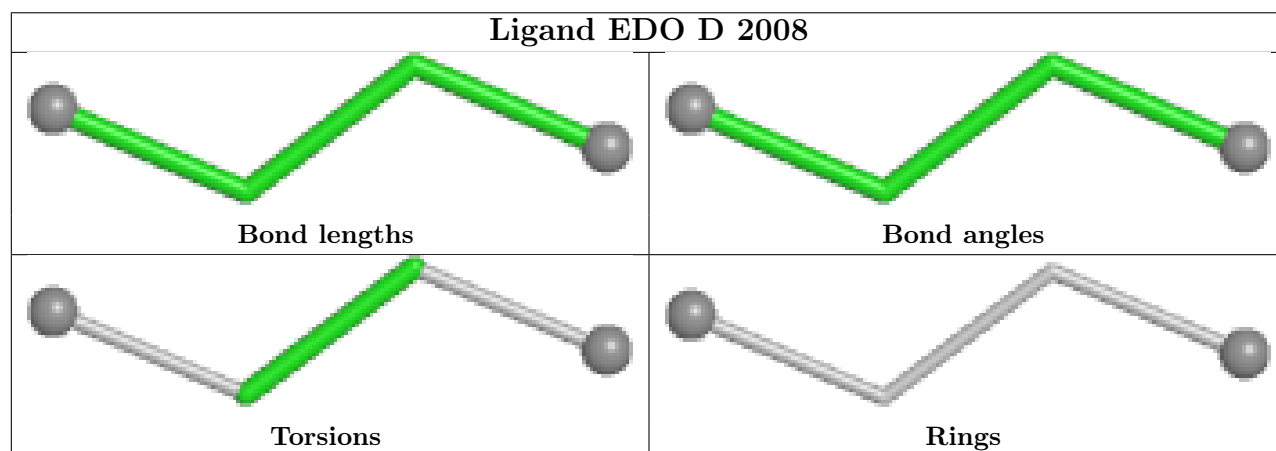
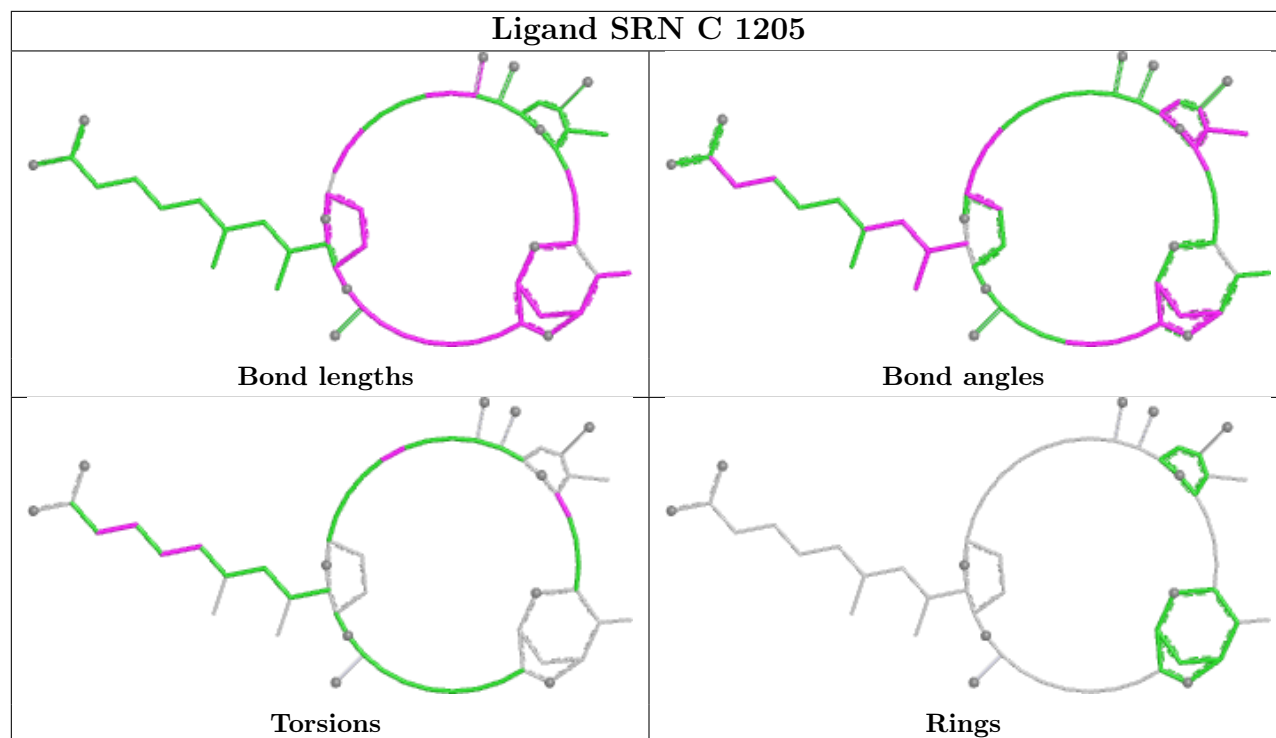


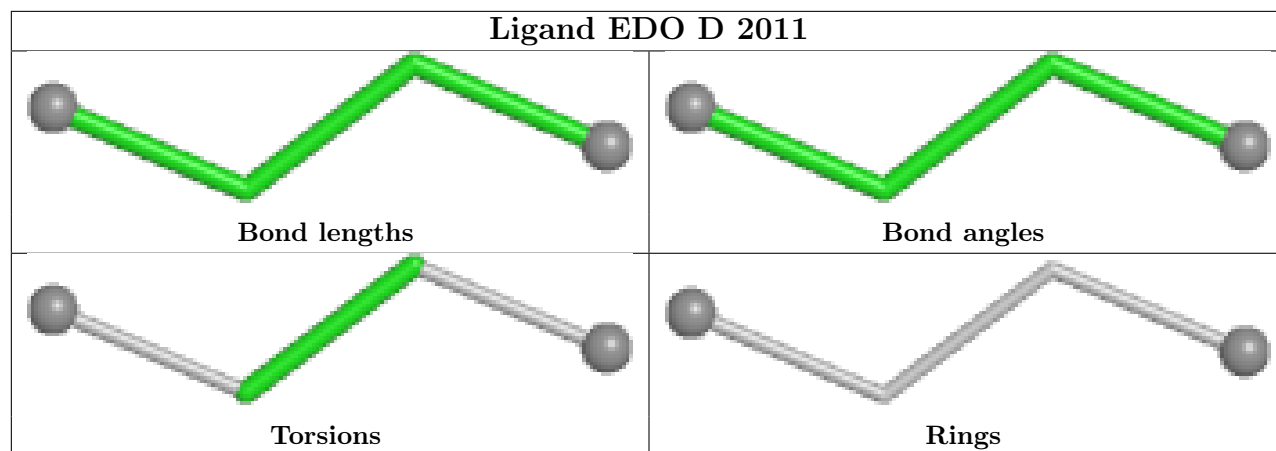












5.7 Other polymers [i](#)

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%)	-0.03	1 (0%) 87 73	76, 105, 138, 165	0
1	B	233/350 (66%)	0.06	2 (0%) 81 63	98, 133, 157, 174	0
1	T	53/350 (15%)	0.21	0 100 100	128, 168, 199, 204	0
2	C	1099/1169 (94%)	-0.06	10 (0%) 81 63	54, 104, 178, 205	0
3	D	1246/1317 (94%)	-0.26	1 (0%) 92 86	46, 91, 152, 196	0
4	E	76/107 (71%)	-0.25	1 (1%) 75 56	67, 98, 140, 151	0
5	F	305/466 (65%)	-0.35	0 100 100	50, 90, 142, 186	0
6	G	0/17	-	-	-	-
7	J	83/114 (72%)	-0.08	3 (3%) 46 26	80, 117, 166, 183	0
8	O	31/31 (100%)	-0.83	0 100 100	64, 81, 105, 111	0
9	P	26/26 (100%)	-0.72	0 100 100	76, 87, 113, 119	0
All	All	3370/4297 (78%)	-0.16	18 (0%) 87 73	46, 101, 169, 205	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1171	SER	3.3
2	C	145	MET	3.0
2	C	329	VAL	2.9
2	C	228	LEU	2.8
7	J	26	PRO	2.7
1	B	217	GLU	2.6
2	C	979	LEU	2.6
2	C	104	ASP	2.5
4	E	24	SER	2.4
2	C	32	PHE	2.4
2	C	332	THR	2.3
2	C	254	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	968	PHE	2.3
2	C	573	SER	2.2
1	A	26	LEU	2.2
7	J	72	PRO	2.2
1	B	152	ASN	2.0
7	J	42	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	EDO	C	1207	4/4	0.49	0.27	107,129,144,144	0
10	SO4	F	504	5/5	0.55	0.10	133,134,157,163	0
11	EDO	D	2007	4/4	0.59	0.17	102,123,135,156	0
11	EDO	D	2008	4/4	0.60	0.18	93,111,125,126	0
10	SO4	C	1202	5/5	0.67	0.10	116,120,146,158	0
10	SO4	C	1203	5/5	0.69	0.09	114,140,180,183	0
10	SO4	C	1201	5/5	0.71	0.08	133,138,162,170	0
11	EDO	F	506	4/4	0.72	0.15	101,121,130,156	0
11	EDO	D	2011	4/4	0.78	0.24	76,107,133,133	0
11	EDO	C	1204	4/4	0.81	0.17	61,88,105,113	0
10	SO4	F	501	5/5	0.81	0.06	122,128,139,153	0
10	SO4	F	503	5/5	0.84	0.11	105,109,129,136	0
10	SO4	D	2006	5/5	0.86	0.11	113,121,139,140	0
10	SO4	D	2005	5/5	0.87	0.07	104,115,141,154	0
10	SO4	D	2010	5/5	0.88	0.11	94,120,151,152	0
10	SO4	C	1206	5/5	0.89	0.08	127,131,156,410	0
10	SO4	F	505	5/5	0.91	0.31	116,128,134,152	0

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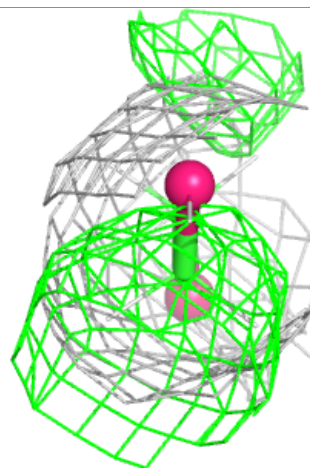
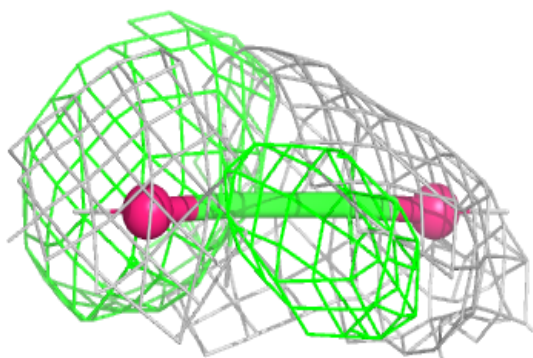
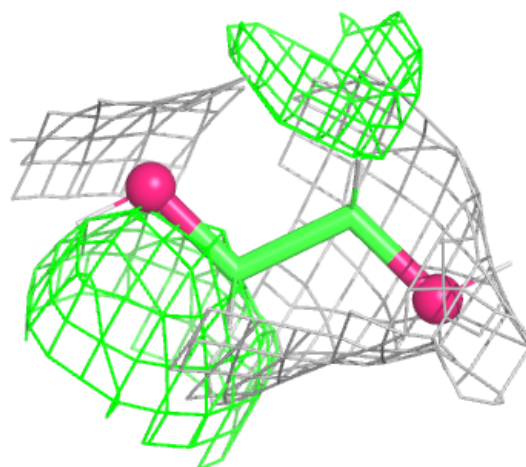
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	SRN	C	1205	58/58	0.92	0.12	79,97,136,149	0
11	EDO	D	2009	4/4	0.93	0.14	90,108,124,137	0
10	SO4	F	502	5/5	0.93	0.05	90,91,130,137	0
10	SO4	D	2003	5/5	0.94	0.07	74,87,102,109	0
10	SO4	D	2004	5/5	0.94	0.07	98,103,114,125	0
13	ZN	D	2002	1/1	0.99	0.05	134,134,134,134	0
13	ZN	D	2001	1/1	1.00	0.03	77,77,77,77	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.

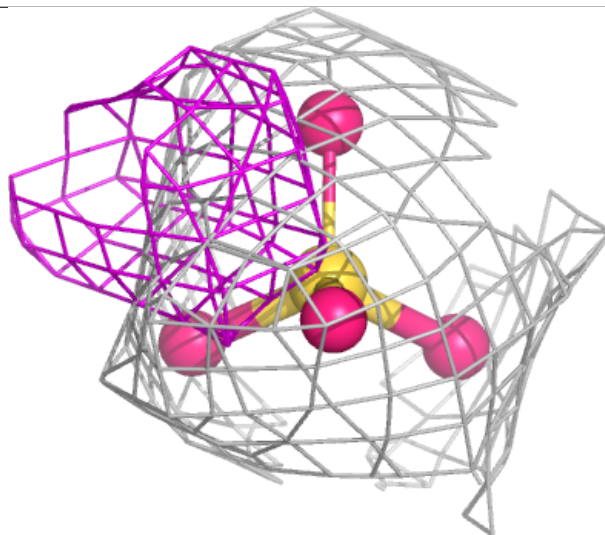
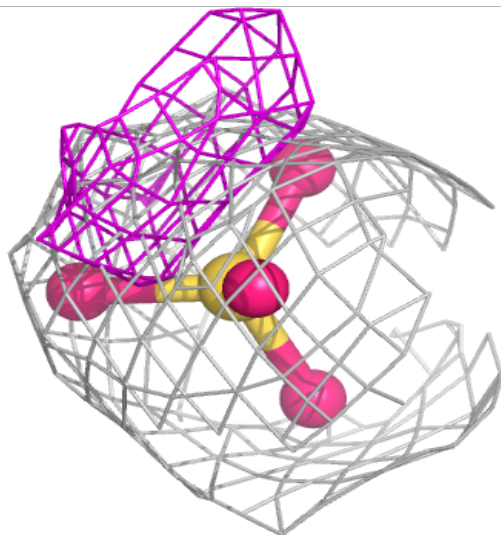
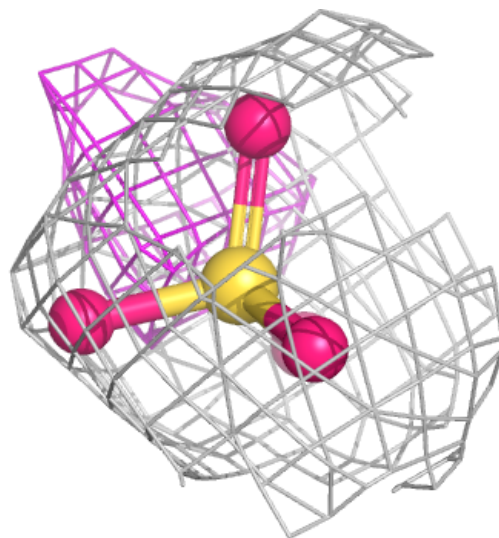
Electron density around EDO C 1207:

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



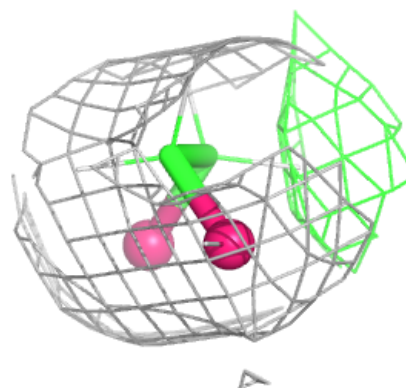
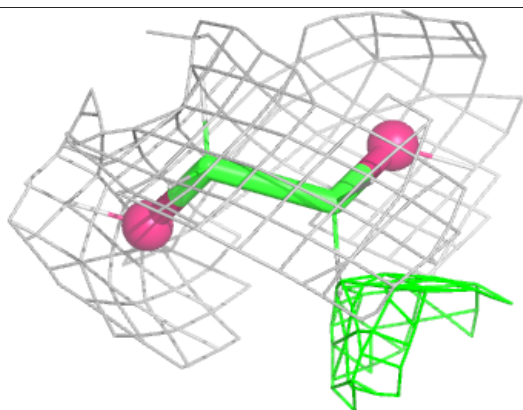
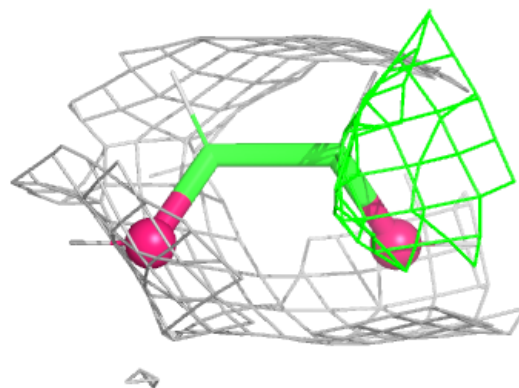
Electron density around SO4 F 504:

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



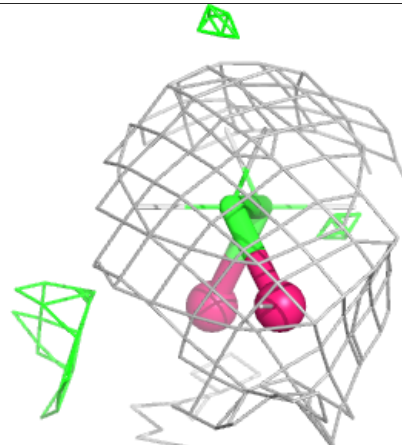
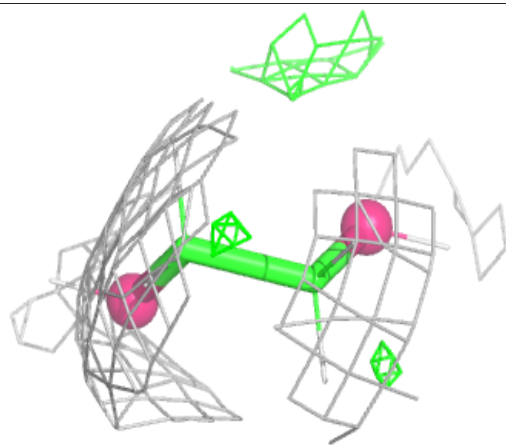
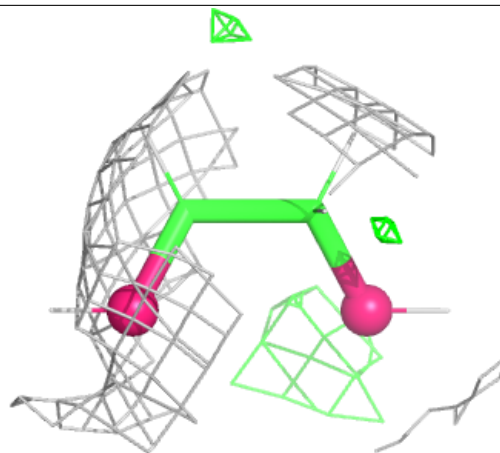
Electron density around EDO D 2007:

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



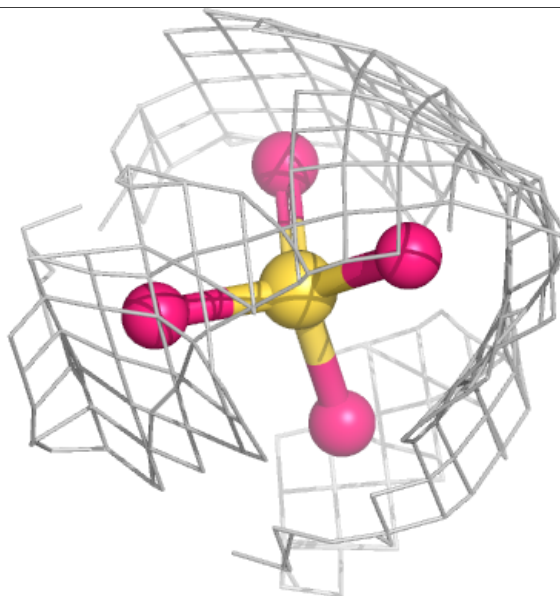
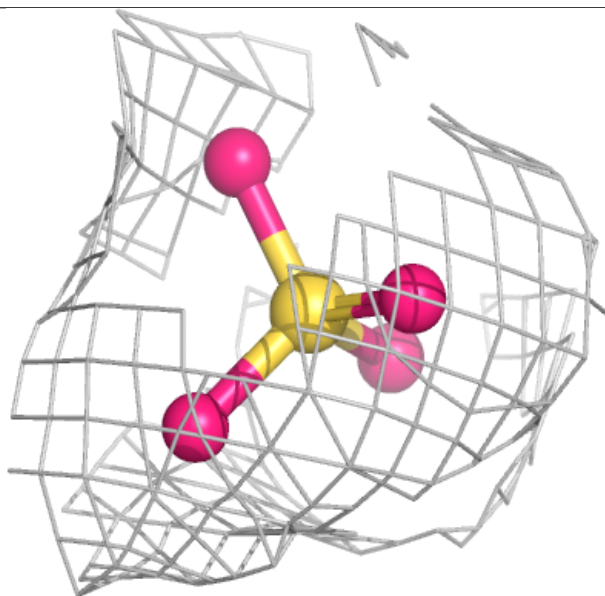
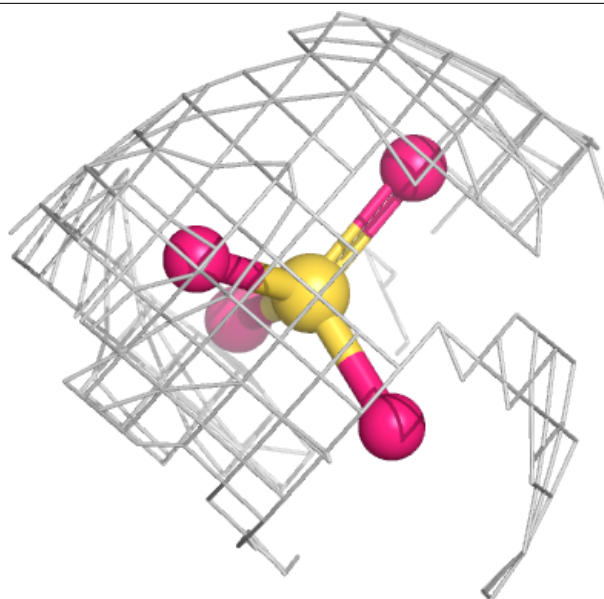
Electron density around EDO D 2008:

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



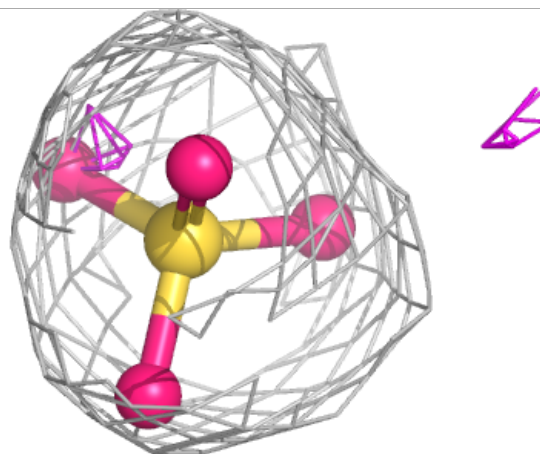
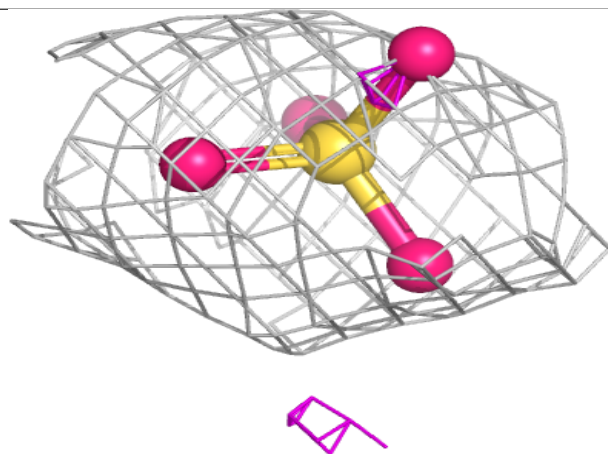
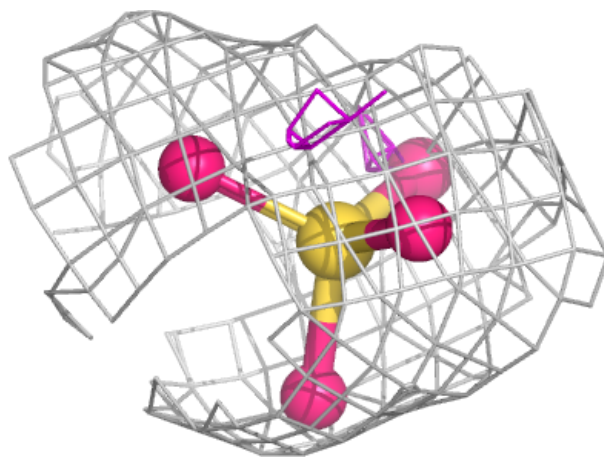
Electron density around SO4 C 1202:

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



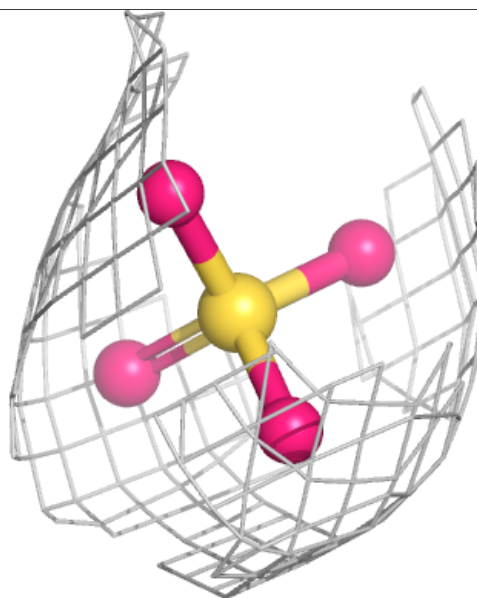
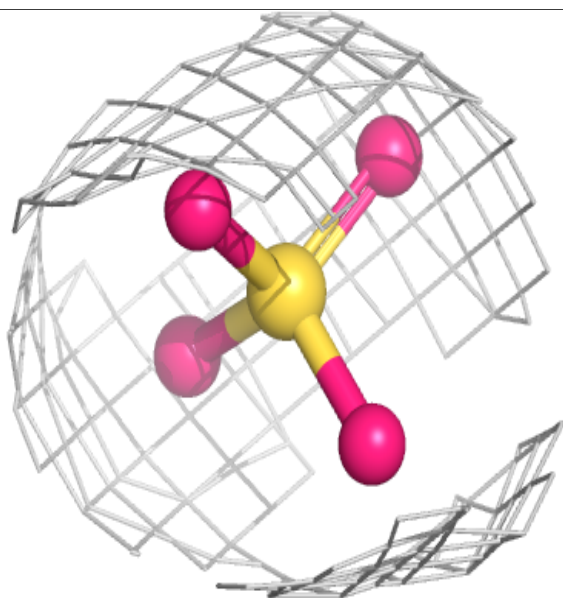
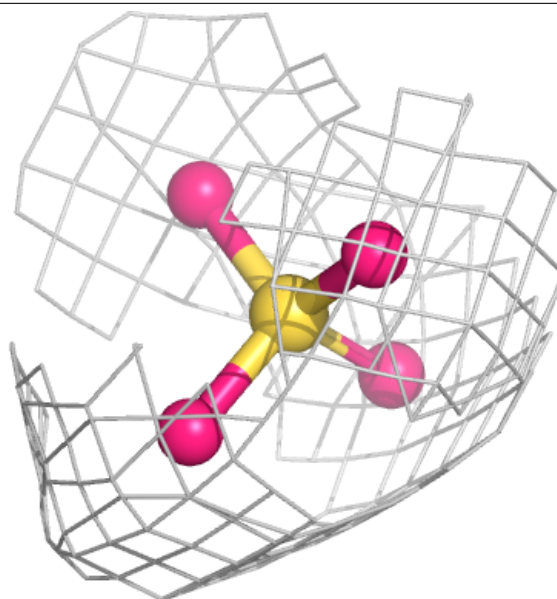
Electron density around SO4 C 1203:

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



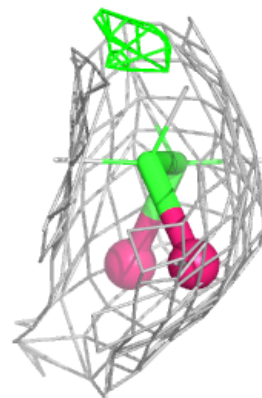
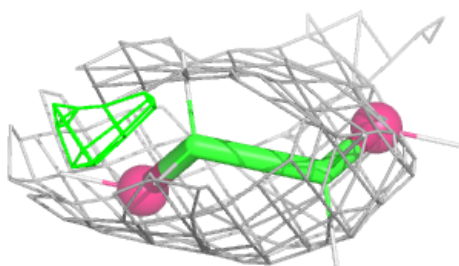
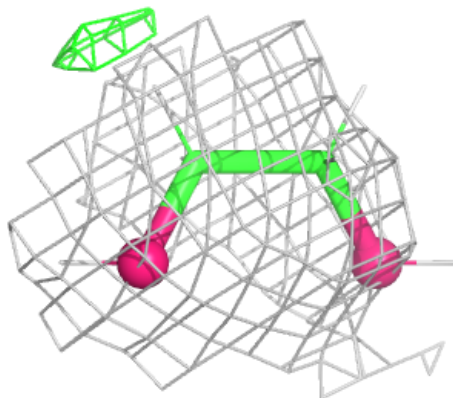
Electron density around SO4 C 1201:

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and green (positive)

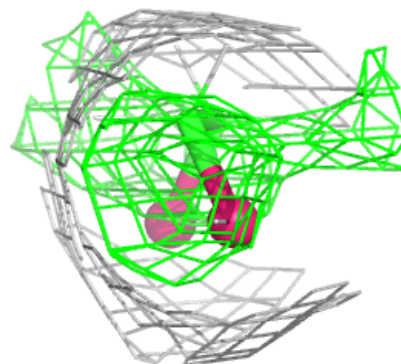
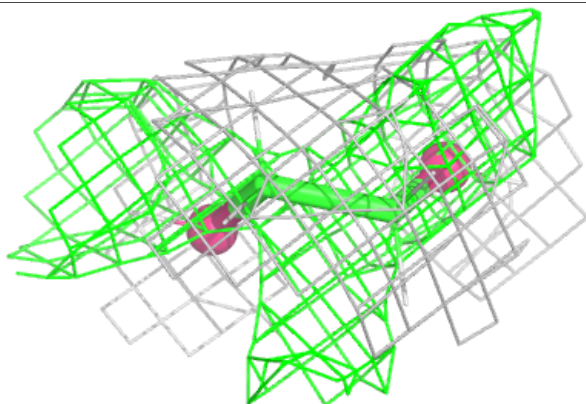
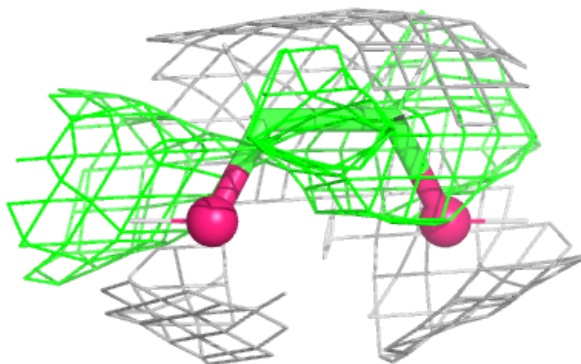


Electron density around EDO F 506:

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

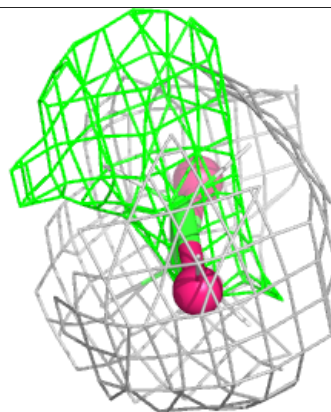
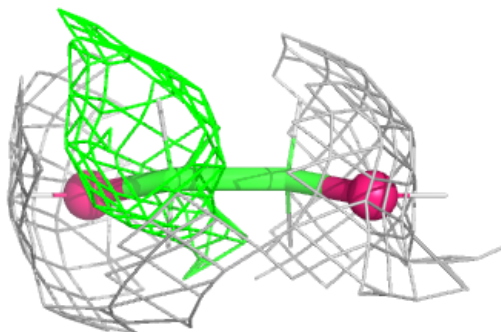
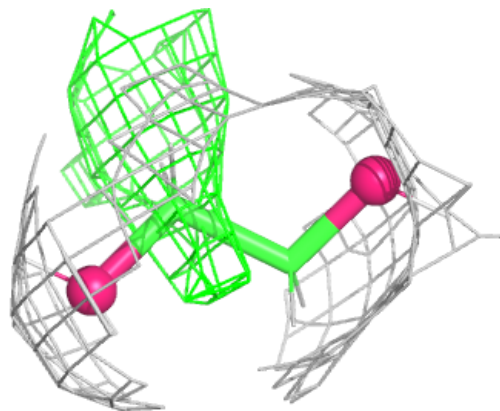
**Electron density around EDO D 2011:**

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



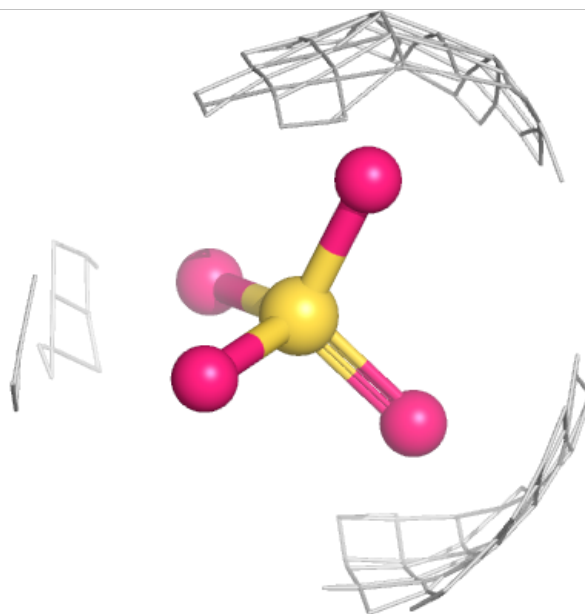
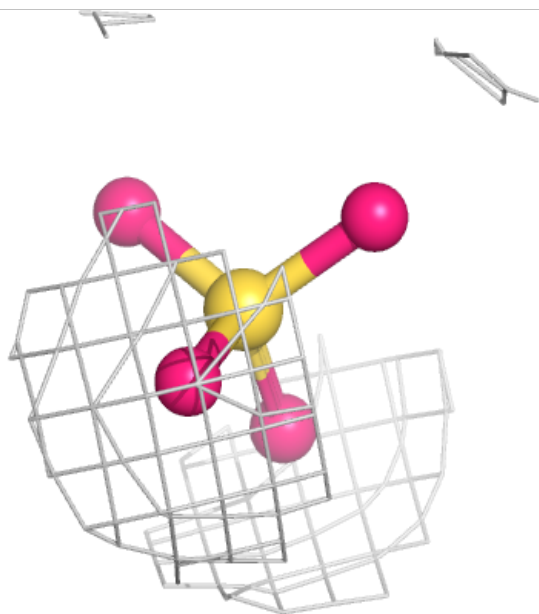
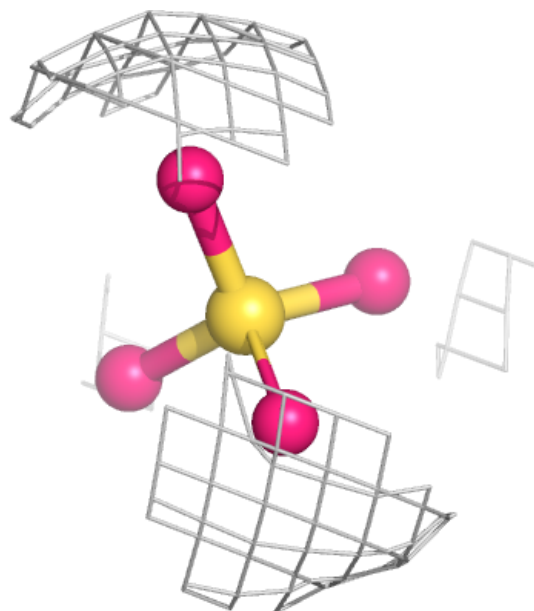
Electron density around EDO C 1204:

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



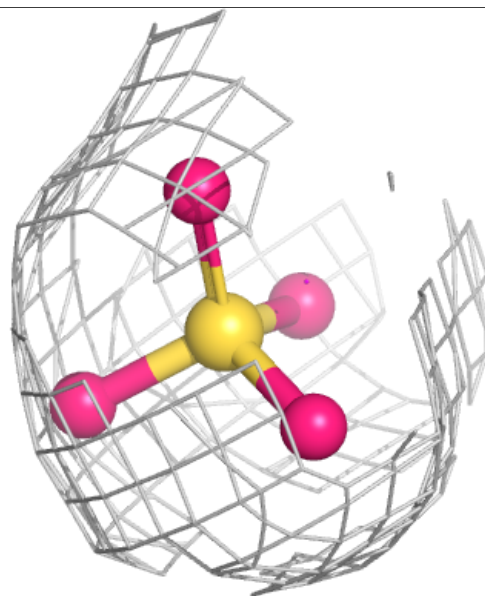
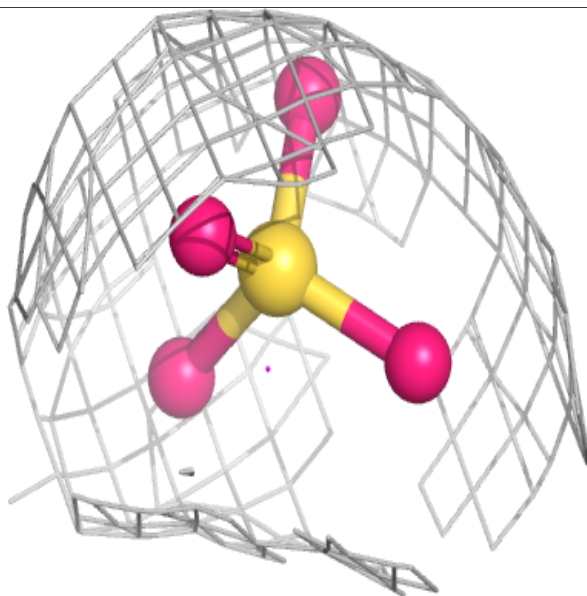
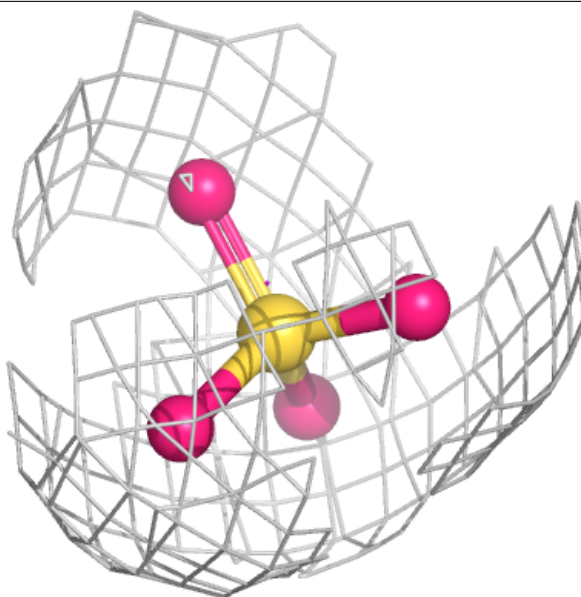
Electron density around SO4 F 501:

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



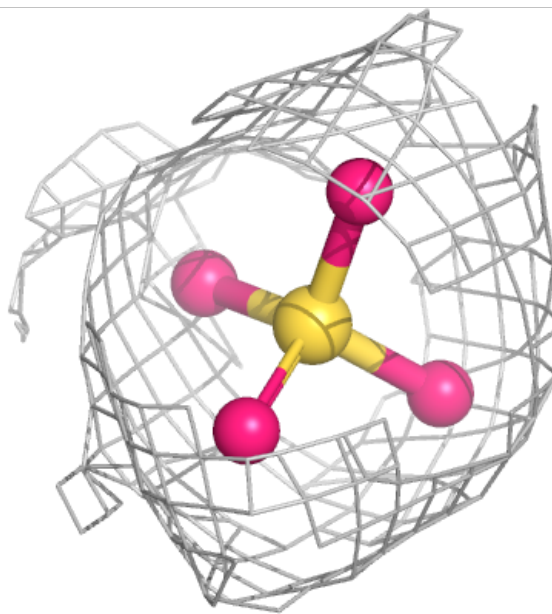
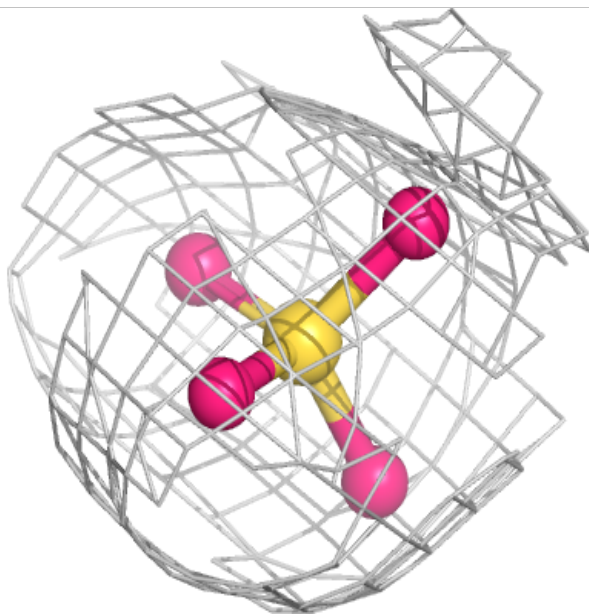
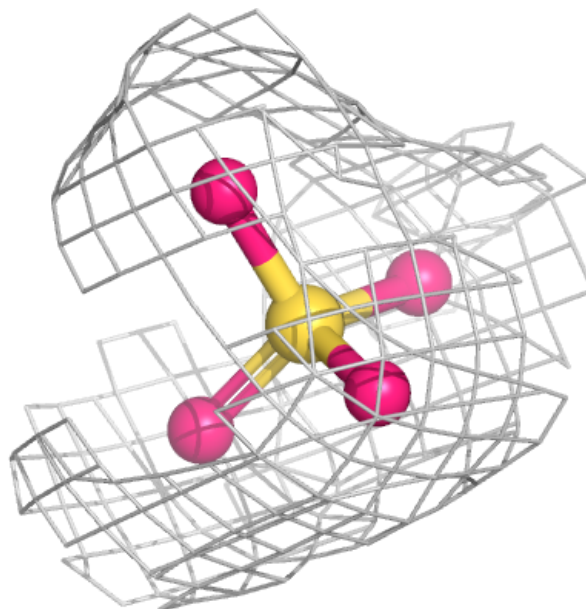
Electron density around SO4 F 503:

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



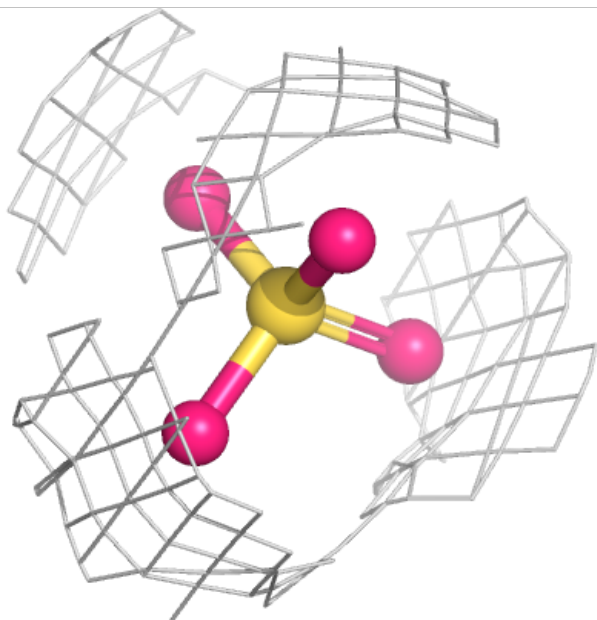
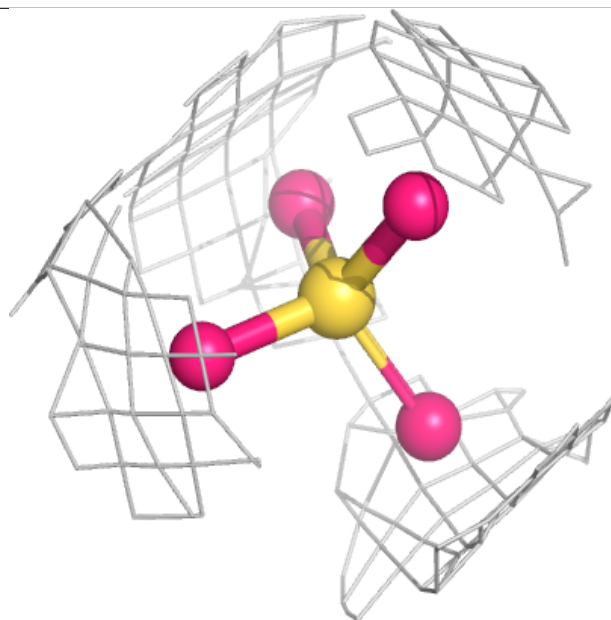
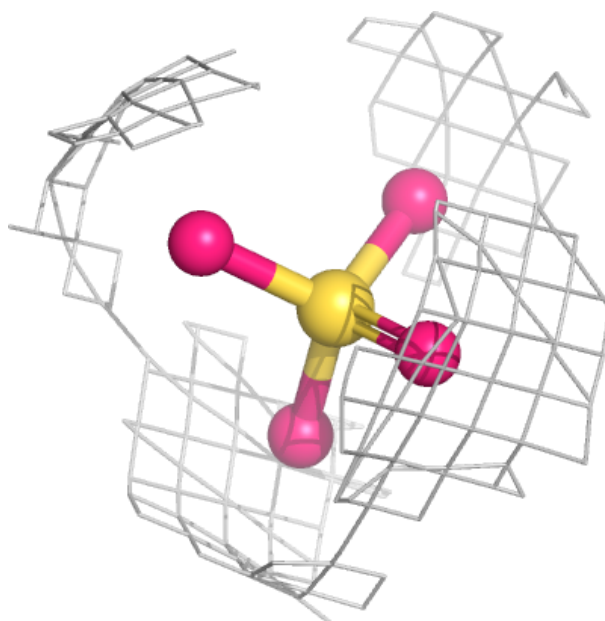
Electron density around SO4 D 2006:

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



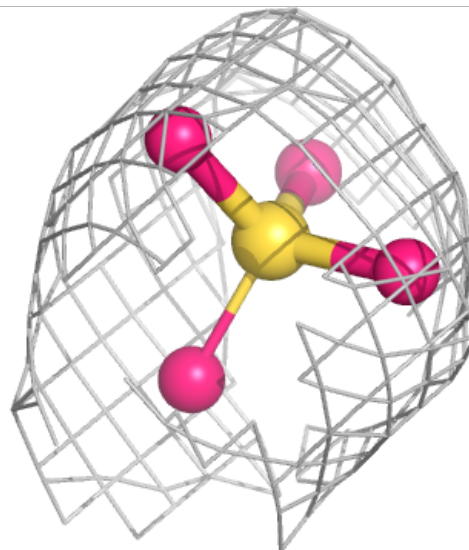
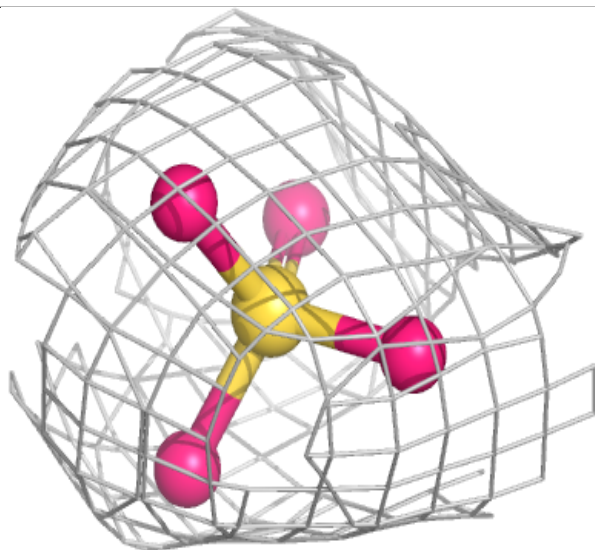
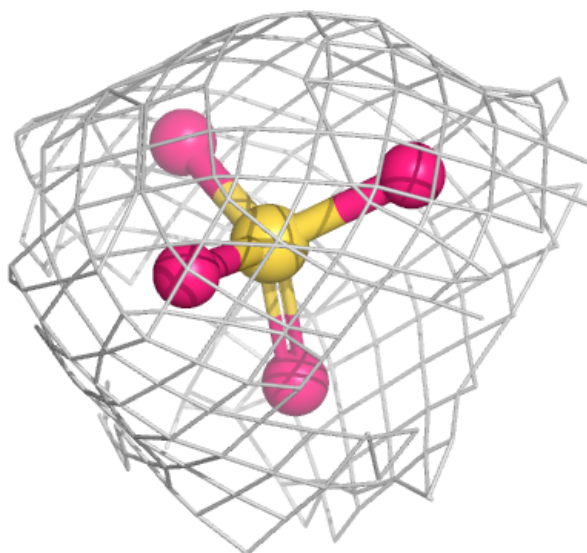
Electron density around SO4 D 2005:

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



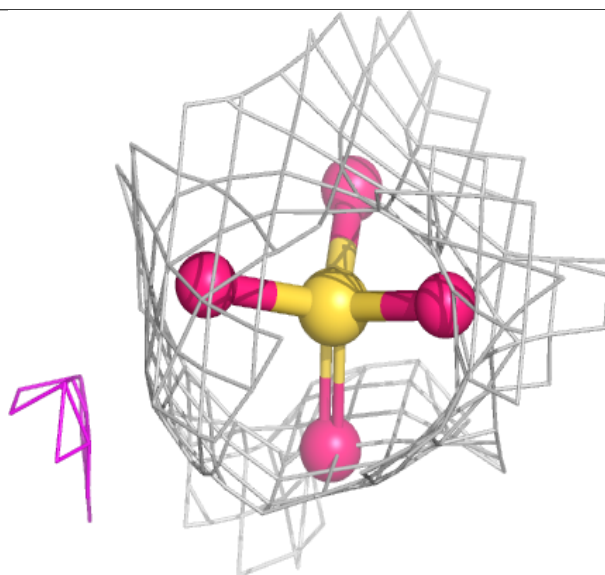
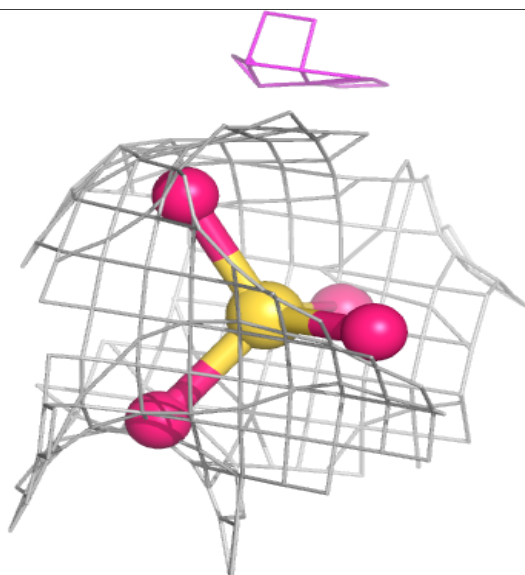
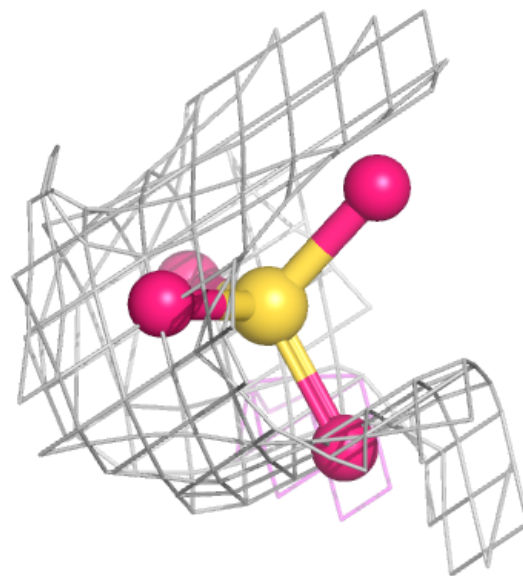
Electron density around SO4 D 2010:

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



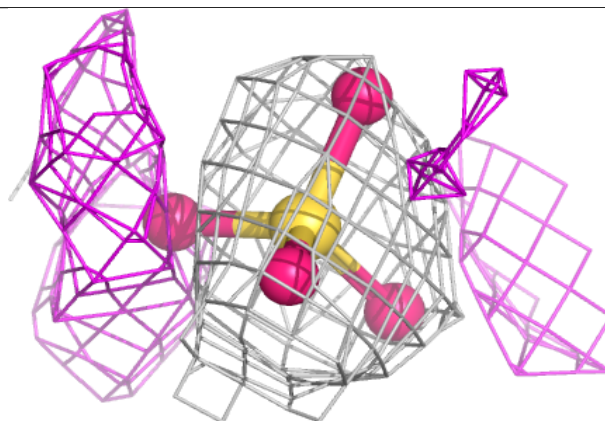
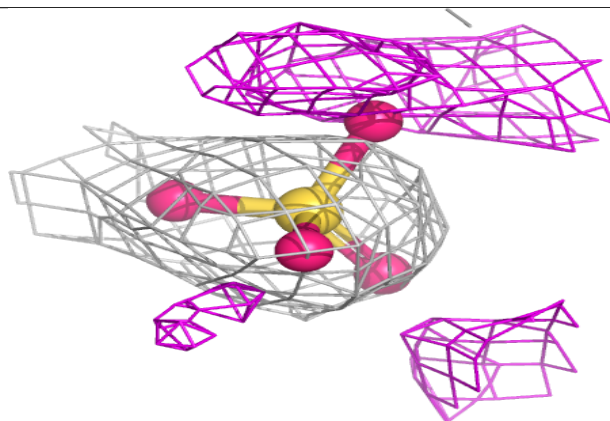
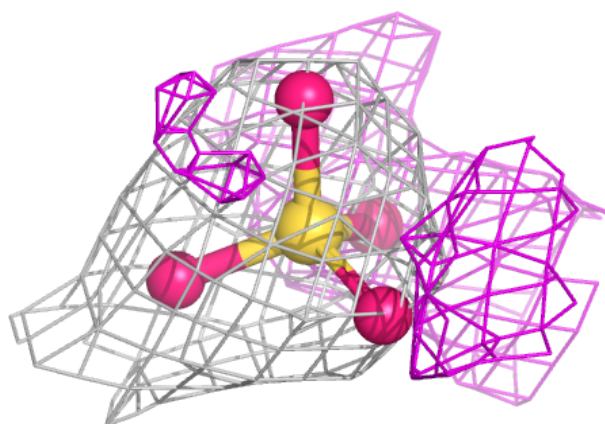
Electron density around SO4 C 1206:

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



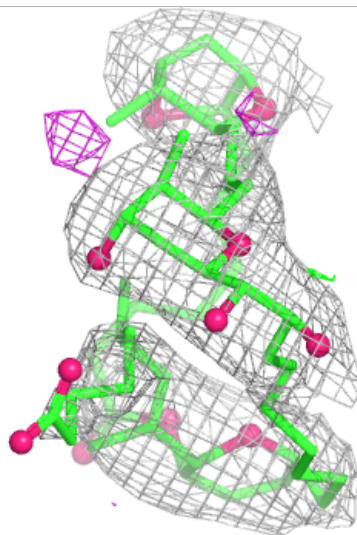
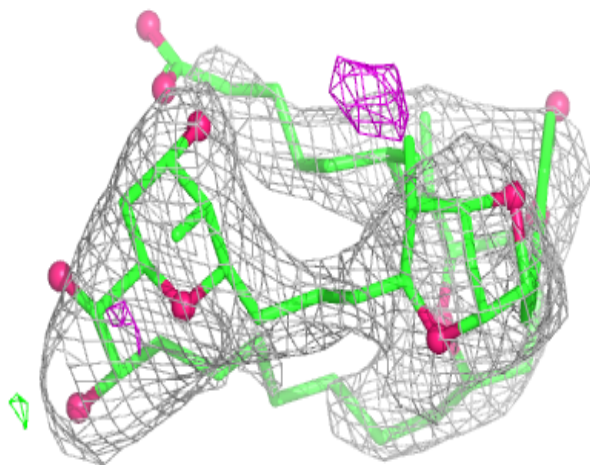
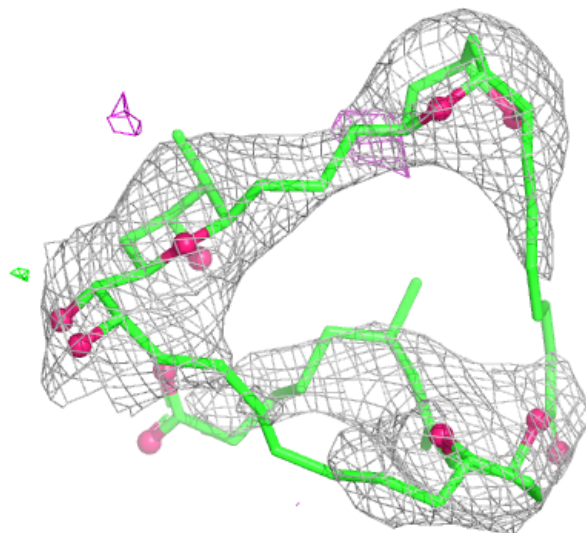
Electron density around SO4 F 505:

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



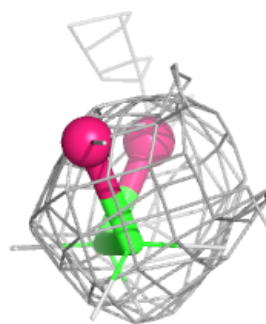
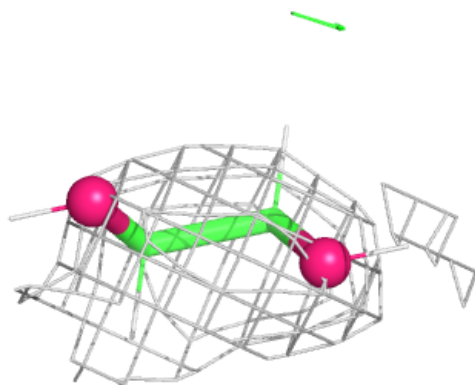
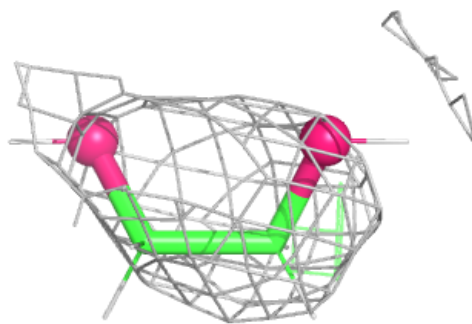
Electron density around SRN C 1205:

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



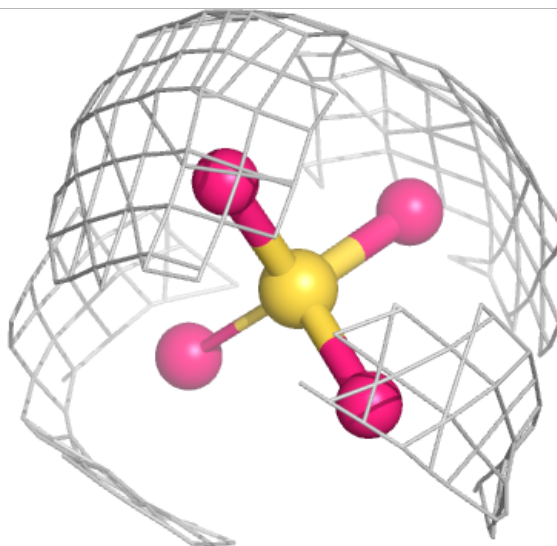
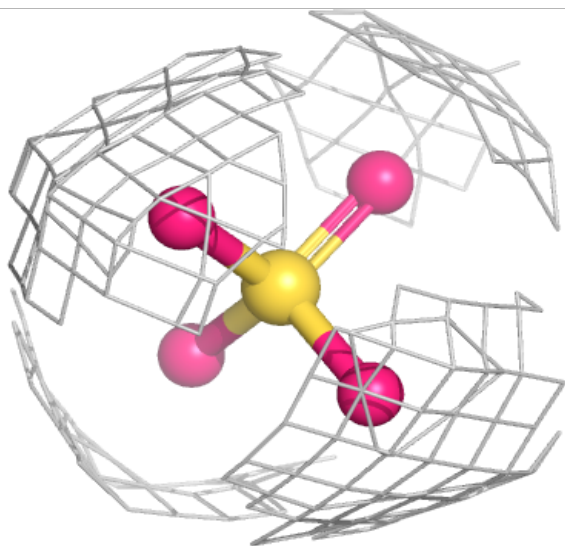
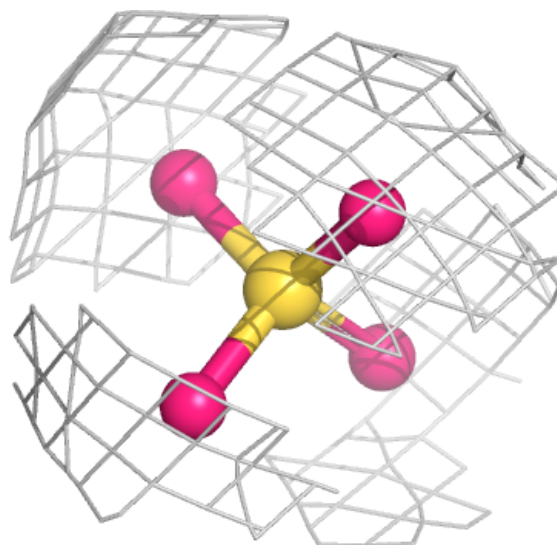
Electron density around EDO D 2009:

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



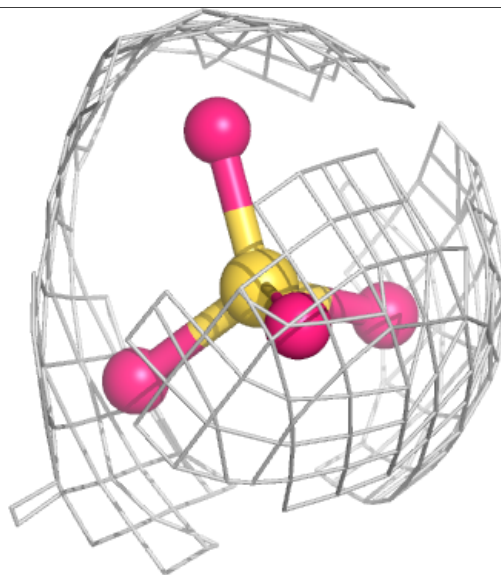
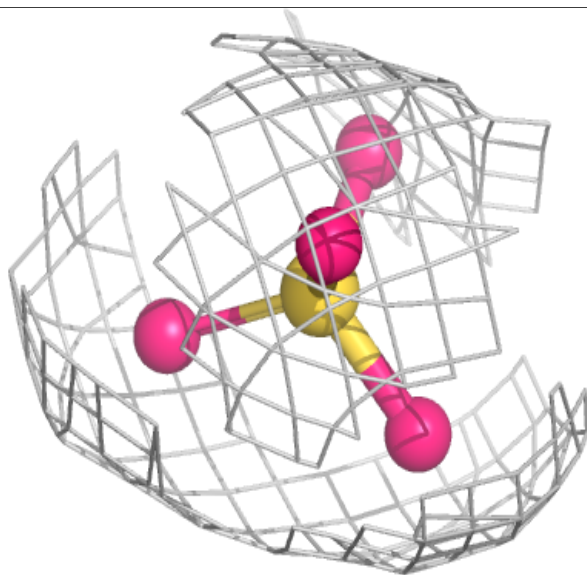
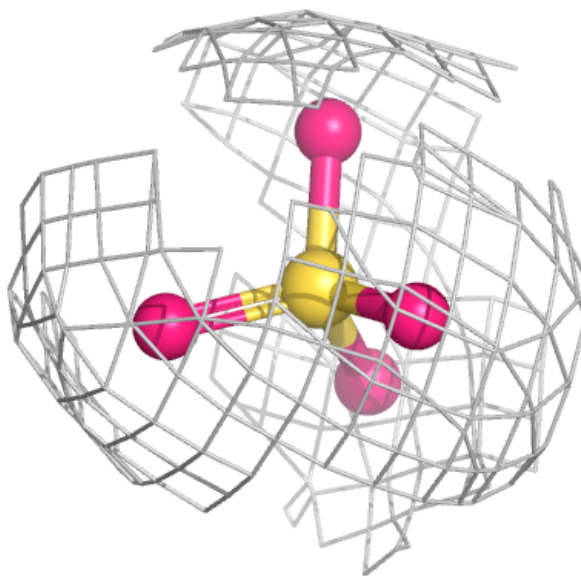
Electron density around SO4 F 502:

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



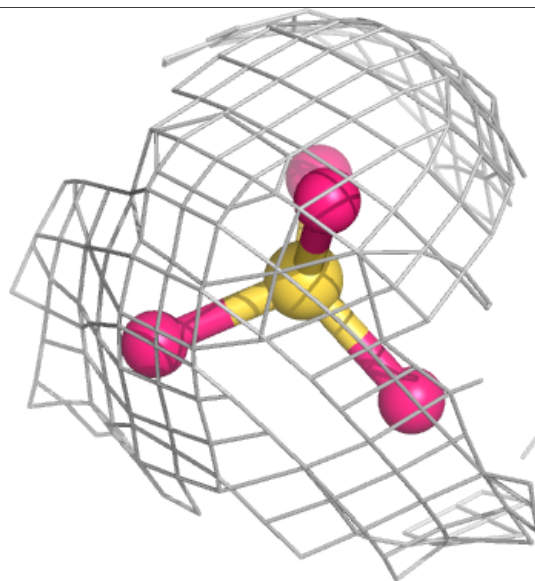
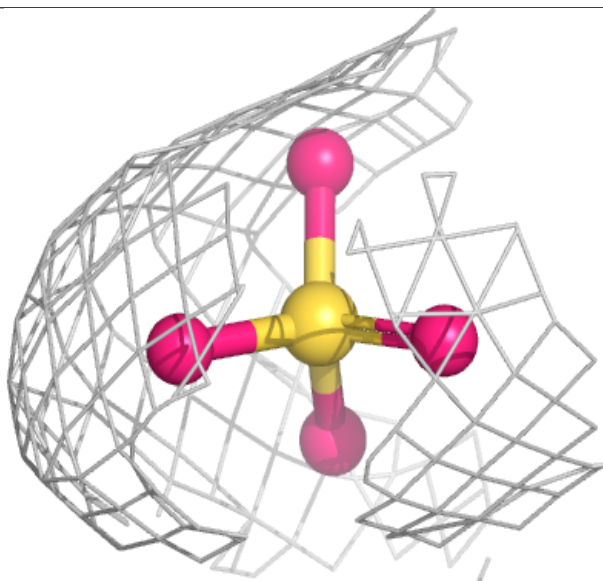
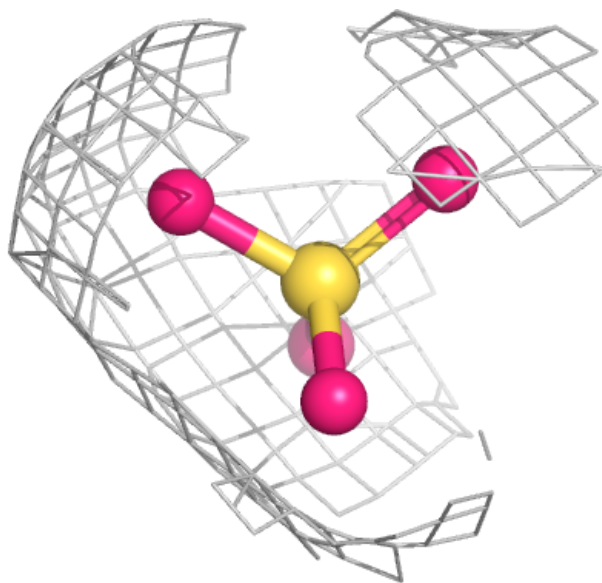
Electron density around SO4 D 2003:

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



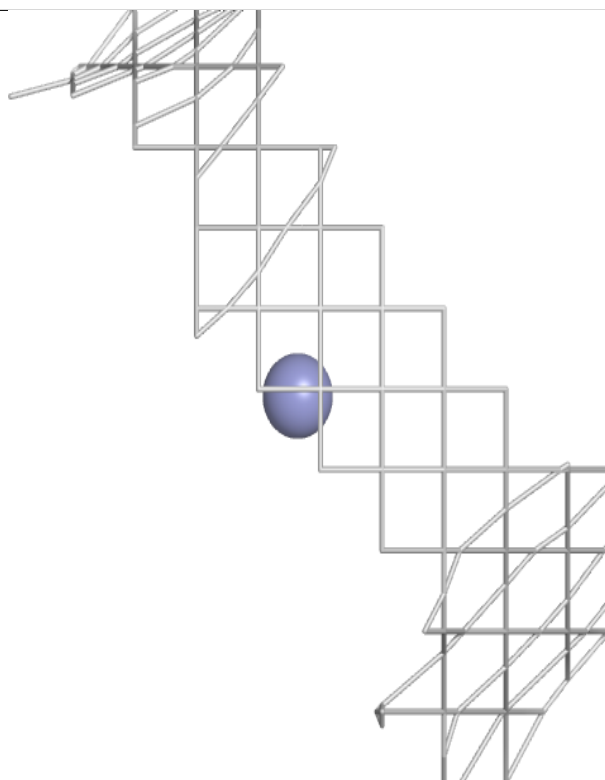
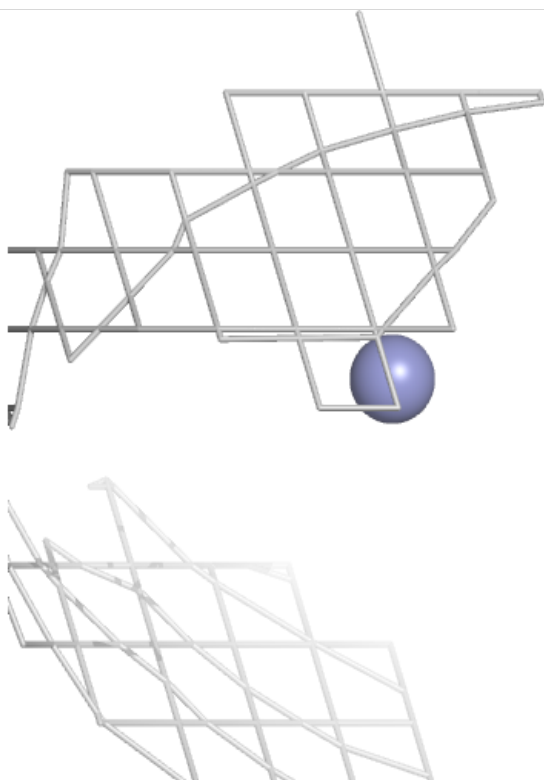
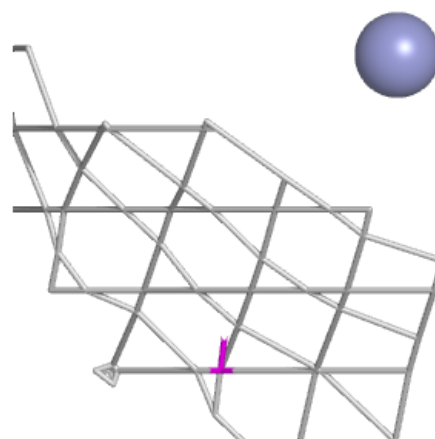
Electron density around SO4 D 2004:

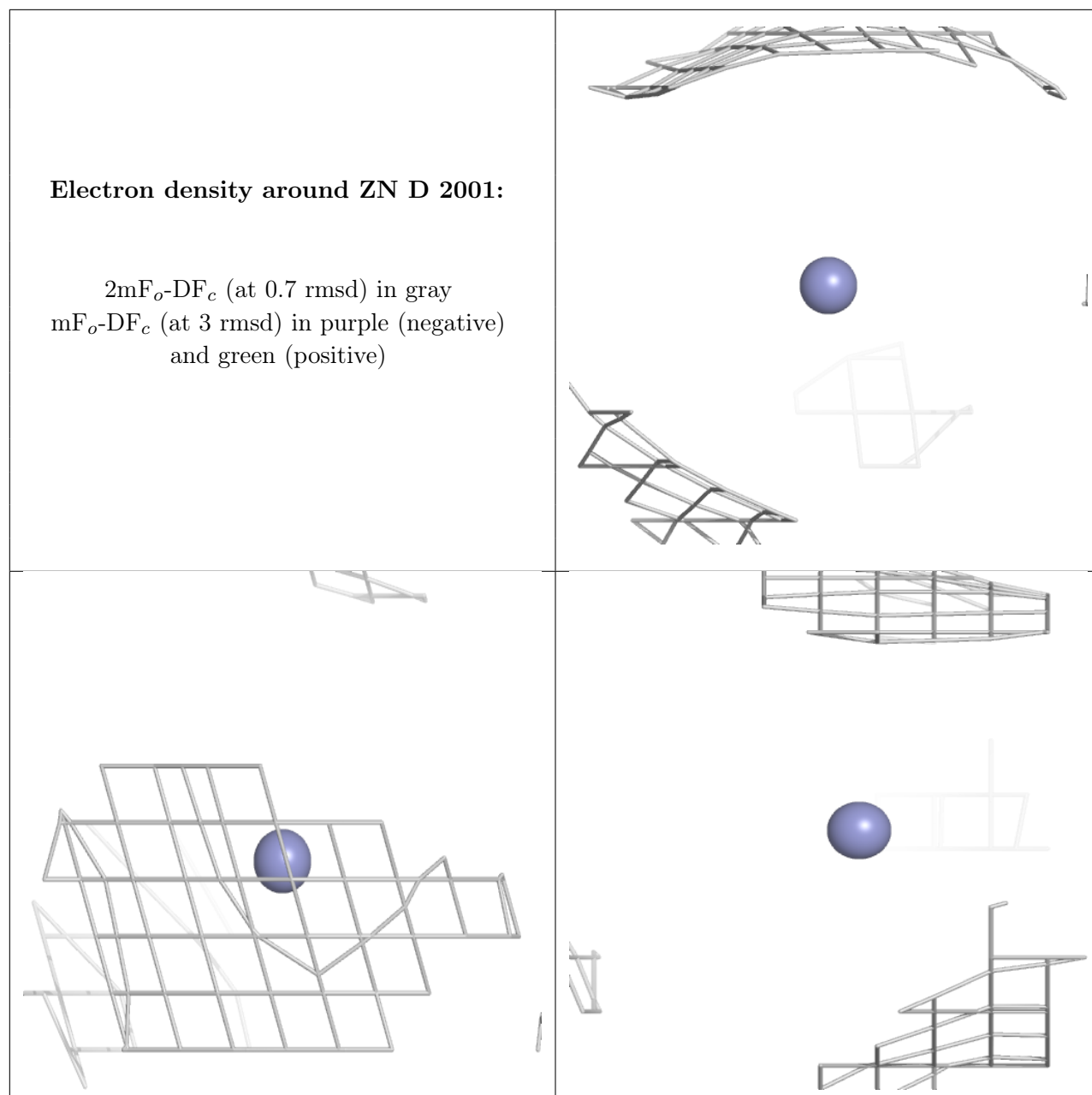
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.