



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:58 PM UTC

PDB ID : 8DOL / pdb_00008dol
Title : Mechanism of regulation of the Helicobacter pylori Cagbeta ATPase by CagZ
Authors : Wu, X.; Zhao, Y.; Yang, W.; Sun, L.; Ye, X.; Jiang, M.; Wang, Q.; Wang, Q.;
Zhang, X.; Wu, Y.
Deposited on : 2022-07-13
Resolution : 2.80 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

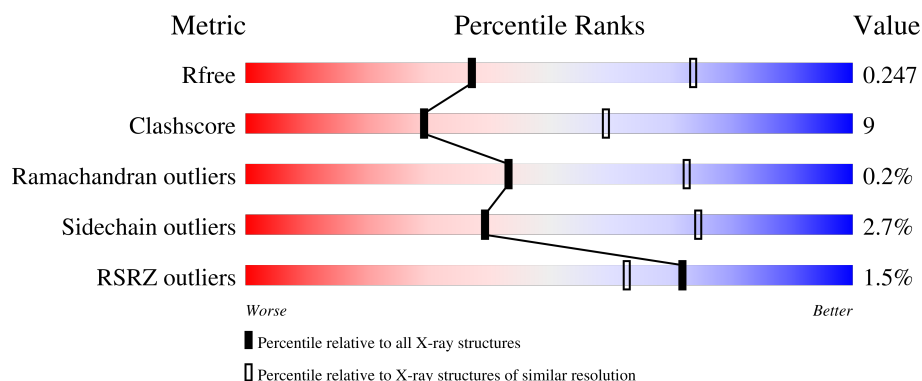
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	593	0.2% 74% 16% 9%
1	B	593	0.2% 64% 20% 16%
1	C	593	2% 66% 19% 14%
1	D	593	0.2% 72% 17% 11%
1	E	593	2% 70% 20% 9%

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Mol	Chain	Length	Quality of chain
1	F	593	2% 65% 23% • 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24565 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cag pathogenicity island protein (Cag5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4301	2760	716	797	28			
1	B	498	Total	C	N	O	S	0	0	0
			3861	2480	643	714	24			
1	C	510	Total	C	N	O	S	0	0	0
			3741	2390	635	697	19			
1	D	530	Total	C	N	O	S	0	0	0
			4186	2688	693	778	27			
1	E	540	Total	C	N	O	S	0	0	0
			4273	2739	713	794	27			
1	F	527	Total	C	N	O	S	0	0	0
			4120	2648	677	770	25			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP O25260
A	157	THR	-	expression tag	UNP O25260
A	158	SER	-	expression tag	UNP O25260
A	159	SER	-	expression tag	UNP O25260
A	160	MET	-	expression tag	UNP O25260
A	161	ALA	-	expression tag	UNP O25260
A	162	ASP	-	expression tag	UNP O25260
A	163	ILE	-	expression tag	UNP O25260
A	164	GLY	-	expression tag	UNP O25260
A	165	SER	-	expression tag	UNP O25260
B	156	GLY	-	expression tag	UNP O25260
B	157	THR	-	expression tag	UNP O25260
B	158	SER	-	expression tag	UNP O25260
B	159	SER	-	expression tag	UNP O25260
B	160	MET	-	expression tag	UNP O25260
B	161	ALA	-	expression tag	UNP O25260
B	162	ASP	-	expression tag	UNP O25260

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Chain	Residue	Modelled	Actual	Comment	Reference
B	163	ILE	-	expression tag	UNP O25260
B	164	GLY	-	expression tag	UNP O25260
B	165	SER	-	expression tag	UNP O25260
C	156	GLY	-	expression tag	UNP O25260
C	157	THR	-	expression tag	UNP O25260
C	158	SER	-	expression tag	UNP O25260
C	159	SER	-	expression tag	UNP O25260
C	160	MET	-	expression tag	UNP O25260
C	161	ALA	-	expression tag	UNP O25260
C	162	ASP	-	expression tag	UNP O25260
C	163	ILE	-	expression tag	UNP O25260
C	164	GLY	-	expression tag	UNP O25260
C	165	SER	-	expression tag	UNP O25260
D	156	GLY	-	expression tag	UNP O25260
D	157	THR	-	expression tag	UNP O25260
D	158	SER	-	expression tag	UNP O25260
D	159	SER	-	expression tag	UNP O25260
D	160	MET	-	expression tag	UNP O25260
D	161	ALA	-	expression tag	UNP O25260
D	162	ASP	-	expression tag	UNP O25260
D	163	ILE	-	expression tag	UNP O25260
D	164	GLY	-	expression tag	UNP O25260
D	165	SER	-	expression tag	UNP O25260
E	156	GLY	-	expression tag	UNP O25260
E	157	THR	-	expression tag	UNP O25260
E	158	SER	-	expression tag	UNP O25260
E	159	SER	-	expression tag	UNP O25260
E	160	MET	-	expression tag	UNP O25260
E	161	ALA	-	expression tag	UNP O25260
E	162	ASP	-	expression tag	UNP O25260
E	163	ILE	-	expression tag	UNP O25260
E	164	GLY	-	expression tag	UNP O25260
E	165	SER	-	expression tag	UNP O25260
F	156	GLY	-	expression tag	UNP O25260
F	157	THR	-	expression tag	UNP O25260
F	158	SER	-	expression tag	UNP O25260
F	159	SER	-	expression tag	UNP O25260
F	160	MET	-	expression tag	UNP O25260
F	161	ALA	-	expression tag	UNP O25260
F	162	ASP	-	expression tag	UNP O25260
F	163	ILE	-	expression tag	UNP O25260
F	164	GLY	-	expression tag	UNP O25260

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Chain	Residue	Modelled	Actual	Comment	Reference
F	165	SER	-	expression tag	UNP O25260

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		

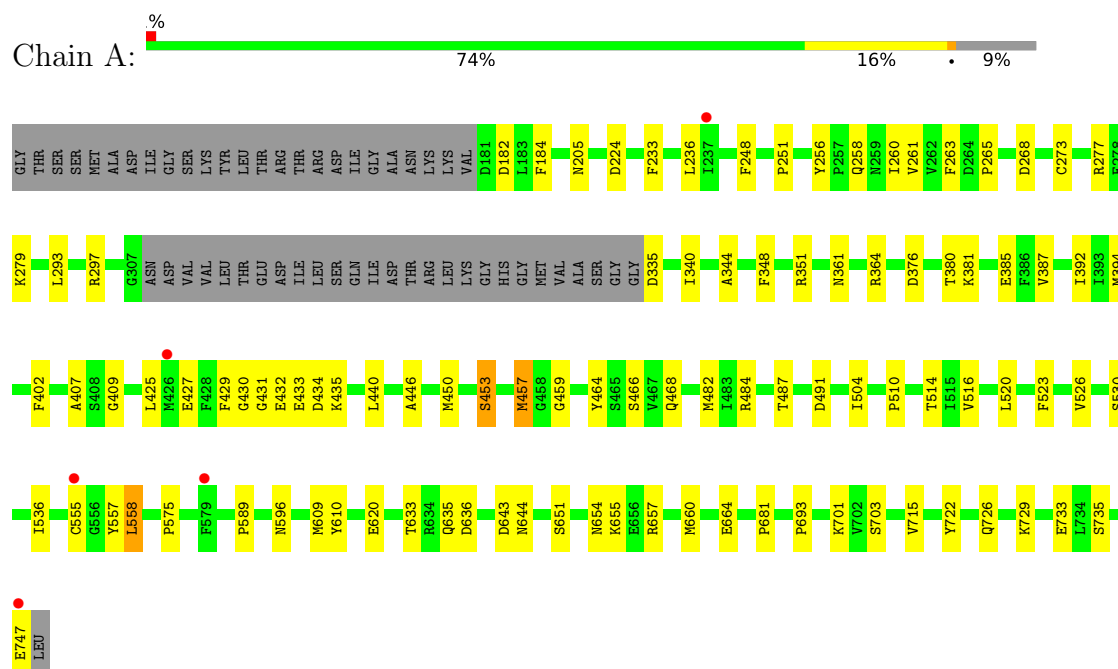
- Molecule 4 is water.

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

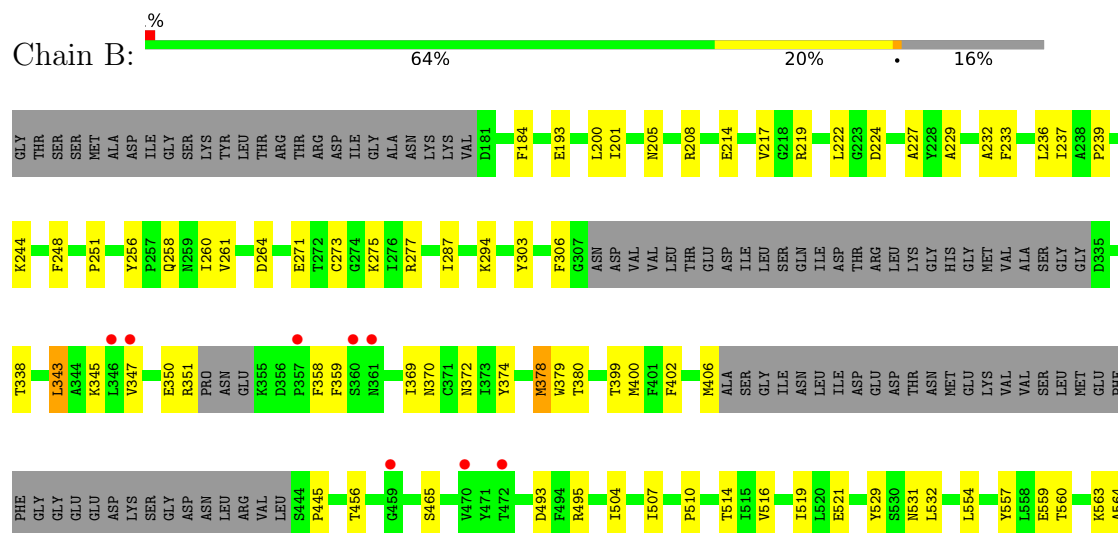
3 Residue-property plots

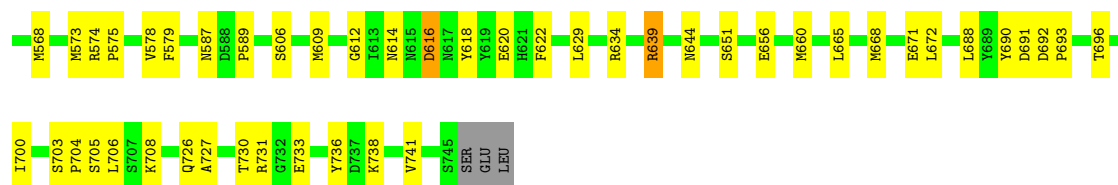
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Cag pathogenicity island protein (Cag5)

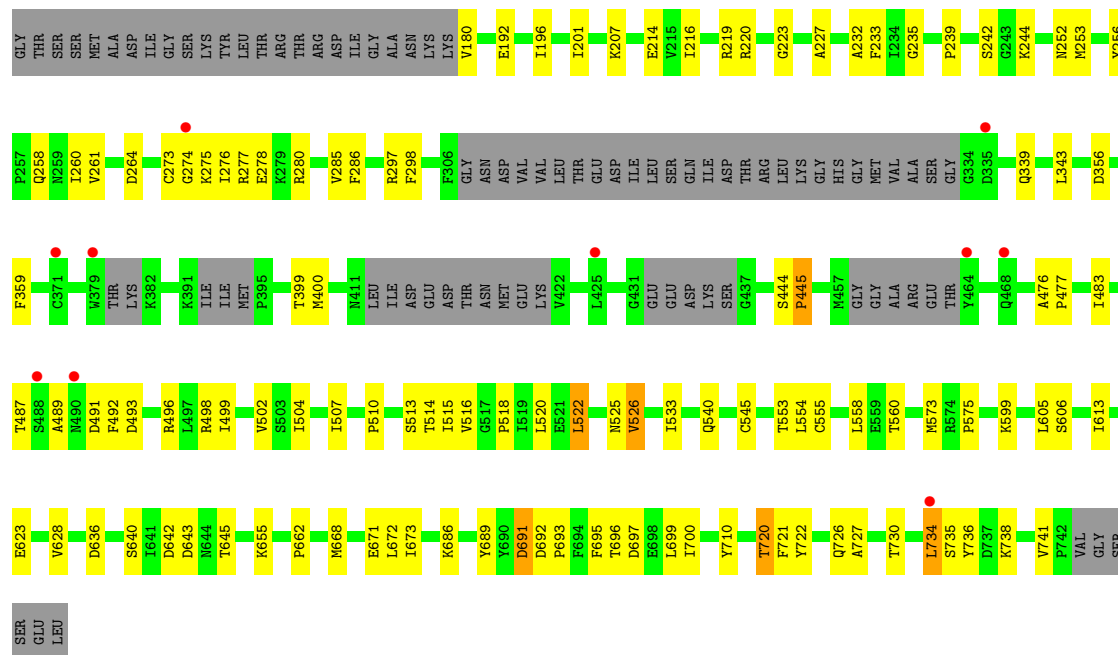


- Molecule 1: Cag pathogenicity island protein (Cag5)

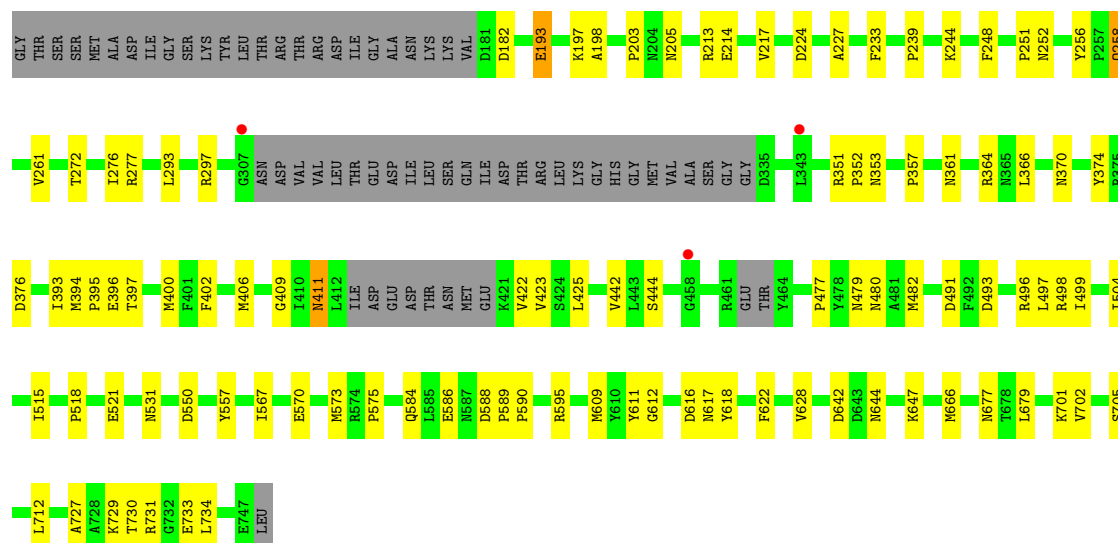




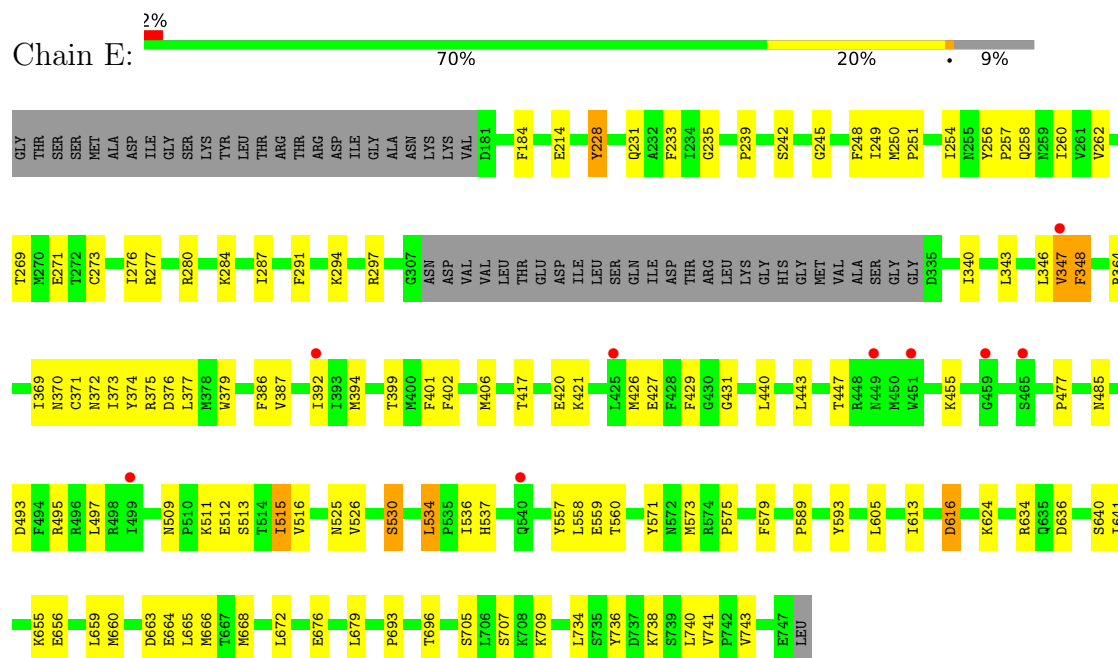
• Molecule 1: Cag pathogenicity island protein (Cag5)



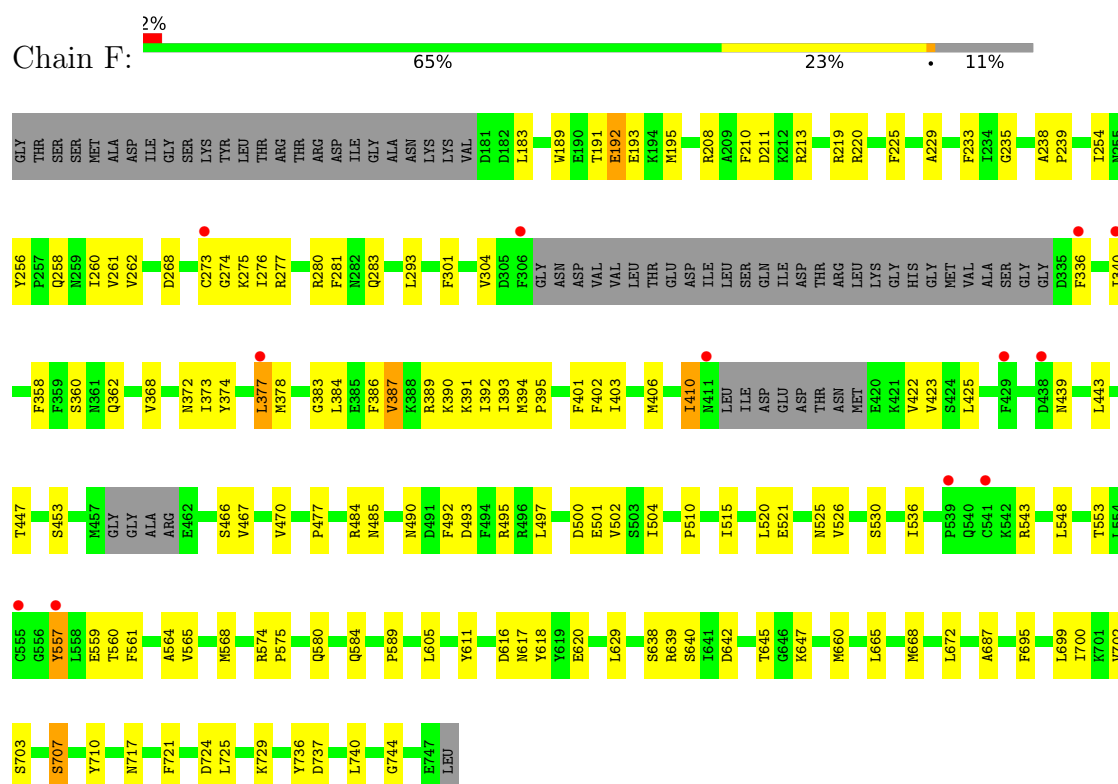
• Molecule 1: Cag pathogenicity island protein (Cag5)



- Molecule 1: Cag pathogenicity island protein (Cag5)



- Molecule 1: Cag pathogenicity island protein (Cag5)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.11Å 163.28Å 112.22Å 90.00° 93.33° 90.00°	Depositor
Resolution (Å)	40.79 – 2.80 40.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.79-2.80) 99.3 (40.79-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.247 0.198 , 0.247	Depositor DCC
R_{free} test set	1988 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24565	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/4397	0.30	0/5932
1	B	0.13	0/3946	0.34	2/5334 (0.0%)
1	C	0.14	0/3814	0.33	0/5170
1	D	0.13	0/4280	0.30	0/5780
1	E	0.12	0/4368	0.30	0/5898
1	F	0.12	0/4211	0.30	0/5695
All	All	0.13	0/25016	0.31	2/33809 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	PRO	N-CA-CB	6.40	110.31	103.52
1	B	378	MET	CB-CG-SD	5.17	128.20	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4301	0	4260	59	0
1	B	3861	0	3707	74	0
1	C	3741	0	3439	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4186	0	4097	62	0
1	E	4273	0	4199	77	0
1	F	4120	0	4009	92	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	7	0	10	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	7	0	10	0	0
3	E	7	0	10	0	0
3	F	7	0	10	1	0
4	A	3	0	0	2	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	3	0	0	1	0
4	F	1	0	0	0	0
All	All	24565	0	23771	416	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ASP:OD1	1:C:359:PHE:N	2.10	0.84
1:F:192:GLU:OE2	1:F:220:ARG:NH1	2.13	0.80
1:D:611:TYR:O	4:D:901:HOH:O	2.02	0.78
1:E:493:ASP:OD1	1:E:495:ARG:HG3	1.86	0.75
1:A:596:ASN:OD1	1:B:587:ASN:ND2	2.19	0.74
1:A:205:ASN:ND2	1:A:224:ASP:OD1	2.16	0.73
1:A:487:THR:O	4:A:901:HOH:O	2.05	0.73
1:E:271:GLU:OE2	1:E:738:LYS:NZ	2.17	0.73
1:D:293:LEU:HG	1:D:482:MET:HE1	1.72	0.72
1:B:705:SER:HA	1:B:708:LYS:HE2	1.76	0.68
1:D:677:ASN:HB3	1:E:613:ILE:HD12	1.75	0.68
1:A:482:MET:HE3	1:A:482:MET:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:LEU:O	1:D:370:ASN:ND2	2.26	0.67
1:E:427:GLU:HA	1:E:431:GLY:HA3	1.76	0.67
1:E:525:ASN:HA	1:E:560:THR:HG21	1.77	0.67
1:F:268:ASP:OD1	1:F:729:LYS:NZ	2.27	0.67
1:F:642:ASP:OD1	1:F:645:THR:N	2.24	0.66
1:D:586:GLU:HG2	1:D:595:ARG:HA	1.78	0.66
1:E:376:ASP:OD2	1:E:447:THR:OG1	2.06	0.66
1:D:731:ARG:NH2	1:D:733:GLU:OE2	2.29	0.65
1:F:189:TRP:HE1	3:F:802:PEG:H11	1.61	0.65
1:C:239:PRO:HG2	1:C:613:ILE:HG12	1.79	0.64
1:E:477:PRO:HB3	1:E:515:ILE:HB	1.78	0.64
1:B:261:VAL:HG22	1:B:504:ILE:HB	1.80	0.64
1:C:275:LYS:N	1:C:735:SER:O	2.30	0.64
1:D:297:ARG:N	1:D:491:ASP:OD2	2.23	0.64
1:A:268:ASP:OD1	1:A:729:LYS:NZ	2.30	0.64
1:C:492:PHE:HZ	1:C:502:VAL:HG11	1.63	0.64
1:C:693:PRO:O	1:C:697:ASP:HB2	1.97	0.63
1:B:531:ASN:HB2	1:B:573:MET:HE2	1.81	0.63
1:C:261:VAL:HG22	1:C:504:ILE:HB	1.80	0.62
1:B:639:ARG:NH2	1:C:643:ASP:OD2	2.33	0.62
1:E:348:PHE:C	1:E:364:ARG:HH12	2.08	0.61
1:C:493:ASP:HB3	1:C:496:ARG:HG3	1.82	0.61
1:A:536:ILE:HG12	1:B:730:THR:HG21	1.83	0.61
1:F:358:PHE:C	1:F:362:GLN:HE22	2.09	0.61
1:C:297:ARG:HE	1:C:489:ALA:HB3	1.65	0.60
1:F:485:ASN:HD21	1:F:744:GLY:HA3	1.66	0.60
1:A:644:ASN:HD22	1:F:647:LYS:HD3	1.66	0.60
1:B:369:ILE:HA	1:B:372:ASN:HB2	1.83	0.60
1:C:235:GLY:HA3	1:C:605:LEU:HD13	1.83	0.60
1:C:339:GLN:O	1:C:343:LEU:HD12	2.01	0.59
1:F:261:VAL:HG22	1:F:504:ILE:HB	1.85	0.59
1:B:184:PHE:HB3	1:B:656:GLU:HB3	1.84	0.59
1:D:731:ARG:HH21	1:D:733:GLU:CD	2.10	0.59
1:F:256:TYR:HB3	1:F:260:ILE:HD11	1.83	0.59
1:A:387:VAL:HG13	1:A:392:ILE:HB	1.85	0.59
1:F:275:LYS:HG2	1:F:702:VAL:HB	1.84	0.59
1:D:361:ASN:HA	1:D:364:ARG:HH12	1.66	0.59
1:B:205:ASN:ND2	1:B:224:ASP:OD1	2.31	0.59
1:F:389:ARG:HD2	1:F:390:LYS:HD3	1.85	0.59
1:A:256:TYR:HB3	1:A:260:ILE:HD11	1.85	0.58
1:B:629:LEU:HD12	1:B:660:MET:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:GLY:N	1:C:692:ASP:OD2	2.37	0.58
1:C:700:ILE:HD13	1:C:710:TYR:HB2	1.85	0.58
1:B:214:GLU:HB3	1:B:227:ALA:HB1	1.85	0.58
1:F:620:GLU:H	1:F:620:GLU:CD	2.12	0.58
1:D:182:ASP:OD1	1:E:634:ARG:NH2	2.29	0.57
1:F:737:ASP:HB3	1:F:740:LEU:HD13	1.85	0.57
1:F:392:ILE:HG23	1:F:410:ILE:HG23	1.86	0.57
1:A:526:VAL:O	1:A:530:SER:HB2	2.05	0.57
1:C:273:CYS:O	1:C:277:ARG:HG2	2.04	0.57
1:B:516:VAL:HA	1:B:519:ILE:HD13	1.87	0.56
1:D:477:PRO:HB3	1:D:515:ILE:HG23	1.86	0.56
1:D:374:TYR:OH	1:D:396:GLU:O	2.22	0.56
1:D:193:GLU:HG2	1:D:197:LYS:HE3	1.88	0.56
1:A:394:MET:HG2	1:A:402:PHE:CZ	2.41	0.56
1:D:493:ASP:HB3	1:D:496:ARG:HG3	1.88	0.56
1:A:261:VAL:HG22	1:A:504:ILE:HB	1.88	0.56
1:A:660:MET:HE2	1:A:664:GLU:HB3	1.88	0.55
1:C:399:THR:OG1	1:C:487:THR:O	2.20	0.55
1:B:519:ILE:HD12	1:B:519:ILE:H	1.72	0.55
1:E:399:THR:HG22	1:E:401:PHE:H	1.71	0.55
1:E:239:PRO:HB2	1:E:613:ILE:HG13	1.88	0.55
1:B:222:LEU:HD22	1:B:692:ASP:HA	1.89	0.55
1:E:377:LEU:HD21	1:E:386:PHE:HD2	1.72	0.55
1:A:348:PHE:O	1:A:364:ARG:NH1	2.38	0.55
1:C:297:ARG:NE	1:C:489:ALA:HB3	2.22	0.55
1:D:357:PRO:O	1:D:361:ASN:ND2	2.32	0.55
1:D:642:ASP:OD1	1:D:644:ASN:N	2.38	0.55
1:D:214:GLU:HB3	1:D:227:ALA:HB1	1.88	0.54
1:E:429:PHE:HB3	1:E:440:LEU:HD13	1.88	0.54
1:B:233:PHE:CE1	1:B:575:PRO:HD2	2.42	0.54
1:D:409:GLY:HA2	1:D:425:LEU:HD22	1.89	0.54
1:A:557:TYR:HB2	1:A:589:PRO:O	2.08	0.54
1:C:214:GLU:HB3	1:C:227:ALA:HB1	1.89	0.54
1:E:294:LYS:HZ2	1:E:741:VAL:HB	1.71	0.54
1:B:665:LEU:O	1:B:668:MET:HG3	2.08	0.54
1:E:660:MET:HE2	1:E:664:GLU:HB3	1.89	0.54
1:F:485:ASN:ND2	1:F:744:GLY:HA3	2.23	0.54
1:A:293:LEU:HD13	1:A:482:MET:HE1	1.90	0.53
1:B:557:TYR:HB2	1:B:589:PRO:O	2.08	0.53
1:A:453:SER:O	1:A:457:MET:HG3	2.08	0.53
1:F:377:LEU:HD21	1:F:443:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:HG2	1:A:555:CYS:HA	1.90	0.53
1:C:727:ALA:O	1:C:730:THR:OG1	2.22	0.53
1:D:480:ASN:OD1	1:D:482:MET:N	2.42	0.53
1:D:497:LEU:HD23	1:D:573:MET:HE1	1.91	0.53
1:C:636:ASP:HB2	1:C:655:LYS:HG3	1.91	0.52
1:F:233:PHE:CE1	1:F:575:PRO:HD2	2.43	0.52
1:D:394:MET:HG3	1:D:402:PHE:CZ	2.44	0.52
1:A:182:ASP:OD1	1:B:634:ARG:NH2	2.41	0.52
1:A:635:GLN:NE2	1:A:654:ASN:OD1	2.42	0.52
1:A:703:SER:OG	1:A:733:GLU:OE1	2.27	0.52
1:B:193:GLU:H	1:B:193:GLU:CD	2.18	0.52
1:C:518:PRO:O	1:C:522:LEU:HG	2.09	0.52
1:F:629:LEU:HD12	1:F:660:MET:HB2	1.90	0.52
1:B:287:ILE:HG13	1:B:736:TYR:CZ	2.44	0.52
1:D:272:THR:HG23	1:D:729:LYS:HD2	1.91	0.52
1:C:400:MET:HB2	1:C:487:THR:HG21	1.92	0.52
1:D:233:PHE:CE1	1:D:575:PRO:HD2	2.43	0.52
1:D:701:LYS:HG3	1:D:712:LEU:HD21	1.91	0.52
1:B:704:PRO:O	1:B:708:LYS:HG3	2.09	0.52
1:D:616:ASP:OD1	1:D:617:ASN:N	2.43	0.52
1:C:286:PHE:CD2	1:C:492:PHE:HD2	2.28	0.52
1:B:620:GLU:CD	1:B:620:GLU:H	2.18	0.52
1:F:510:PRO:HG3	1:F:520:LEU:HD12	1.92	0.52
1:F:390:LYS:HB2	1:F:392:ILE:HD11	1.91	0.51
1:E:291:PHE:HZ	1:E:515:ILE:HD11	1.75	0.51
1:B:256:TYR:CE2	1:B:258:GLN:HB2	2.45	0.51
1:B:347:VAL:HG22	1:B:400:MET:HE1	1.92	0.51
1:E:370:ASN:HA	1:E:373:ILE:HD12	1.92	0.51
1:A:273:CYS:O	1:A:277:ARG:HG2	2.10	0.51
1:E:256:TYR:HB3	1:E:260:ILE:HD11	1.93	0.51
1:F:521:GLU:OE2	1:F:559:GLU:N	2.31	0.51
1:E:373:ILE:HG23	1:E:443:LEU:HD21	1.93	0.50
1:B:668:MET:HB3	1:B:671:GLU:HB2	1.93	0.50
1:E:387:VAL:HA	1:E:392:ILE:HD12	1.91	0.50
1:F:273:CYS:O	1:F:277:ARG:HG2	2.12	0.50
1:A:335:ASP:N	1:A:335:ASP:OD1	2.45	0.50
1:B:651:SER:HA	1:C:640:SER:HA	1.93	0.50
1:C:555:CYS:HB3	1:C:558:LEU:HD23	1.92	0.50
1:E:374:TYR:HB2	1:E:406:MET:HE1	1.92	0.50
1:F:340:ILE:HG22	1:F:368:VAL:HG22	1.93	0.50
1:F:403:ILE:HA	1:F:406:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PHE:CE1	1:A:575:PRO:HD2	2.47	0.50
1:A:636:ASP:OD2	1:A:655:LYS:NZ	2.42	0.50
1:A:409:GLY:HA2	1:A:425:LEU:HD23	1.94	0.50
1:A:344:ALA:HB1	1:A:364:ARG:HG3	1.93	0.49
1:B:727:ALA:O	1:B:730:THR:OG1	2.30	0.49
1:D:351:ARG:HD3	1:D:352:PRO:HD2	1.93	0.49
1:E:509:ASN:ND2	1:E:512:GLU:OE2	2.44	0.49
1:F:219:ARG:HA	1:F:225:PHE:HA	1.93	0.49
1:F:235:GLY:HA3	1:F:605:LEU:HD13	1.94	0.49
1:F:378:MET:SD	1:F:394:MET:SD	3.10	0.49
1:B:264:ASP:HB3	1:B:507:ILE:HD13	1.94	0.49
1:F:387:VAL:O	1:F:391:LYS:N	2.45	0.49
1:D:705:SER:CB	1:D:731:ARG:HH22	2.25	0.49
1:E:250:MET:HA	1:E:250:MET:HE2	1.94	0.49
1:F:378:MET:SD	1:F:378:MET:N	2.85	0.49
1:C:196:ILE:HG13	1:C:201:ILE:HG13	1.95	0.49
1:D:258:GLN:O	1:D:277:ARG:NH2	2.45	0.49
1:D:261:VAL:HG22	1:D:504:ILE:HB	1.93	0.49
1:A:520:LEU:O	1:A:523:PHE:HB3	2.12	0.49
1:B:688:LEU:HD12	1:B:690:TYR:CE2	2.46	0.49
1:C:233:PHE:CE1	1:C:575:PRO:HD2	2.48	0.49
1:A:681:PRO:HD3	1:B:614:ASN:HD21	1.77	0.49
1:C:699:LEU:HD22	1:C:734:LEU:HD11	1.93	0.49
1:A:446:ALA:O	1:A:450:MET:HG3	2.13	0.49
1:B:358:PHE:CG	1:B:359:PHE:N	2.81	0.49
1:E:343:LEU:O	1:E:347:VAL:HG23	2.13	0.49
1:D:394:MET:HE2	1:D:402:PHE:HZ	1.78	0.49
1:F:262:VAL:HG23	1:F:548:LEU:HB2	1.95	0.49
1:F:710:TYR:OH	1:F:724:ASP:OD2	2.26	0.49
1:A:361:ASN:OD1	1:A:364:ARG:NH2	2.46	0.49
1:A:427:GLU:HA	1:A:431:GLY:HA3	1.94	0.49
1:C:297:ARG:HG3	1:C:491:ASP:N	2.28	0.49
1:F:493:ASP:OD2	1:F:495:ARG:NH2	2.45	0.49
1:A:487:THR:HB	4:A:901:HOH:O	2.12	0.48
1:D:361:ASN:HA	1:D:364:ARG:NH1	2.28	0.48
1:E:526:VAL:O	1:E:530:SER:OG	2.27	0.48
1:F:283:GLN:HG2	1:F:501:GLU:HB3	1.94	0.48
1:D:198:ALA:HB2	1:D:679:LEU:HD11	1.95	0.48
1:C:525:ASN:OD1	1:C:560:THR:OG1	2.32	0.48
1:D:705:SER:OG	1:D:731:ARG:NH2	2.36	0.48
1:E:273:CYS:HA	1:E:276:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:ASP:OD1	1:F:211:ASP:N	2.45	0.48
1:A:236:LEU:HD13	1:A:609:MET:HB2	1.95	0.48
1:B:273:CYS:O	1:B:277:ARG:HG2	2.12	0.48
1:C:483:ILE:O	1:C:487:THR:HG22	2.13	0.48
1:D:642:ASP:OD1	1:D:642:ASP:C	2.57	0.48
1:E:273:CYS:O	1:E:277:ARG:HG2	2.14	0.48
1:A:432:GLU:O	1:A:435:LYS:NZ	2.45	0.48
1:B:731:ARG:HD2	1:B:733:GLU:OE2	2.14	0.48
1:B:493:ASP:OD1	1:B:495:ARG:HG3	2.14	0.48
1:C:298:PHE:HE1	1:C:526:VAL:HG11	1.79	0.48
1:F:233:PHE:CD1	1:F:575:PRO:HD2	2.48	0.48
1:B:294:LYS:HZ2	1:B:741:VAL:HB	1.78	0.48
1:F:410:ILE:HB	1:F:423:VAL:HG22	1.94	0.48
1:F:616:ASP:OD1	1:F:617:ASN:N	2.46	0.48
1:C:692:ASP:O	1:C:696:THR:HG23	2.14	0.48
1:E:676:GLU:HB3	1:E:679:LEU:HB2	1.95	0.48
1:F:700:ILE:HD11	1:F:721:PHE:HE2	1.78	0.48
1:D:374:TYR:OH	1:D:395:PRO:O	2.32	0.48
1:E:705:SER:O	1:E:709:LYS:HG3	2.14	0.48
1:F:395:PRO:HD2	1:F:402:PHE:CE1	2.49	0.48
1:C:274:GLY:HA3	1:C:736:TYR:HB3	1.96	0.48
1:E:214:GLU:HA	1:E:228:TYR:O	2.13	0.47
1:E:636:ASP:OD2	1:E:655:LYS:NZ	2.47	0.47
1:F:553:THR:HG21	1:F:584:GLN:HG2	1.96	0.47
1:A:555:CYS:HB3	1:A:558:LEU:HD22	1.97	0.47
1:D:239:PRO:HB3	1:D:618:TYR:CZ	2.49	0.47
1:B:529:TYR:HA	1:B:532:LEU:HD21	1.95	0.47
1:E:262:VAL:HG21	1:E:269:THR:HG21	1.96	0.47
1:F:208:ARG:HD2	1:F:210:PHE:CD2	2.50	0.47
1:A:256:TYR:CE2	1:A:258:GLN:HB2	2.50	0.47
1:D:248:PHE:C	1:D:251:PRO:HD2	2.40	0.47
1:B:493:ASP:OD2	1:B:495:ARG:NH1	2.47	0.47
1:B:521:GLU:OE2	1:B:560:THR:HG23	2.14	0.47
1:C:232:ALA:HB1	1:C:606:SER:HB2	1.97	0.47
1:C:496:ARG:HA	1:C:499:ILE:HG13	1.96	0.47
1:D:244:LYS:NZ	1:D:550:ASP:OD1	2.47	0.47
1:E:287:ILE:HG13	1:E:736:TYR:CZ	2.49	0.47
1:F:401:PHE:CD2	1:F:484:ARG:HD3	2.49	0.47
1:C:700:ILE:HD11	1:C:721:PHE:HE2	1.80	0.47
1:F:229:ALA:O	1:F:574:ARG:NH2	2.48	0.47
1:E:369:ILE:O	1:E:373:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:SER:OG	1:B:733:GLU:OE1	2.31	0.46
1:E:245:GLY:HA2	1:E:249:ILE:HB	1.97	0.46
1:F:374:TYR:HA	1:F:378:MET:HG2	1.97	0.46
1:C:573:MET:HE2	1:C:573:MET:HA	1.97	0.46
1:F:373:ILE:O	1:F:378:MET:HE2	2.14	0.46
1:F:191:THR:O	1:F:195:MET:HG3	2.15	0.46
1:F:239:PRO:HB3	1:F:618:TYR:CZ	2.50	0.46
1:B:232:ALA:HB1	1:B:606:SER:HB2	1.97	0.46
1:A:701:LYS:HB3	1:A:701:LYS:HE3	1.77	0.46
1:D:400:MET:HE3	1:D:400:MET:HB3	1.77	0.46
1:E:254:ILE:O	1:E:280:ARG:NH1	2.48	0.46
1:E:294:LYS:HG3	1:E:743:VAL:HG22	1.97	0.46
1:D:193:GLU:O	1:D:197:LYS:HE2	2.15	0.46
1:E:233:PHE:CE1	1:E:575:PRO:HD2	2.51	0.46
1:E:426:MET:HE3	1:E:426:MET:O	2.16	0.46
1:E:426:MET:SD	1:E:455:LYS:HD3	2.56	0.46
1:E:624:LYS:NZ	1:F:620:GLU:OE2	2.29	0.46
1:A:381:LYS:HE3	1:A:385:GLU:OE2	2.14	0.46
1:B:510:PRO:HD2	1:B:554:LEU:HD23	1.98	0.46
1:E:613:ILE:O	1:E:666:MET:HG2	2.16	0.46
1:F:193:GLU:OE2	1:F:193:GLU:N	2.48	0.46
1:F:703:SER:O	1:F:707:SER:OG	2.32	0.46
1:A:722:TYR:O	1:A:726:GLN:HG2	2.16	0.45
1:C:256:TYR:CE2	1:C:258:GLN:HB2	2.51	0.45
1:F:256:TYR:CE2	1:F:258:GLN:HB2	2.51	0.45
1:A:184:PHE:HD2	1:A:633:THR:HG23	1.82	0.45
1:B:378:MET:HB3	1:B:379:TRP:CE3	2.51	0.45
1:E:256:TYR:CE2	1:E:258:GLN:HB2	2.51	0.45
1:C:628:VAL:HG22	1:D:666:MET:HE1	1.98	0.45
1:E:239:PRO:O	1:E:242:SER:OG	2.27	0.45
1:F:526:VAL:O	1:F:530:SER:OG	2.29	0.45
1:B:350:GLU:O	1:B:351:ARG:HD2	2.16	0.45
1:F:557:TYR:CD2	1:F:589:PRO:HB3	2.52	0.45
1:B:306:PHE:HB3	1:B:379:TRP:CD2	2.52	0.45
1:F:377:LEU:HA	1:F:383:GLY:HA3	1.98	0.45
1:F:394:MET:HB2	1:F:394:MET:HE3	1.57	0.45
1:A:279:LYS:HA	1:A:279:LYS:HD3	1.72	0.45
1:A:429:PHE:HB3	1:A:440:LEU:HD12	1.99	0.45
1:B:200:LEU:O	1:B:208:ARG:NH2	2.48	0.45
1:A:233:PHE:CD1	1:A:575:PRO:HD2	2.52	0.45
1:C:278:GLU:HG3	1:C:285:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:GLN:O	1:B:730:THR:HG23	2.16	0.45
1:E:513:SER:O	1:E:516:VAL:HG12	2.17	0.44
1:F:387:VAL:HA	1:F:392:ILE:HD12	1.99	0.44
1:B:345:LYS:HB3	1:B:345:LYS:HE3	1.82	0.44
1:F:390:LYS:HB2	1:F:392:ILE:CD1	2.48	0.44
1:F:564:ALA:O	1:F:568:MET:HG3	2.18	0.44
1:A:430:GLY:H	1:A:434:ASP:HB3	1.82	0.44
1:B:244:LYS:HD3	1:B:578:VAL:HG11	2.00	0.44
1:B:303:TYR:HA	1:B:495:ARG:HH21	1.82	0.44
1:E:284:LYS:HE2	1:E:740:LEU:HD23	1.99	0.44
1:C:207:LYS:HA	1:C:207:LYS:HD3	1.86	0.44
1:B:693:PRO:HA	1:B:696:THR:OG1	2.18	0.44
1:F:393:ILE:C	1:F:394:MET:HG3	2.42	0.44
1:F:611:TYR:HE1	1:F:672:LEU:HD13	1.82	0.44
1:A:484:ARG:NH1	1:A:747:GLU:O	2.50	0.44
1:B:612:GLY:HA2	1:B:622:PHE:CZ	2.53	0.44
1:C:623:GLU:HA	1:C:662:PRO:HG3	1.98	0.44
1:C:668:MET:HB3	1:C:671:GLU:HB2	1.99	0.44
1:D:612:GLY:HA2	1:D:622:PHE:CZ	2.53	0.44
1:F:213:ARG:NH2	1:F:543:ARG:HA	2.32	0.44
1:B:248:PHE:C	1:B:251:PRO:HD2	2.43	0.44
1:C:510:PRO:HD2	1:C:554:LEU:HD22	1.99	0.44
1:F:238:ALA:O	1:F:580:GLN:HA	2.17	0.44
1:F:561:PHE:O	1:F:565:VAL:HB	2.17	0.44
1:A:459:GLY:HA2	1:A:464:TYR:HD2	1.83	0.44
1:A:643:ASP:OD2	1:F:639:ARG:NH2	2.50	0.44
1:B:236:LEU:HD13	1:B:609:MET:HB2	2.00	0.44
1:B:237:ILE:HG13	1:B:579:PHE:HE1	1.82	0.44
1:F:280:ARG:HD3	1:F:281:PHE:CZ	2.53	0.44
1:A:427:GLU:HB3	1:A:433:GLU:HG2	1.99	0.44
1:C:253:MET:HE2	1:C:260:ILE:HG21	2.00	0.44
1:F:466:SER:O	1:F:470:VAL:HG13	2.17	0.44
1:A:263:PHE:CE2	1:A:265:PRO:HG3	2.53	0.43
1:B:303:TYR:HA	1:B:495:ARG:NH2	2.33	0.43
1:B:343:LEU:HD23	1:B:343:LEU:HA	1.82	0.43
1:C:242:SER:O	1:C:686:LYS:NZ	2.51	0.43
1:F:386:PHE:CE2	1:F:439:ASN:HA	2.53	0.43
1:B:219:ARG:HH12	1:B:691:ASP:HB3	1.82	0.43
1:B:700:ILE:HG12	1:B:706:LEU:HB3	2.00	0.43
1:C:233:PHE:CD1	1:C:575:PRO:HD2	2.53	0.43
1:F:276:ILE:HD11	1:F:699:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:TYR:HA	1:B:532:LEU:CD2	2.47	0.43
1:B:688:LEU:HD13	1:B:688:LEU:HA	1.89	0.43
1:E:417:THR:OG1	1:E:421:LYS:NZ	2.50	0.43
1:F:377:LEU:HB2	1:F:378:MET:CE	2.49	0.43
1:D:498:ARG:HE	1:D:531:ASN:HB3	1.82	0.43
1:C:498:ARG:HH22	1:C:533:ILE:HG13	1.83	0.43
1:C:642:ASP:OD1	1:C:645:THR:HG23	2.18	0.43
1:E:256:TYR:HA	1:E:257:PRO:HD3	1.88	0.43
1:F:374:TYR:O	1:F:378:MET:HG2	2.19	0.43
1:B:239:PRO:HB3	1:B:618:TYR:CZ	2.53	0.43
1:E:231:GLN:HB3	4:E:903:HOH:O	2.18	0.43
1:E:248:PHE:C	1:E:251:PRO:HD2	2.43	0.43
1:F:254:ILE:HD13	1:F:695:PHE:HB3	2.01	0.43
1:F:301:PHE:CZ	1:F:403:ILE:HG13	2.54	0.43
1:F:301:PHE:CE2	1:F:403:ILE:HG13	2.53	0.43
1:F:402:PHE:CE2	1:F:406:MET:HE2	2.54	0.43
1:A:657:ARG:HG3	1:F:183:LEU:O	2.17	0.43
1:E:497:LEU:HD23	1:E:573:MET:HE1	2.01	0.43
1:C:244:LYS:HG2	2:C:801:SO4:O3	2.19	0.43
1:F:402:PHE:O	1:F:406:MET:HG2	2.19	0.43
1:C:738:LYS:O	1:C:741:VAL:HG22	2.19	0.43
1:D:351:ARG:HG3	1:D:353:ASN:H	1.83	0.43
1:E:663:ASP:HA	1:E:666:MET:HE3	1.99	0.43
1:E:394:MET:HG2	1:E:402:PHE:HZ	1.84	0.43
1:F:525:ASN:ND2	1:F:560:THR:OG1	2.52	0.43
1:B:374:TYR:HB2	1:B:406:MET:HE1	2.00	0.42
1:E:558:LEU:HB2	1:E:593:TYR:OH	2.19	0.42
1:F:490:ASN:ND2	1:F:492:PHE:O	2.52	0.42
1:C:192:GLU:OE1	1:C:220:ARG:NH1	2.52	0.42
1:C:286:PHE:HB2	1:C:504:ILE:HD12	2.02	0.42
1:C:444:SER:O	1:C:445:PRO:C	2.63	0.42
1:C:499:ILE:HD12	1:C:540:GLN:HG2	2.01	0.42
1:D:205:ASN:ND2	1:D:224:ASP:OD1	2.36	0.42
1:E:297:ARG:HG2	1:E:485:ASN:O	2.18	0.42
1:E:372:ASN:HB3	1:E:447:THR:HG23	2.01	0.42
1:F:699:LEU:HD23	1:F:725:LEU:HD11	2.00	0.42
1:A:693:PRO:HD3	1:A:715:VAL:HG22	2.00	0.42
1:B:275:LYS:HA	1:B:275:LYS:HD3	1.92	0.42
1:D:248:PHE:O	1:D:252:ASN:ND2	2.42	0.42
1:E:184:PHE:HB3	1:E:656:GLU:HB3	2.00	0.42
1:F:219:ARG:HD3	1:F:687:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ILE:HD12	1:E:371:CYS:HB3	2.00	0.42
1:E:402:PHE:HE2	1:E:406:MET:HE3	1.84	0.42
1:F:274:GLY:HA3	1:F:736:TYR:HB3	2.00	0.42
1:A:248:PHE:C	1:A:251:PRO:HD2	2.44	0.42
1:C:264:ASP:O	1:C:507:ILE:HD13	2.20	0.42
1:C:297:ARG:HG3	1:C:491:ASP:H	1.85	0.42
1:A:620:GLU:H	1:A:620:GLU:HG2	1.70	0.42
1:C:298:PHE:CE1	1:C:526:VAL:HG11	2.55	0.42
1:C:476:ALA:N	1:C:477:PRO:HD2	2.35	0.42
1:C:276:ILE:O	1:C:280:ARG:HB2	2.20	0.41
1:C:720:THR:O	1:C:720:THR:OG1	2.38	0.41
1:E:348:PHE:HB2	1:E:364:ARG:NH1	2.34	0.41
1:F:401:PHE:CE2	1:F:484:ARG:HD3	2.55	0.41
1:F:536:ILE:H	1:F:536:ILE:HG13	1.63	0.41
1:B:201:ILE:HA	1:B:208:ARG:NH2	2.35	0.41
1:C:673:ILE:HD13	1:C:673:ILE:HA	1.84	0.41
1:D:518:PRO:O	1:D:521:GLU:HB3	2.20	0.41
1:F:336:PHE:O	1:F:340:ILE:HG12	2.19	0.41
1:F:403:ILE:H	1:F:403:ILE:HG12	1.75	0.41
1:A:297:ARG:NH2	1:A:491:ASP:OD1	2.53	0.41
1:A:376:ASP:O	1:A:380:THR:OG1	2.38	0.41
1:B:271:GLU:OE2	1:B:738:LYS:NZ	2.31	0.41
1:D:393:ILE:HB	1:D:411:ASN:HB2	2.03	0.41
1:E:276:ILE:N	1:E:276:ILE:HD12	2.36	0.41
1:C:516:VAL:HG12	1:C:520:LEU:HG	2.01	0.41
1:E:343:LEU:HD23	1:E:343:LEU:HA	1.84	0.41
1:E:375:ARG:HG2	1:E:379:TRP:HB2	2.01	0.41
1:F:301:PHE:O	1:F:304:VAL:HG12	2.20	0.41
1:A:340:ILE:HD13	1:A:340:ILE:HA	1.90	0.41
1:B:399:THR:HG23	1:B:402:PHE:H	1.85	0.41
1:C:219:ARG:HH12	1:C:691:ASP:HB3	1.84	0.41
1:D:276:ILE:HG12	1:D:702:VAL:HG21	2.02	0.41
1:A:407:ALA:O	1:A:468:GLN:NE2	2.54	0.41
1:E:534:LEU:HD22	1:E:571:TYR:CE1	2.55	0.41
1:D:370:ASN:HB3	1:D:406:MET:HE2	2.01	0.41
1:F:362:GLN:CD	1:F:362:GLN:H	2.28	0.41
1:B:378:MET:C	1:B:380:THR:H	2.28	0.41
1:D:570:GLU:CD	1:D:570:GLU:H	2.29	0.41
1:E:534:LEU:HB2	1:E:537:HIS:CD2	2.55	0.41
1:B:229:ALA:O	1:B:574:ARG:NH2	2.53	0.41
1:B:559:GLU:O	1:B:563:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ALA:O	1:B:568:MET:HG3	2.20	0.41
1:C:216:ILE:N	1:C:252:ASN:OD1	2.53	0.41
1:C:545:CYS:HB3	1:C:573:MET:CE	2.51	0.41
1:D:233:PHE:CD1	1:D:575:PRO:HD2	2.55	0.41
1:D:557:TYR:HB2	1:D:589:PRO:O	2.21	0.41
1:D:567:ILE:HD13	1:E:511:LYS:HB3	2.03	0.41
1:D:727:ALA:O	1:D:731:ARG:HG3	2.21	0.41
1:E:659:LEU:HD12	1:E:659:LEU:HA	1.91	0.41
1:B:217:VAL:O	1:B:609:MET:HE3	2.20	0.41
1:B:237:ILE:HG13	1:B:579:PHE:CE1	2.56	0.41
1:B:256:TYR:HB3	1:B:260:ILE:HD11	2.02	0.41
1:E:536:ILE:H	1:E:536:ILE:HG12	1.74	0.41
1:D:628:VAL:HG21	1:E:616:ASP:HB2	2.02	0.40
1:E:235:GLY:HA3	1:E:605:LEU:HD13	2.02	0.40
1:C:722:TYR:O	1:C:726:GLN:HG2	2.21	0.40
1:D:217:VAL:O	1:D:609:MET:HE3	2.20	0.40
1:D:376:ASP:OD2	1:D:444:SER:HB3	2.22	0.40
1:D:588:ASP:HB3	1:D:590:PRO:HD2	2.02	0.40
1:F:665:LEU:HA	1:F:668:MET:HG3	2.03	0.40
1:C:689:TYR:HA	1:C:695:PHE:CD2	2.56	0.40
1:D:479:ASN:OD1	1:D:479:ASN:N	2.54	0.40
1:E:557:TYR:HB2	1:E:589:PRO:O	2.21	0.40
1:E:613:ILE:HD13	1:E:613:ILE:HA	1.88	0.40
1:E:693:PRO:HA	1:E:696:THR:OG1	2.21	0.40
1:F:500:ASP:HB3	1:F:502:VAL:HG13	2.03	0.40
1:E:233:PHE:CD1	1:E:575:PRO:HD2	2.56	0.40
1:E:427:GLU:H	1:E:427:GLU:HG2	1.77	0.40
1:E:665:LEU:HA	1:E:668:MET:HG3	2.04	0.40
1:F:372:ASN:HB3	1:F:447:THR:HG22	2.03	0.40
1:F:477:PRO:HB3	1:F:515:ILE:HB	2.03	0.40
1:A:610:TYR:OH	1:B:616:ASP:OD2	2.22	0.40
1:D:256:TYR:CE2	1:D:258:GLN:HB3	2.57	0.40
1:D:496:ARG:HA	1:D:499:ILE:HD12	2.04	0.40
1:E:346:LEU:HD13	1:E:346:LEU:HA	1.93	0.40
1:F:492:PHE:HE1	1:F:497:LEU:HD13	1.86	0.40

There are no symmetry-related clashes.

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	536/593 (90%)	508 (95%)	28 (5%)	0	100	100
1	B	490/593 (83%)	465 (95%)	24 (5%)	1 (0%)	43	72
1	C	496/593 (84%)	469 (95%)	26 (5%)	1 (0%)	43	72
1	D	522/593 (88%)	500 (96%)	19 (4%)	3 (1%)	21	51
1	E	536/593 (90%)	516 (96%)	19 (4%)	1 (0%)	43	72
1	F	519/593 (88%)	501 (96%)	18 (4%)	0	100	100
All	All	3099/3558 (87%)	2959 (96%)	134 (4%)	6 (0%)	43	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	445	PRO
1	B	456	THR
1	E	347	VAL
1	D	193	GLU
1	D	213	ARG
1	D	203	PRO

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	469/520 (90%)	460 (98%)	9 (2%)	50	81
1	B	399/520 (77%)	390 (98%)	9 (2%)	44	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	354/520 (68%)	342 (97%)	12 (3%)	32	68
1	D	452/520 (87%)	442 (98%)	10 (2%)	45	78
1	E	461/520 (89%)	447 (97%)	14 (3%)	36	72
1	F	442/520 (85%)	426 (96%)	16 (4%)	31	66
All	All	2577/3120 (83%)	2507 (97%)	70 (3%)	39	74

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	ARG
1	A	453	SER
1	A	457	MET
1	A	466	SER
1	A	514	THR
1	A	516	VAL
1	A	558	LEU
1	A	651	SER
1	A	735	SER
1	B	338	THR
1	B	343	LEU
1	B	370	ASN
1	B	465	SER
1	B	514	THR
1	B	616	ASP
1	B	639	ARG
1	B	644	ASN
1	B	672	LEU
1	C	180	VAL
1	C	513	SER
1	C	514	THR
1	C	515	ILE
1	C	522	LEU
1	C	526	VAL
1	C	553	THR
1	C	599	LYS
1	C	672	LEU
1	C	691	ASP
1	C	720	THR
1	C	734	LEU
1	D	258	GLN
1	D	397	THR

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Mol	Chain	Res	Type
1	D	411	ASN
1	D	422	VAL
1	D	423	VAL
1	D	442	VAL
1	D	584	GLN
1	D	647	LYS
1	D	730	THR
1	D	734	LEU
1	E	228	TYR
1	E	348	PHE
1	E	420	GLU
1	E	515	ILE
1	E	530	SER
1	E	534	LEU
1	E	559	GLU
1	E	579	PHE
1	E	616	ASP
1	E	640	SER
1	E	641	ILE
1	E	672	LEU
1	E	707	SER
1	E	734	LEU
1	F	192	GLU
1	F	293	LEU
1	F	360	SER
1	F	377	LEU
1	F	384	LEU
1	F	387	VAL
1	F	410	ILE
1	F	422	VAL
1	F	425	LEU
1	F	453	SER
1	F	467	VAL
1	F	557	TYR
1	F	638	SER
1	F	640	SER
1	F	707	SER
1	F	717	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	362	GLN
1	A	452	ASN
1	A	468	GLN
1	A	644	ASN
1	A	649	ASN
1	B	231	GLN
1	B	282	ASN
1	B	370	ASN
1	B	614	ASN
1	B	617	ASN
1	B	644	ASN
1	B	685	HIS
1	C	255	ASN
1	C	296	HIS
1	D	231	GLN
1	D	468	GLN
1	D	644	ASN
1	E	365	ASN
1	E	509	ASN
1	E	525	ASN
1	E	537	HIS
1	E	608	ASN
1	F	231	GLN
1	F	485	ASN
1	F	525	ASN
1	F	621	HIS
1	F	635	GLN
1	F	649	ASN
1	F	718	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	C	801	-	4,4,4	0.24	0	6,6,6	0.15	0
3	PEG	C	802	-	6,6,6	0.12	0	5,5,5	0.09	0
2	SO4	A	801	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	F	801	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	E	801	-	4,4,4	0.22	0	6,6,6	0.13	0
3	PEG	A	802	-	6,6,6	0.13	0	5,5,5	0.06	0
2	SO4	D	801	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	B	801	-	4,4,4	0.23	0	6,6,6	0.12	0
3	PEG	D	802	-	6,6,6	0.12	0	5,5,5	0.10	0
3	PEG	B	802	-	6,6,6	0.10	0	5,5,5	0.10	0
3	PEG	E	802	-	6,6,6	0.14	0	5,5,5	0.06	0
3	PEG	F	802	-	6,6,6	0.14	0	5,5,5	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	C	802	-	-	2/4/4/4	-
3	PEG	A	802	-	-	2/4/4/4	-
3	PEG	E	802	-	-	2/4/4/4	-
3	PEG	D	802	-	-	1/4/4/4	-
3	PEG	B	802	-	-	1/4/4/4	-
3	PEG	F	802	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

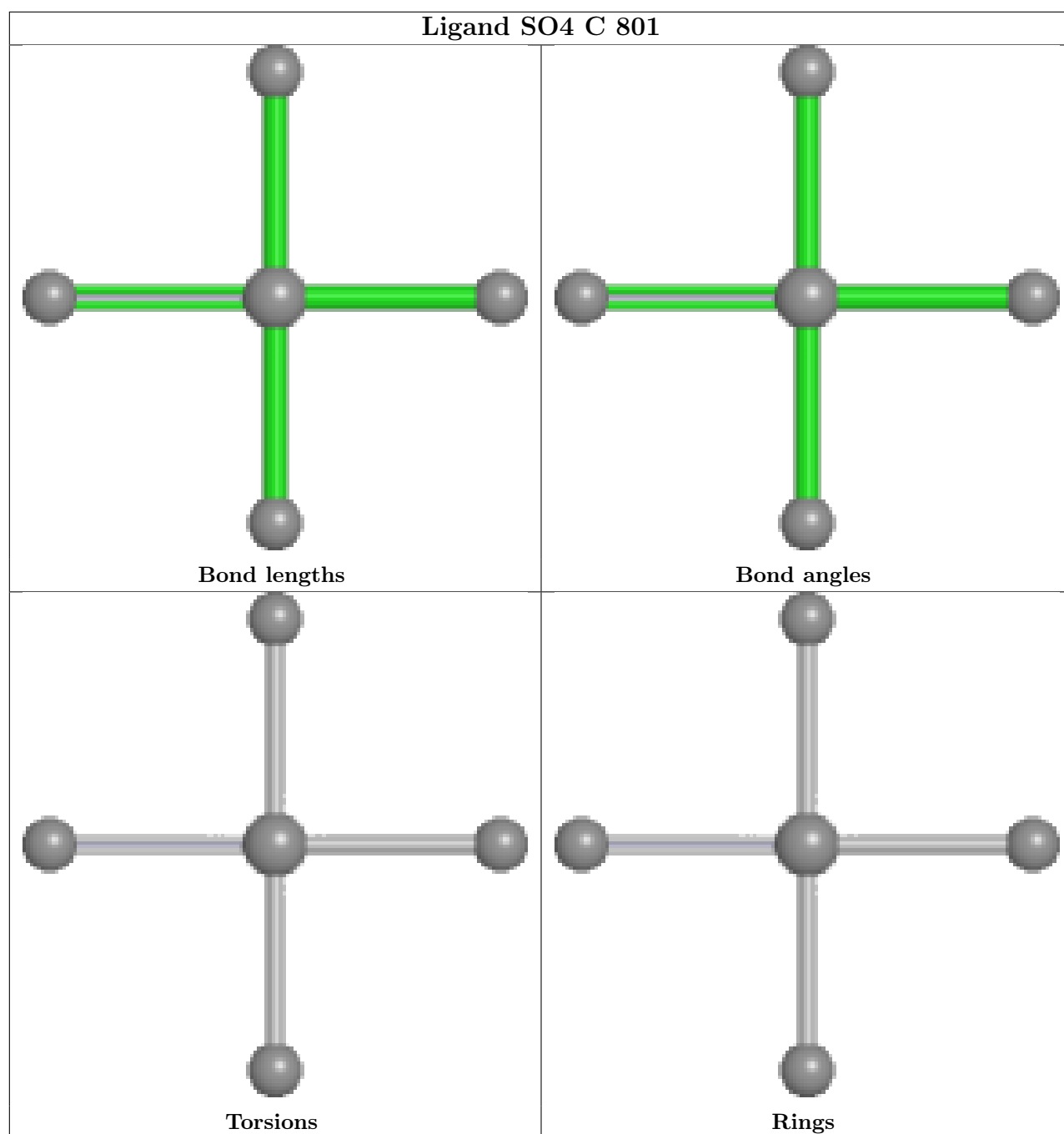
Mol	Chain	Res	Type	Atoms
3	A	802	PEG	O1-C1-C2-O2
3	F	802	PEG	O2-C3-C4-O4
3	C	802	PEG	O1-C1-C2-O2
3	E	802	PEG	O1-C1-C2-O2
3	F	802	PEG	O1-C1-C2-O2
3	E	802	PEG	C4-C3-O2-C2
3	A	802	PEG	C1-C2-O2-C3
3	F	802	PEG	C1-C2-O2-C3
3	C	802	PEG	C1-C2-O2-C3
3	B	802	PEG	C1-C2-O2-C3
3	D	802	PEG	O2-C3-C4-O4

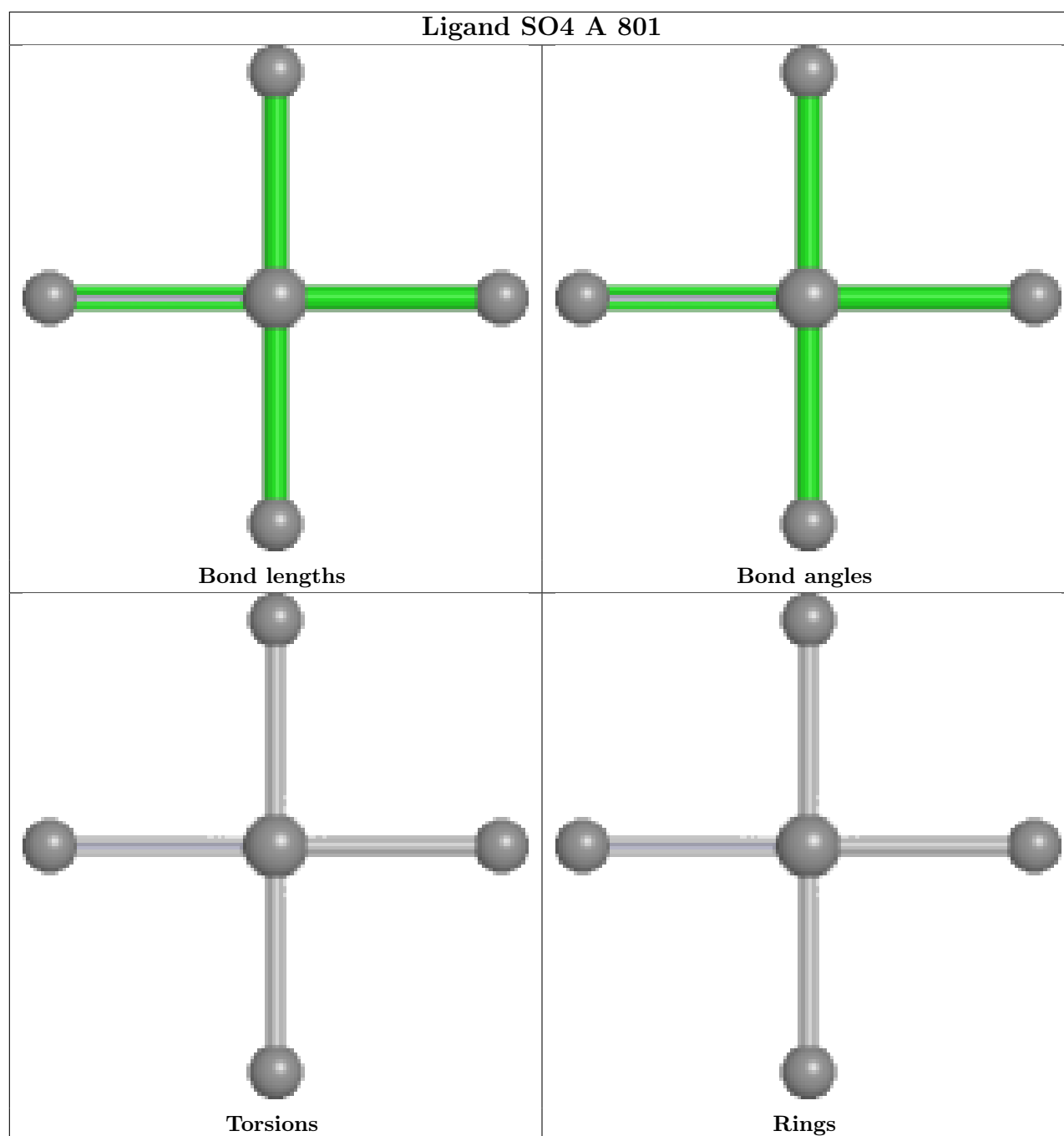
There are no ring outliers.

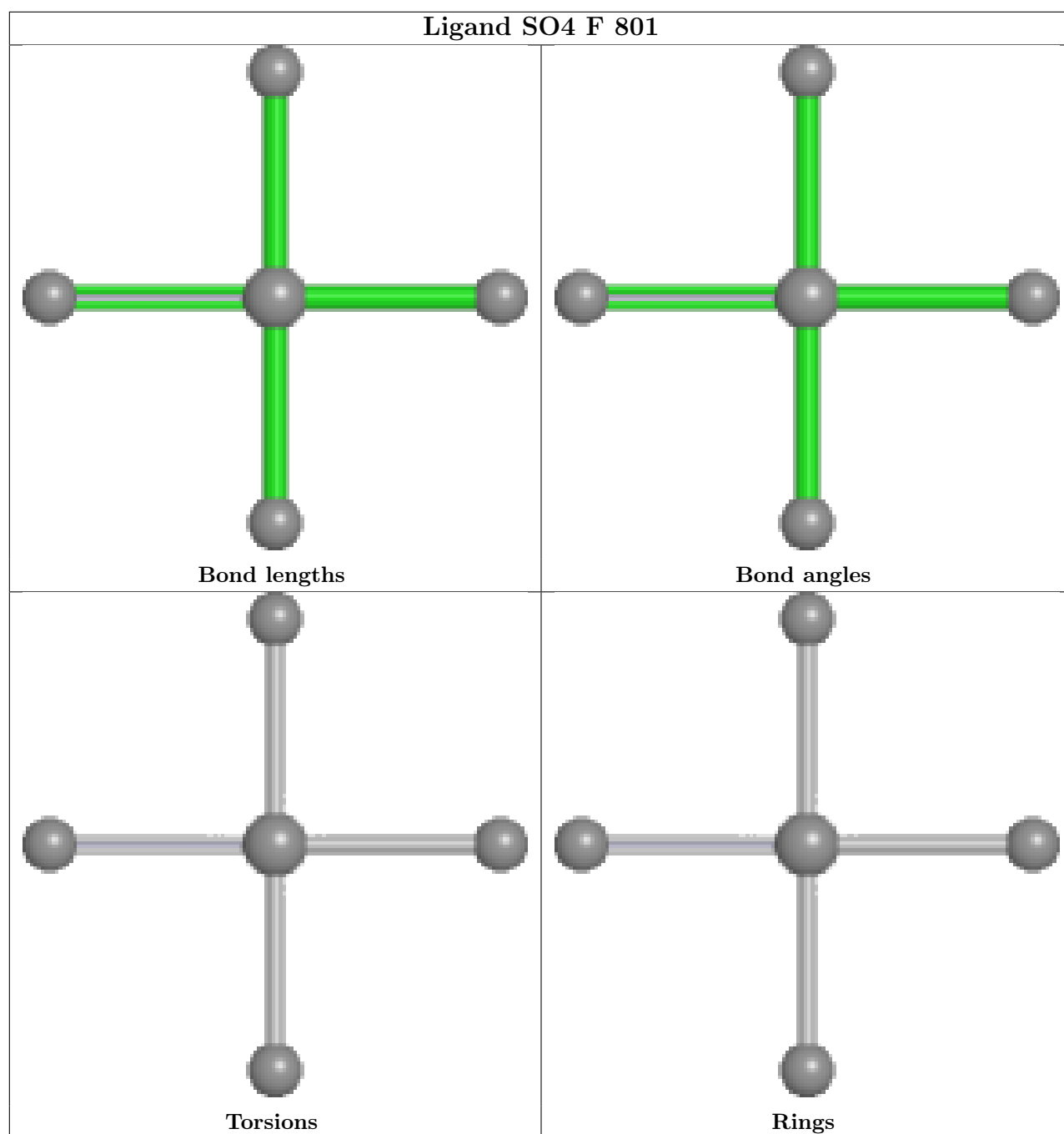
2 monomers are involved in 2 short contacts:

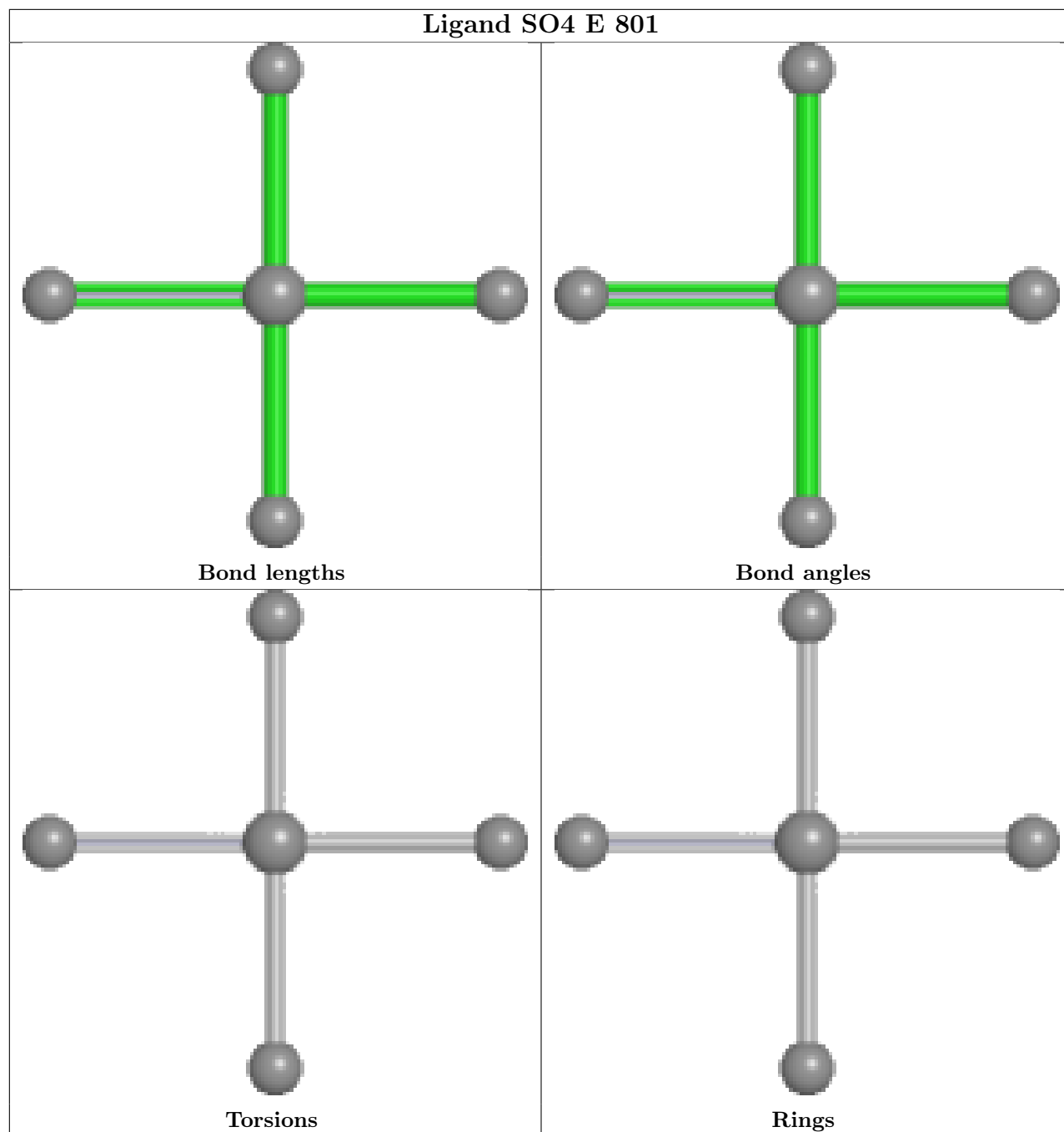
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	SO4	1	0
3	F	802	PEG	1	0

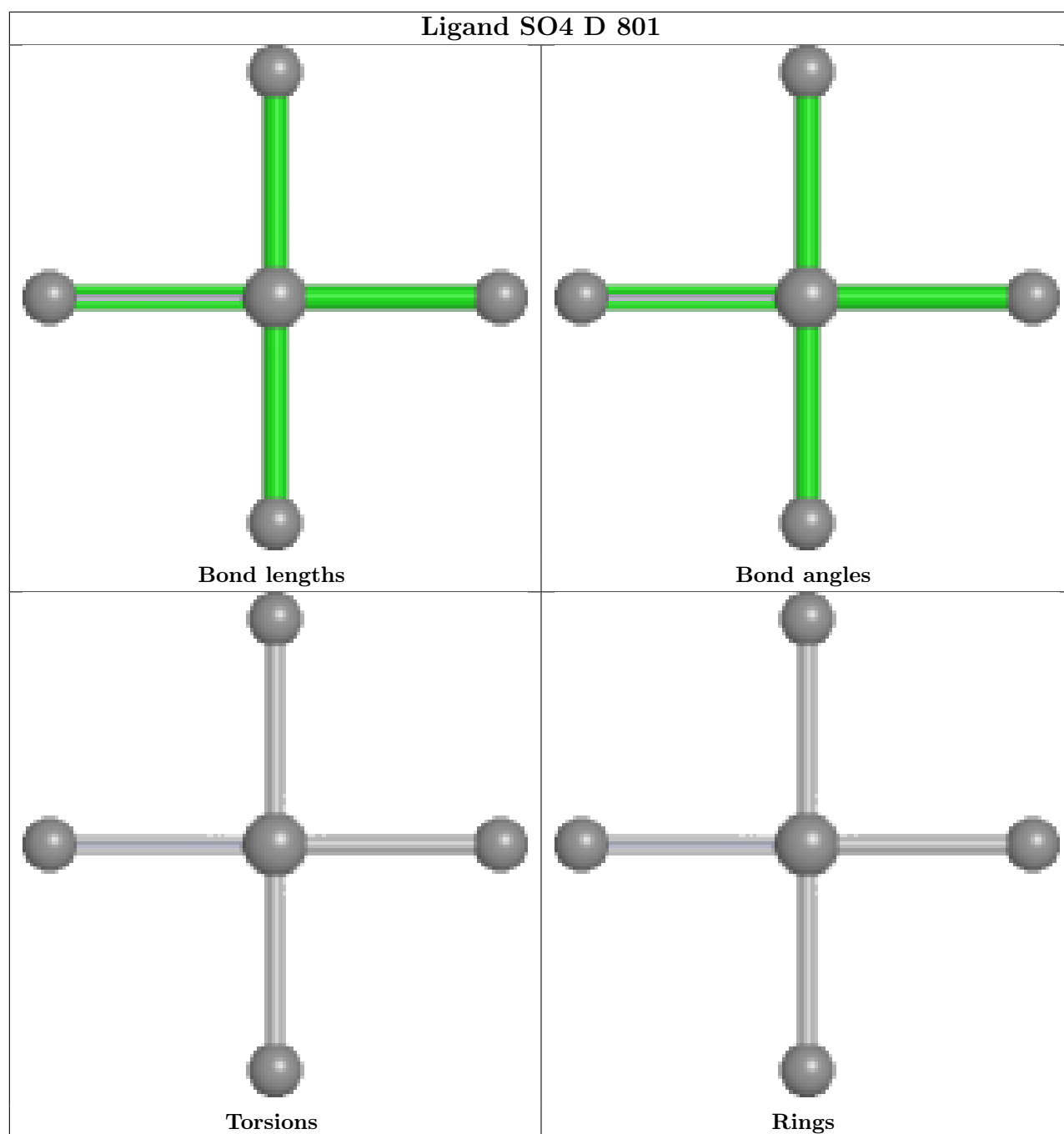
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

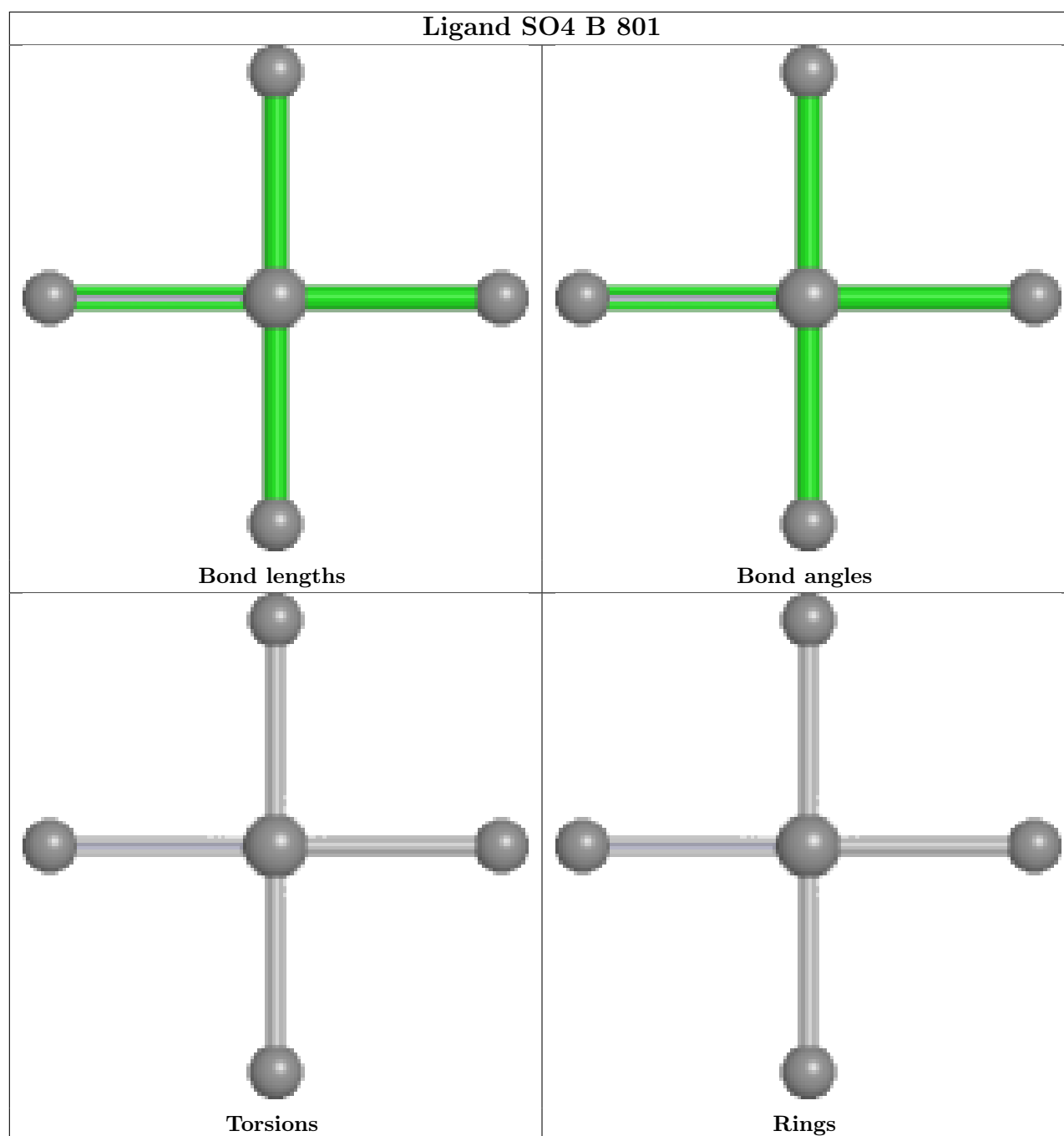












5.7 Other polymers [i](#)

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	540/593 (91%)	-0.33	5 (0%) 81 74	44, 74, 113, 185	0
1	B	498/593 (83%)	-0.03	8 (1%) 70 61	45, 85, 197, 250	0
1	C	510/593 (86%)	0.24	10 (1%) 65 56	47, 109, 216, 272	0
1	D	530/593 (89%)	-0.07	3 (0%) 85 80	45, 96, 172, 230	0
1	E	540/593 (91%)	-0.06	9 (1%) 69 60	44, 80, 175, 214	0
1	F	527/593 (88%)	0.03	12 (2%) 61 51	47, 101, 215, 273	0
All	All	3145/3558 (88%)	-0.04	47 (1%) 72 63	44, 89, 198, 273	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	451	TRP	3.9
1	C	488	SER	3.9
1	C	734	LEU	3.4
1	B	472	THR	3.4
1	F	377	LEU	3.3
1	B	346	LEU	3.2
1	C	464	TYR	3.0
1	C	468	GLN	3.0
1	C	371	CYS	3.0
1	E	499	ILE	2.9
1	B	360	SER	2.8
1	C	379	TRP	2.8
1	F	411	ASN	2.6
1	B	347	VAL	2.6
1	F	541	CYS	2.5
1	A	555	CYS	2.5
1	D	307	GLY	2.4
1	D	458	GLY	2.4
1	E	459	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	747	GLU	2.4
1	E	425	LEU	2.4
1	A	579	PHE	2.4
1	C	490	ASN	2.4
1	F	306	PHE	2.4
1	E	449	ASN	2.3
1	E	540	GLN	2.3
1	A	237	ILE	2.3
1	F	340	ILE	2.3
1	F	438	ASP	2.3
1	B	361	ASN	2.2
1	F	555	CYS	2.2
1	E	347	VAL	2.2
1	C	425	LEU	2.2
1	B	357	PRO	2.2
1	E	392	ILE	2.2
1	A	426	MET	2.2
1	B	459	GLY	2.2
1	C	274	GLY	2.2
1	F	429	PHE	2.2
1	F	539	PRO	2.1
1	F	336	PHE	2.1
1	E	465	SER	2.1
1	B	470	VAL	2.1
1	F	557	TYR	2.1
1	F	273	CYS	2.0
1	D	343	LEU	2.0
1	C	335	ASP	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,

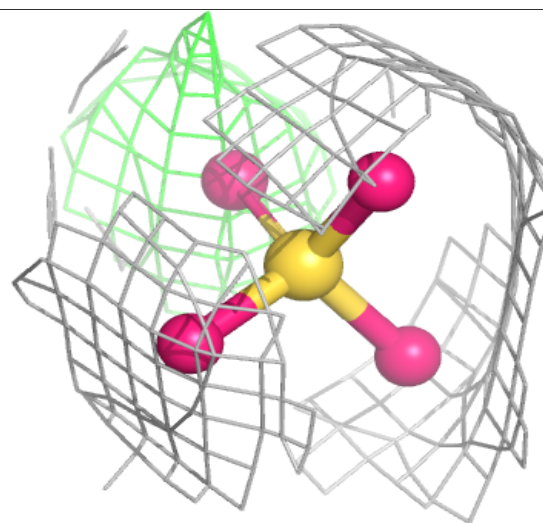
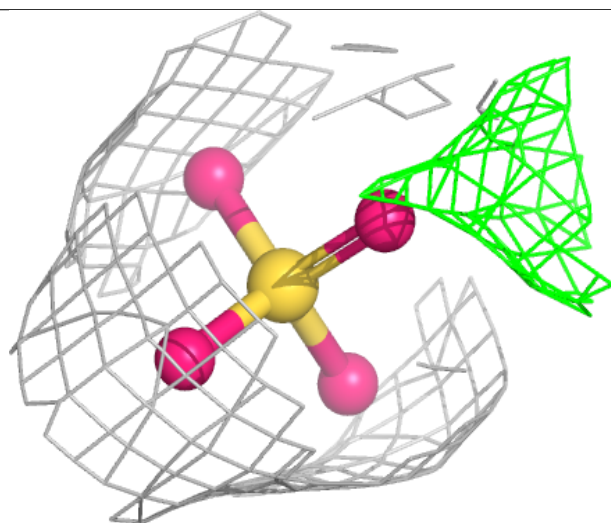
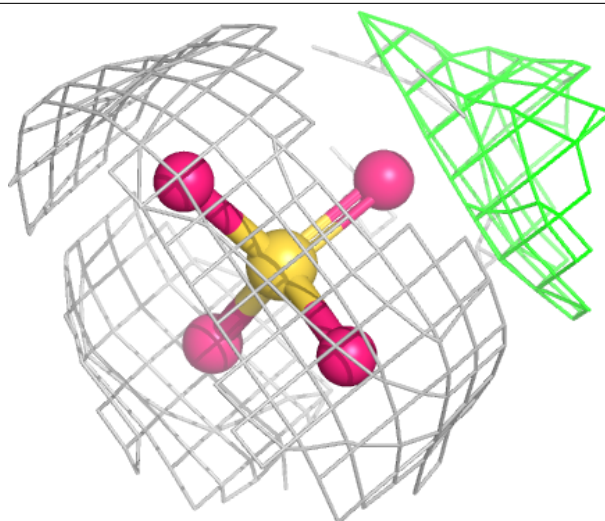
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	801	5/5	0.79	0.10	74,98,106,107	0
3	PEG	E	802	7/7	0.80	0.13	80,100,103,108	0
2	SO4	E	801	5/5	0.82	0.14	63,70,81,306	0
3	PEG	A	802	7/7	0.85	0.11	71,82,97,101	0
2	SO4	F	801	5/5	0.89	0.11	63,72,85,234	0
3	PEG	C	802	7/7	0.90	0.14	72,81,92,92	0
2	SO4	A	801	5/5	0.90	0.08	65,75,80,90	0
3	PEG	F	802	7/7	0.90	0.12	81,89,94,94	0
3	PEG	D	802	7/7	0.91	0.11	74,81,94,99	0
3	PEG	B	802	7/7	0.91	0.10	71,80,89,108	0
2	SO4	D	801	5/5	0.91	0.06	66,66,73,77	0
2	SO4	B	801	5/5	0.94	0.06	72,78,79,83	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

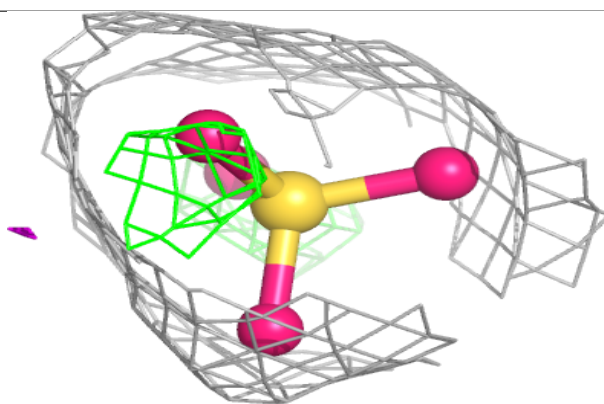
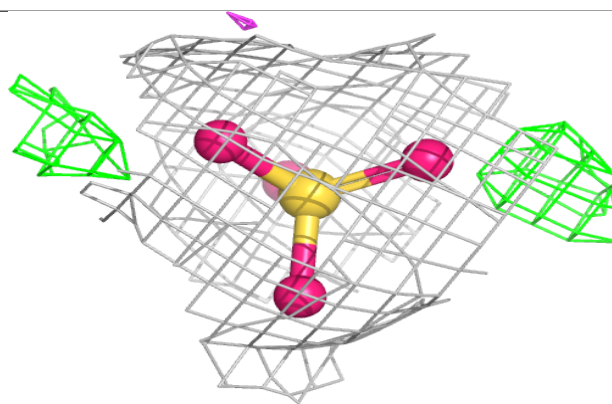
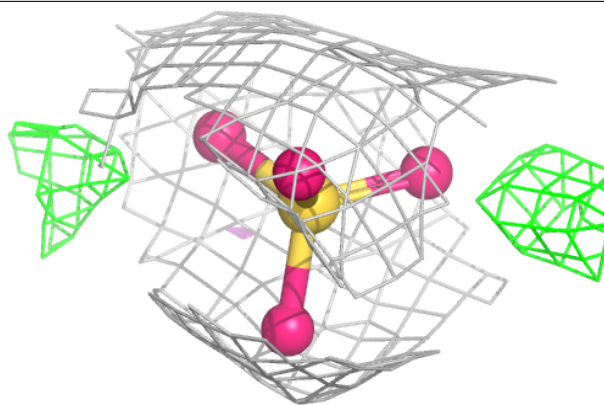
Electron density around SO4 C 801:

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



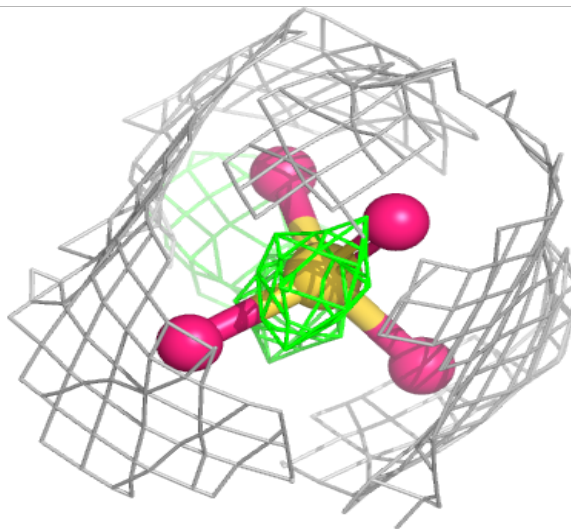
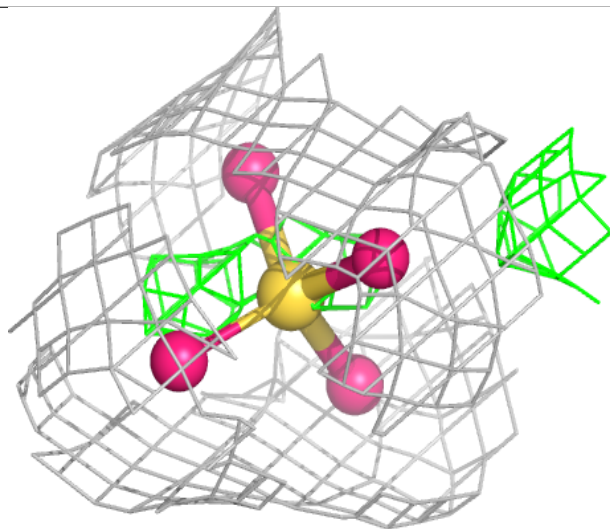
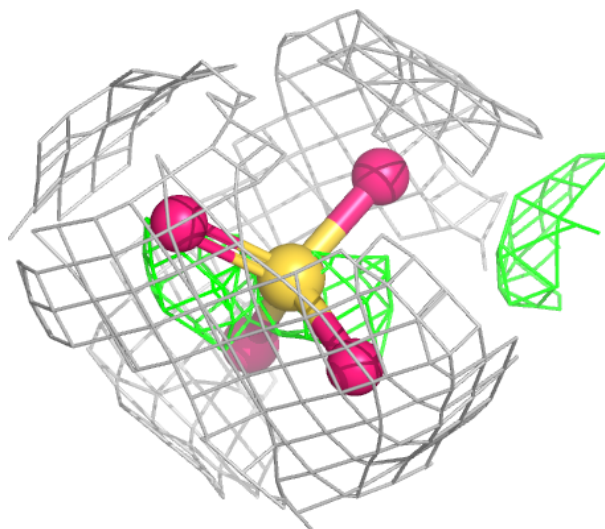
Electron density around SO4 E 801:

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



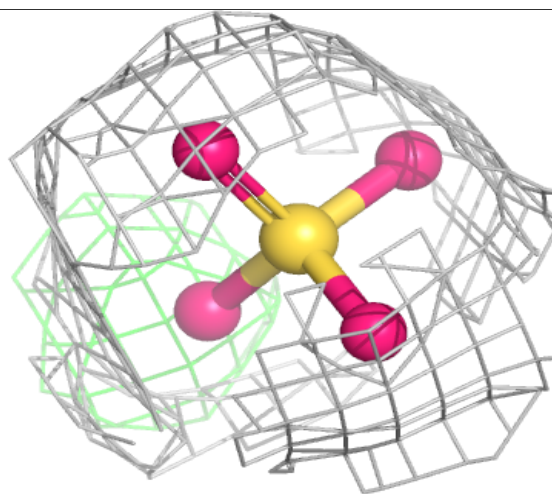
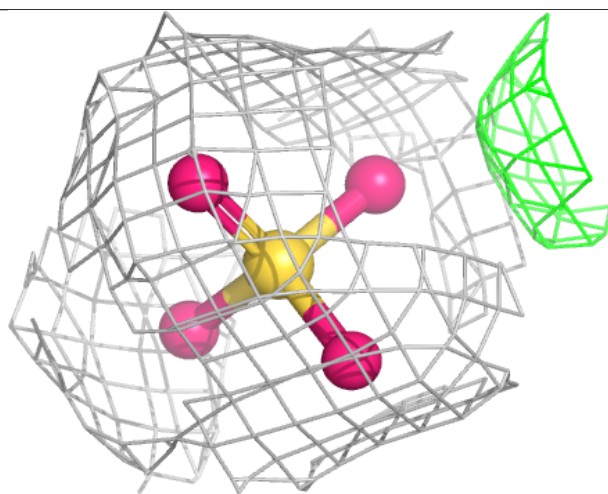
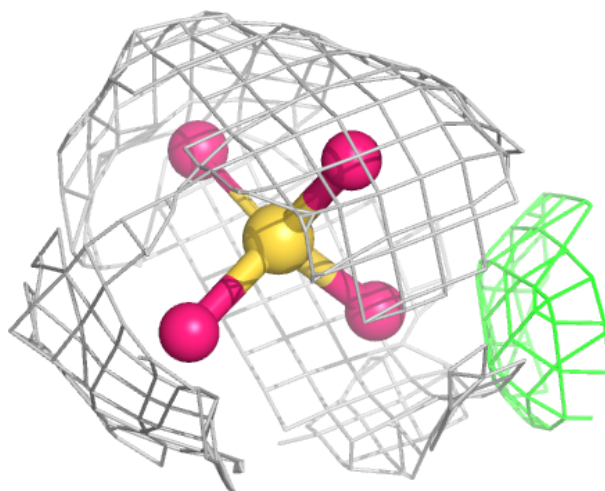
Electron density around SO4 F 801:

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



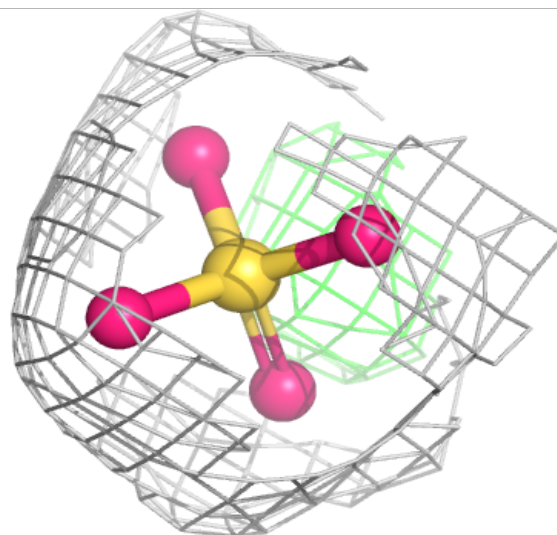
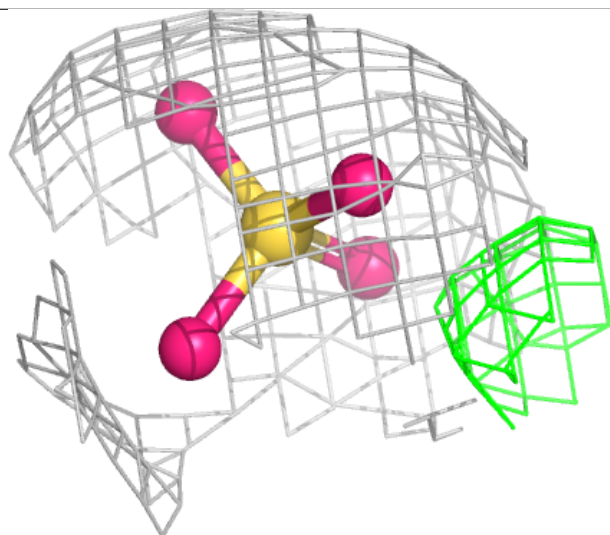
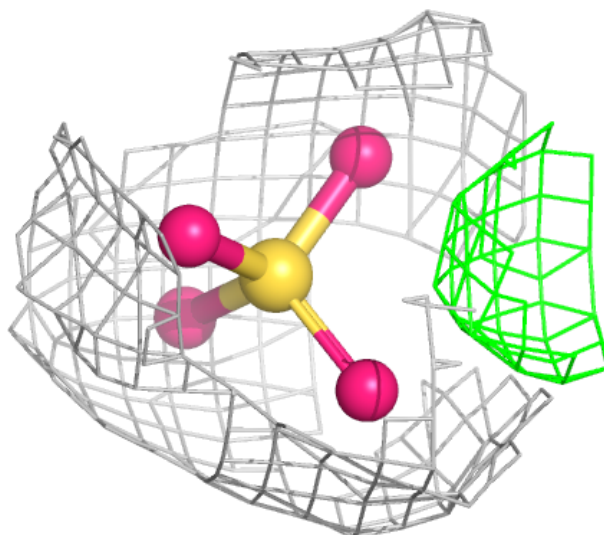
Electron density around SO4 A 801:

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



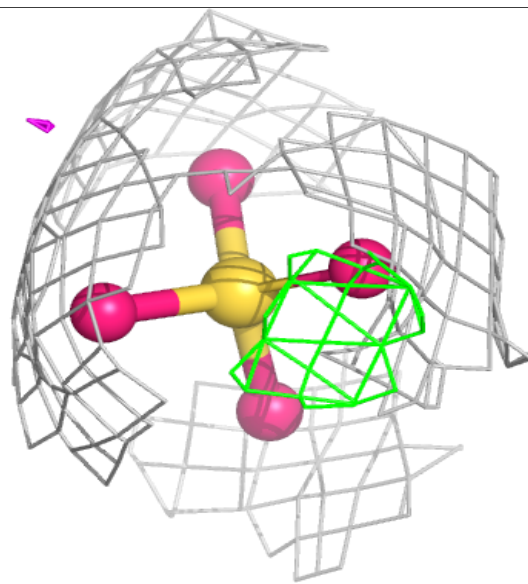
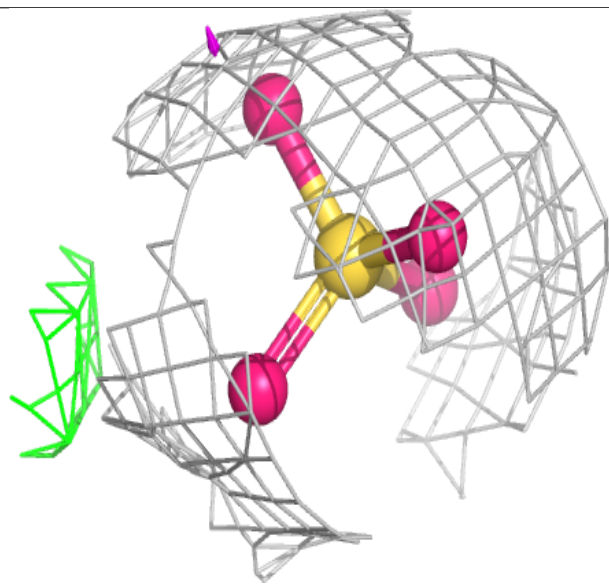
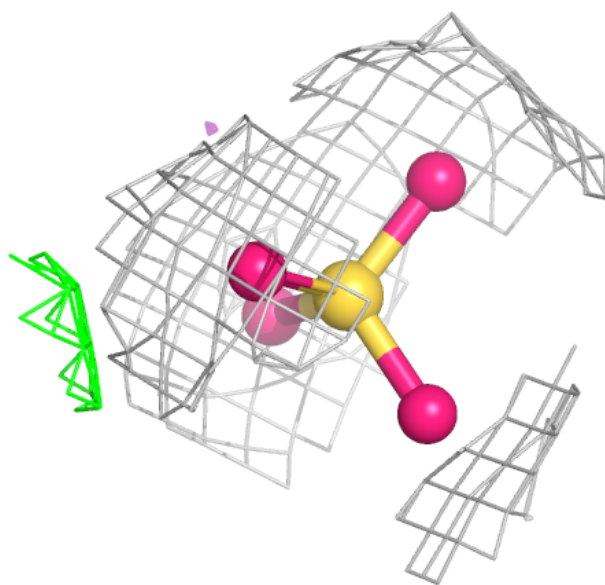
Electron density around SO4 D 801:

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



Electron density around SO4 B 801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.