Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2023 – 03:57 PM EST

PDB ID	:	8DOL
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:

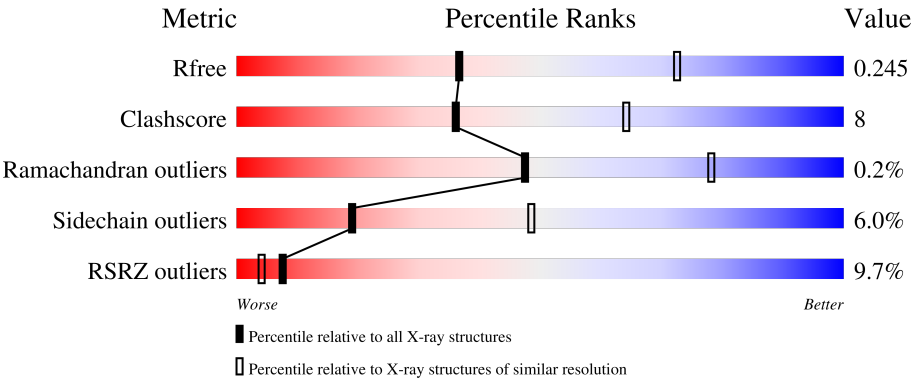
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	% 74% 17% • 9%
1	B	593	8% 63% 20% • 16%
1	C	593	13% 65% 19% • 14%
1	D	593	7% 72% 16% • 11%
1	E	593	7% 70% 20% • 9%

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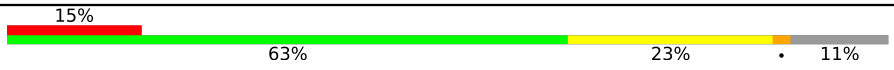
Mol	Chain	Length	Quality of chain
1	F	593	

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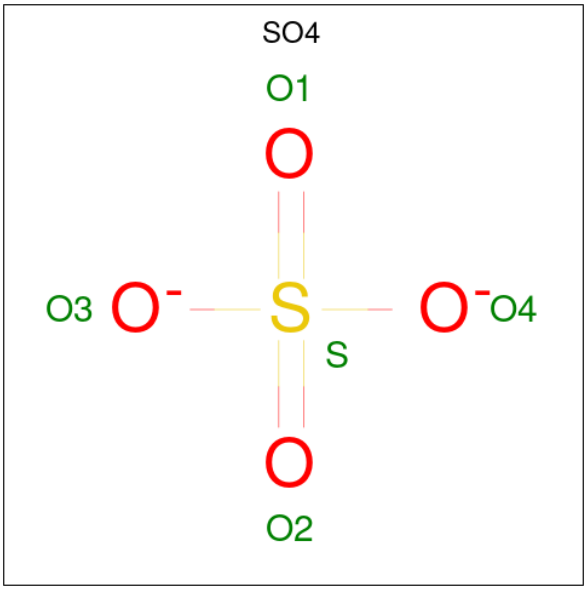
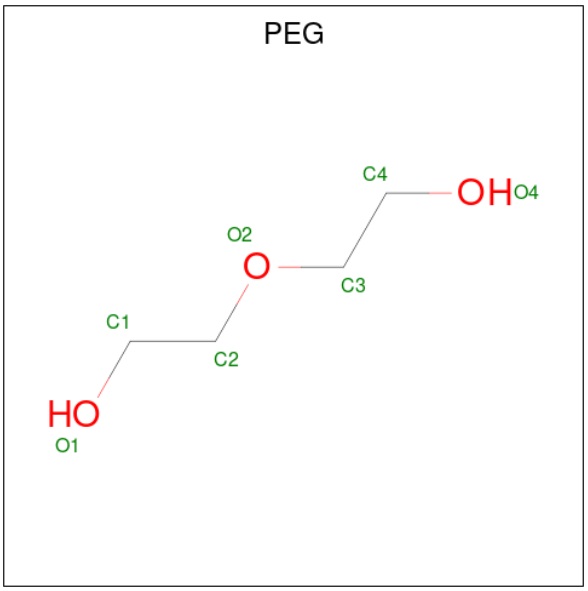
Chain	Residue	Modelled	Actual	Comment	Reference
F	165	SER	-	expression tag	UNP O25260

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is water.

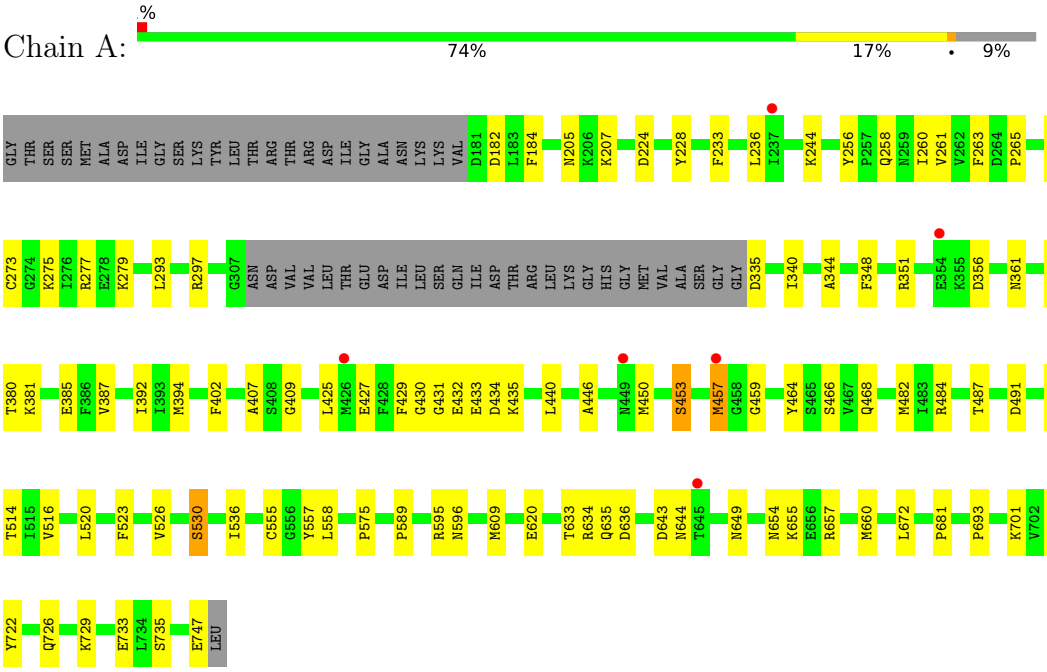
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	B	2	Total O 2 2	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	3	Total O 3 3	0	0
4	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

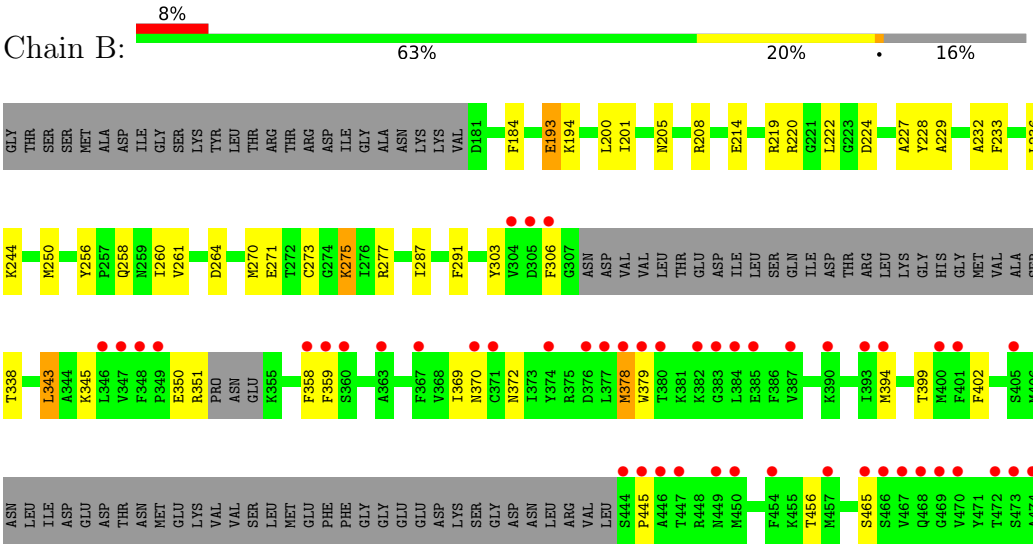
• Molecule 1: Cag pathogenicity island protein (Cag5)

Chain A:



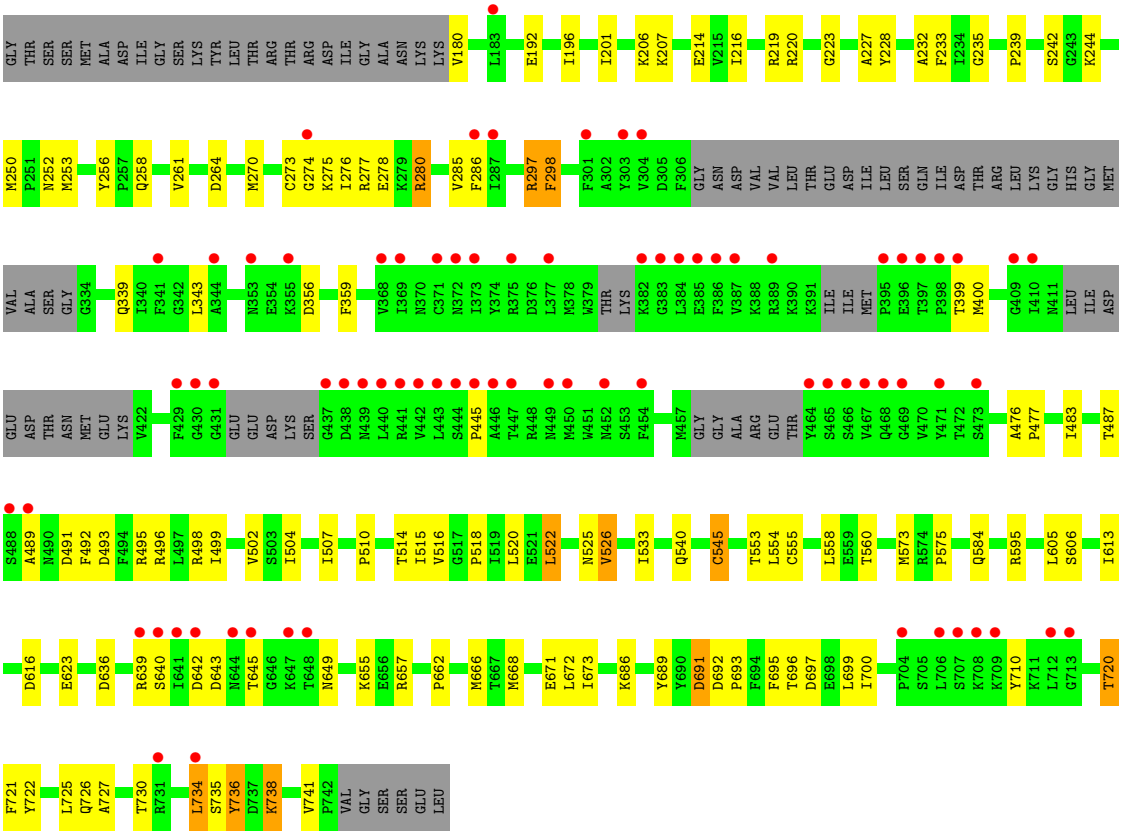
• Molecule 1: Cag pathogenicity island protein (Cag5)

Chain B:



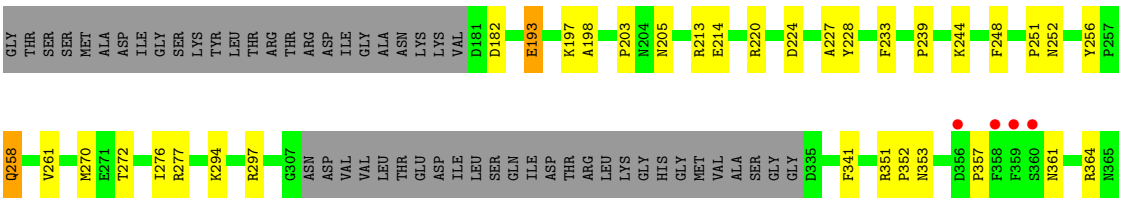
• Molecule 1: Cag pathogenicity island protein (Cag5)

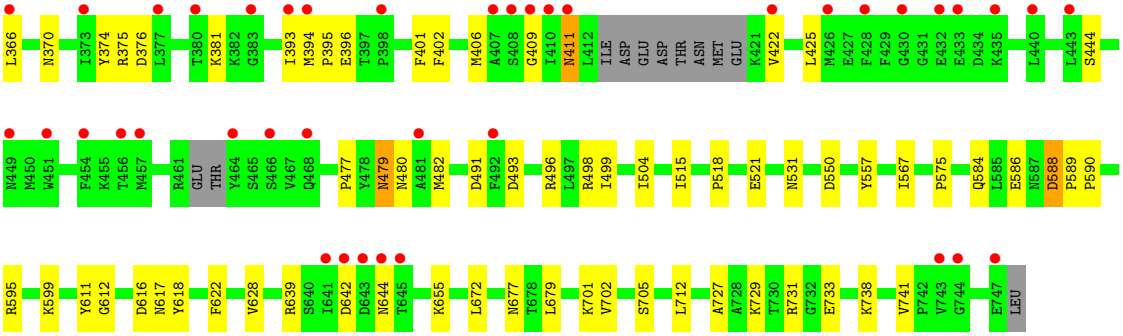
Chain C:



• Molecule 1: Cag pathogenicity island protein (Cag5)

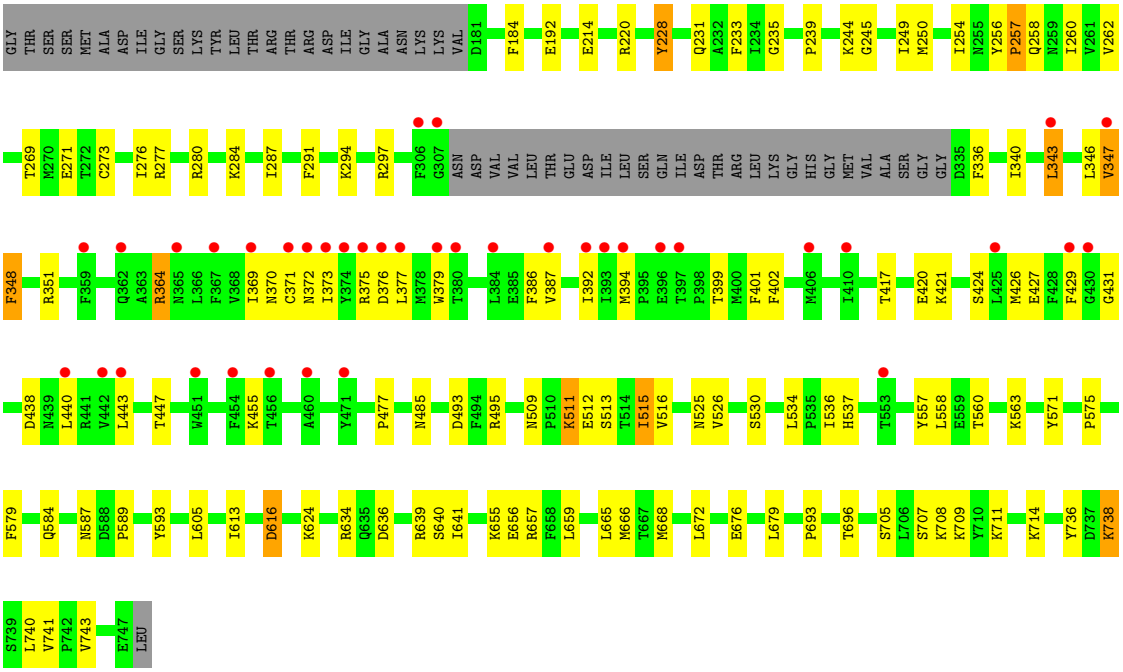
Chain D:





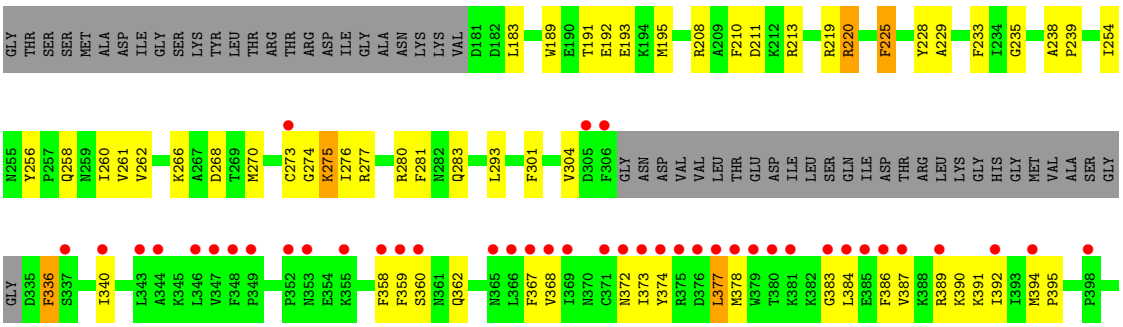
• Molecule 1: Cag pathogenicity island protein (Cag5)

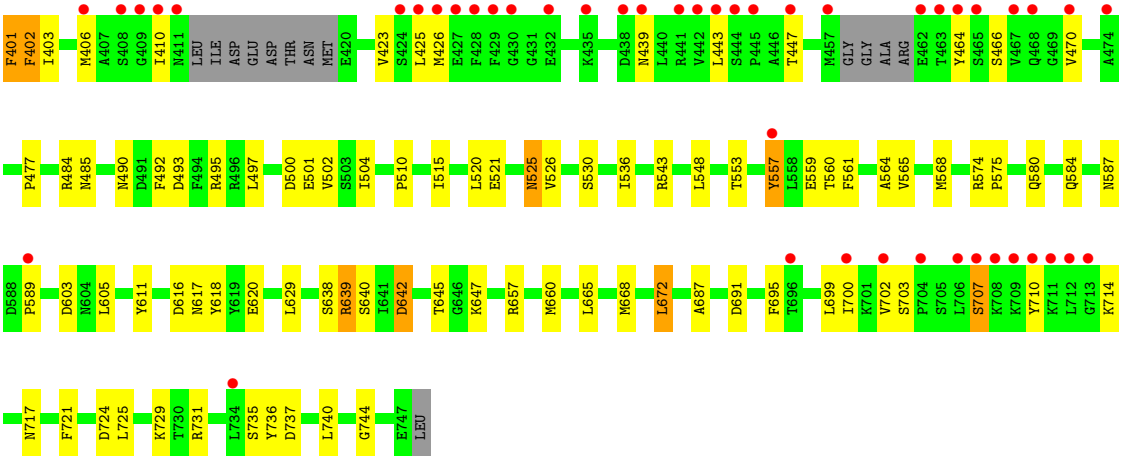
Chain E:



• Molecule 1: Cag pathogenicity island protein (Cag5)

Chain F:




F401 F402 I403 M406 A407 S408 G409 I410 N411 LEU ILE ASP GLU ASP THR ASN MET E420 V423 S424 L425 M426 E427 F428 F429 G430 G431 E432 K435 D438 N439 L440 R441 V442 L443 S444 P445 A446 T447 M457 GLY GLY ALA ARG E462 T463 Y464 S465 S466 V467 Q468 G469 V470 A474
P477 R484 N485 N490 D491 F492 D493 F494 R495 R496 L497 D500 E501 V502 S503 I504 P510 I515 L520 E521 N525 V526 S530 I536 R543 L548 T553 Y557 L558 E559 T560 F561 A564 V565 M568 R574 P575 Q580 Q584 N587
D588 P589 D603 N604 L605 Y611 D616 N617 Y618 Y619 E620 L629 S638 R639 S640 I641 D642 T645 G646 K647 R657 M660 L665 M668 L672 A687 D691 F695 T696 L699 I700 K701 V702 S703 P704 S705 L706 S707 K708 K709 Y710 K711 L712 G713 K714
N717 F721 D724 L725 K729 T730 R731 L734 S735 Y736 D737 L740 G744 E747 LEU

4 Data and refinement statistics (i)

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 48.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.79-2.80) 99.3 (48.95-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.247 0.196 , 0.245	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)	0.31 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.26	0/4397	0.48	0/5932
1	B	0.27	0/3946	0.50	2/5334 (0.0%)
1	C	0.26	0/3814	0.50	0/5170
1	D	0.26	0/4280	0.48	0/5780
1	E	0.26	0/4368	0.48	0/5898
1	F	0.26	0/4211	0.48	0/5695
All	All	0.26	0/25016	0.49	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(^{o})	Ideal(^{o})
1	B	445	PRO	N-CA-CB	5.84	110.31	103.30
1	B	378	MET	CB-CG-SD	5.27	128.20	112.40

There are no chirality outliers.

There are no planarity outliers.

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	4301	0	4260	56	0
1	B	3861	0	3707	66	0
1	C	3741	0	3439	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4186	0	4097	57	0
1	E	4273	0	4199	69	0
1	F	4120	0	4009	88	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	386	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 8.

All (386) 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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:ASN:HA	1:E:560:THR:HG21	1.77	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:F:268:ASP:OD1	1:F:729:LYS:NZ	2.27	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: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: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: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: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: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
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:D:182:ASP:OD1	1:E:634:ARG:NH2	2.29	0.57
1:A:268:ASP:OD1	1:A:729:LYS:NZ	2.30	0.57
1:F:737:ASP:HB3	1:F:740:LEU:HD13	1.85	0.57
1:E:348:PHE:C	1:E:364:ARG:HH12	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:358:PHE:C	1:F:362:GLN:HE22	2.09	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: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:731:ARG:HH21	1:D:733:GLU:CD	2.10	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:B:665:LEU:O	1:B:668:MET:HG3	2.08	0.54
1:F:485:ASN:ND2	1:F:744:GLY:HA3	2.23	0.54
1:B:557:TYR:HB2	1:B:589:PRO:O	2.08	0.53
1:F:620:GLU:H	1:F:620:GLU:CD	2.12	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:250:MET:HA	1:E:250:MET:HE2	1.92	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: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:A:482:MET:HE3	1:A:482:MET:HA	1.92	0.51
1:B:256:TYR:CE2	1:B:258:GLN:HB2	2.45	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:294:LYS:HZ2	1:E:741:VAL:HB	1.77	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:193:GLU:H	1:B:193:GLU:CD	2.18	0.47
1:E:214:GLU:HA	1:E:228:TYR:O	2.13	0.47
1:F:553:THR:HG21	1:F:584:GLN:HG2	1.96	0.47
1:E:636:ASP:OD2	1:E:655:LYS:NZ	2.47	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: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:B:620:GLU:CD	1:B:620:GLU:H	2.18	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: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
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: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: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:SD	1:E:455:LYS:HD3	2.56	0.46
1:E:624:LYS:NZ	1:F:620:GLU:OE2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:293:LEU:N	1:A:482:MET:HE1	2.30	0.45
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:D:294:LYS:NZ	1:D:738:LYS:O	2.39	0.45
1:E:256:TYR:CE2	1:E:258:GLN:HB2	2.51	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:B:727:ALA:O	1:B:730:THR:OG1	2.30	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:642:ASP:OD1	1:D:642:ASP:C	2.57	0.43
1:F:276:ILE:HD11	1:F:699:LEU:HA	2.00	0.43
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:D:244:LYS:NZ	1:D:550:ASP:OD1	2.47	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: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:A:657:ARG:HG3	1:F:183:LEU:O	2.17	0.43
1:D:370:ASN:HB3	1:D:406:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ARG:HG3	1:D:353:ASN:H	1.83	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: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: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:D:248:PHE:C	1:D:251:PRO:HD2	2.40	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
1:E:340:ILE:HD12	1:E:371:CYS:HB3	2.00	0.42
1:F:274:GLY:HA3	1:F:736:TYR:HB3	2.00	0.42
1:E:417:THR:OG1	1:E:421:LYS:NZ	2.50	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:294:LYS:HZ2	1:D:741:VAL:HB	1.85	0.41
1:D:393:ILE:HB	1:D:411:ASN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:477:PRO:HB3	1:F:515:ILE:HB	2.03	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	536/593 (90%)	508 (95%)	28 (5%)	0	100	100
1	B	490/593 (83%)	465 (95%)	24 (5%)	1 (0%)	47	78
1	C	496/593 (84%)	469 (95%)	26 (5%)	1 (0%)	47	78
1	D	522/593 (88%)	500 (96%)	19 (4%)	3 (1%)	25	56
1	E	536/593 (90%)	516 (96%)	19 (4%)	1 (0%)	47	78
1	F	519/593 (88%)	501 (96%)	18 (4%)	0	100	100
All	All	3099/3558 (87%)	2959 (96%)	134 (4%)	6 (0%)	47	78

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/520 (90%)	450 (96%)	19 (4%)	30	64
1	B	399/520 (77%)	375 (94%)	24 (6%)	19	48
1	C	354/520 (68%)	324 (92%)	30 (8%)	10	31
1	D	452/520 (87%)	435 (96%)	17 (4%)	33	67
1	E	461/520 (89%)	431 (94%)	30 (6%)	17	44
1	F	442/520 (85%)	408 (92%)	34 (8%)	13	35
All	All	2577/3120 (83%)	2423 (94%)	154 (6%)	19	48

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	A	228	TYR
1	A	244	LYS
1	A	270	MET
1	A	275	LYS
1	A	351	ARG
1	A	356	ASP
1	A	453	SER
1	A	457	MET
1	A	466	SER
1	A	514	THR
1	A	516	VAL
1	A	530	SER
1	A	595	ARG
1	A	634	ARG
1	A	649	ASN
1	A	660	MET
1	A	672	LEU
1	A	735	SER
1	B	193	GLU
1	B	194	LYS
1	B	220	ARG

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Mol	Chain	Res	Type
1	B	228	TYR
1	B	250	MET
1	B	270	MET
1	B	275	LYS
1	B	291	PHE
1	B	338	THR
1	B	343	LEU
1	B	370	ASN
1	B	394	MET
1	B	465	SER
1	B	513	SER
1	B	579	PHE
1	B	582	LYS
1	B	588	ASP
1	B	595	ARG
1	B	616	ASP
1	B	644	ASN
1	B	647	LYS
1	B	657	ARG
1	B	672	LEU
1	B	711	LYS
1	C	180	VAL
1	C	206	LYS
1	C	228	TYR
1	C	250	MET
1	C	253	MET
1	C	270	MET
1	C	280	ARG
1	C	297	ARG
1	C	298	PHE
1	C	495	ARG
1	C	514	THR
1	C	515	ILE
1	C	522	LEU
1	C	526	VAL
1	C	545	CYS
1	C	553	THR
1	C	584	GLN
1	C	595	ARG
1	C	616	ASP
1	C	639	ARG
1	C	649	ASN

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Mol	Chain	Res	Type
1	C	657	ARG
1	C	666	MET
1	C	672	LEU
1	C	691	ASP
1	C	720	THR
1	C	725	LEU
1	C	734	LEU
1	C	736	TYR
1	C	738	LYS
1	D	220	ARG
1	D	228	TYR
1	D	258	GLN
1	D	270	MET
1	D	341	PHE
1	D	375	ARG
1	D	381	LYS
1	D	401	PHE
1	D	411	ASN
1	D	422	VAL
1	D	479	ASN
1	D	584	GLN
1	D	588	ASP
1	D	599	LYS
1	D	639	ARG
1	D	655	LYS
1	D	672	LEU
1	E	192	GLU
1	E	220	ARG
1	E	228	TYR
1	E	244	LYS
1	E	257	PRO
1	E	336	PHE
1	E	343	LEU
1	E	348	PHE
1	E	351	ARG
1	E	364	ARG
1	E	420	GLU
1	E	424	SER
1	E	438	ASP
1	E	511	LYS
1	E	515	ILE
1	E	563	LYS

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Mol	Chain	Res	Type
1	E	579	PHE
1	E	584	GLN
1	E	587	ASN
1	E	616	ASP
1	E	639	ARG
1	E	640	SER
1	E	641	ILE
1	E	657	ARG
1	E	672	LEU
1	E	707	SER
1	E	708	LYS
1	E	711	LYS
1	E	714	LYS
1	E	738	LYS
1	F	220	ARG
1	F	225	PHE
1	F	228	TYR
1	F	266	LYS
1	F	270	MET
1	F	275	LYS
1	F	293	LEU
1	F	336	PHE
1	F	359	PHE
1	F	360	SER
1	F	367	PHE
1	F	377	LEU
1	F	384	LEU
1	F	401	PHE
1	F	402	PHE
1	F	425	LEU
1	F	426	MET
1	F	464	TYR
1	F	525	ASN
1	F	557	TYR
1	F	587	ASN
1	F	603	ASP
1	F	638	SER
1	F	639	ARG
1	F	640	SER
1	F	642	ASP
1	F	657	ARG
1	F	672	LEU

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Mol	Chain	Res	Type
1	F	691	ASP
1	F	707	SER
1	F	714	LYS
1	F	717	ASN
1	F	731	ARG
1	F	735	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	GLN
1	A	596	ASN
1	A	644	ASN
1	B	282	ASN
1	B	370	ASN
1	B	587	ASN
1	B	644	ASN
1	E	525	ASN
1	F	485	ASN
1	F	525	ASN

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 monosaccharides 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	E	801	-	4,4,4	0.14	0	6,6,6	0.12	0
3	PEG	B	802	-	6,6,6	0.10	0	5,5,5	0.10	0
2	SO4	F	801	-	4,4,4	0.15	0	6,6,6	0.13	0
3	PEG	C	802	-	6,6,6	0.12	0	5,5,5	0.08	0
2	SO4	B	801	-	4,4,4	0.13	0	6,6,6	0.09	0
3	PEG	E	802	-	6,6,6	0.13	0	5,5,5	0.05	0
2	SO4	D	801	-	4,4,4	0.14	0	6,6,6	0.12	0
3	PEG	F	802	-	6,6,6	0.14	0	5,5,5	0.10	0
3	PEG	D	802	-	6,6,6	0.12	0	5,5,5	0.10	0
2	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	C	801	-	4,4,4	0.14	0	6,6,6	0.12	0
3	PEG	A	802	-	6,6,6	0.12	0	5,5,5	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	802	-	-	1/4/4/4	-
3	PEG	C	802	-	-	2/4/4/4	-
3	PEG	E	802	-	-	2/4/4/4	-
3	PEG	F	802	-	-	3/4/4/4	-
3	PEG	D	802	-	-	0/4/4/4	-
3	PEG	A	802	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) 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

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

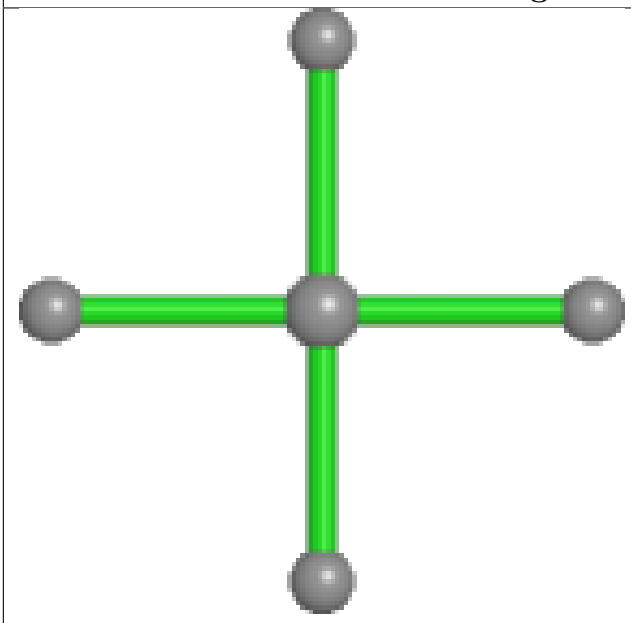
There are no ring outliers.

2 monomers are involved in 2 short contacts:

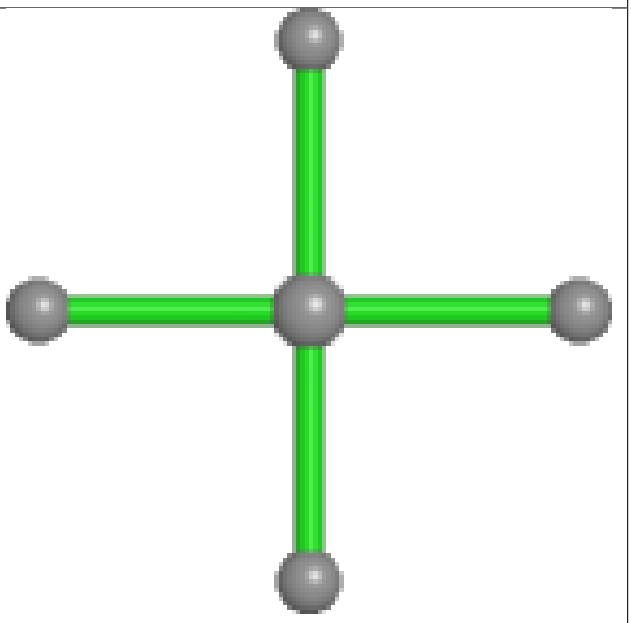
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	802	PEG	1	0
2	C	801	SO4	1	0

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

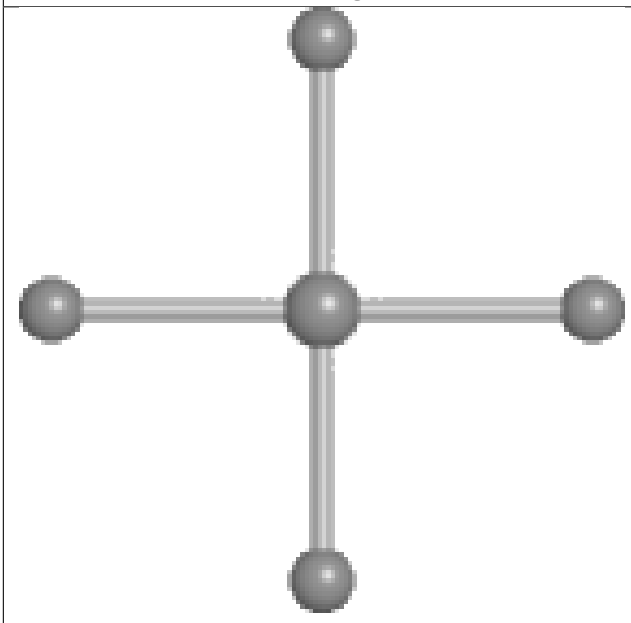
Ligand SO4 E 801



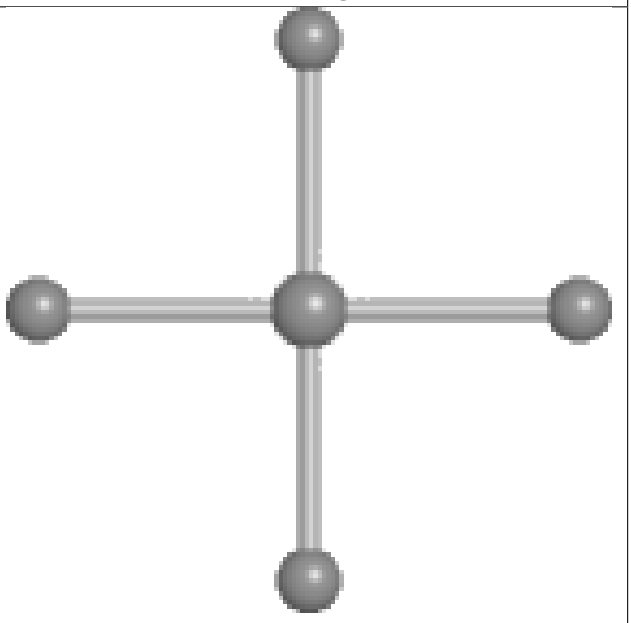
Bond lengths



Bond angles

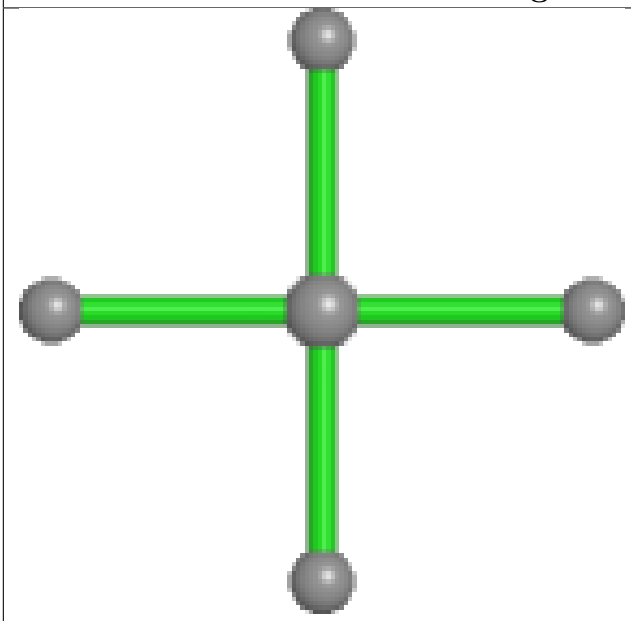


Torsions

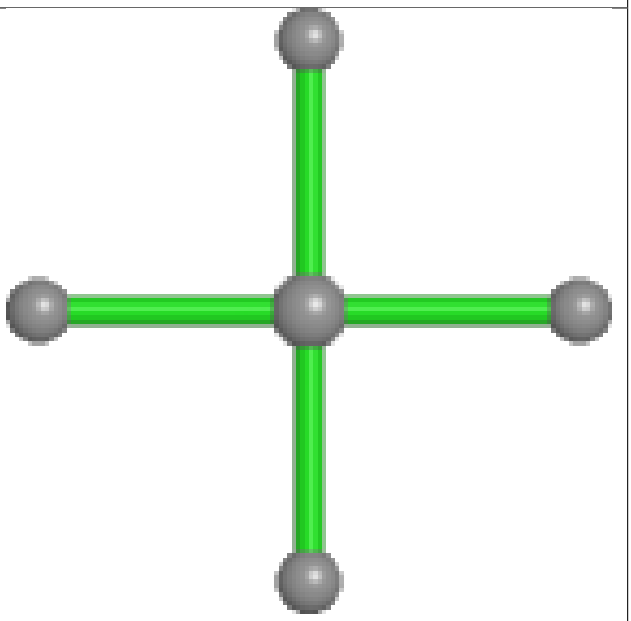


Rings

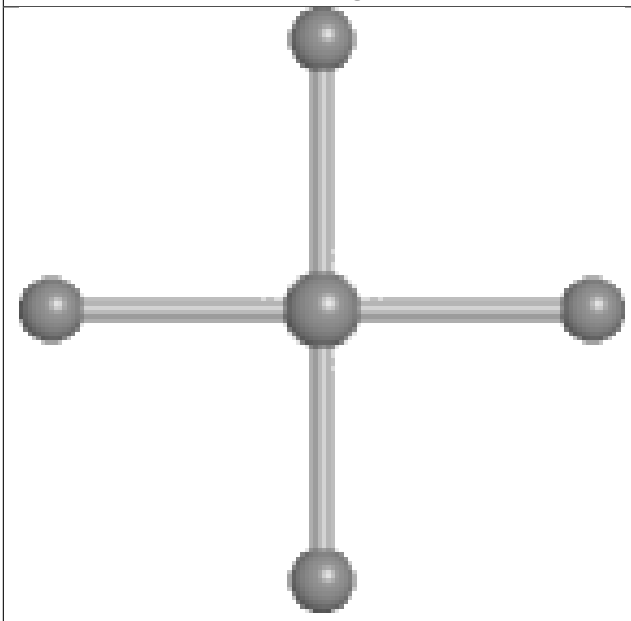
Ligand SO4 F 801



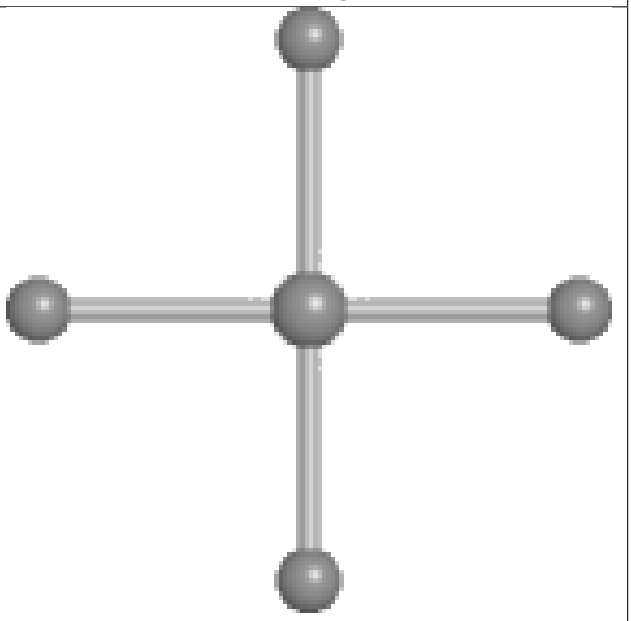
Bond lengths



Bond angles

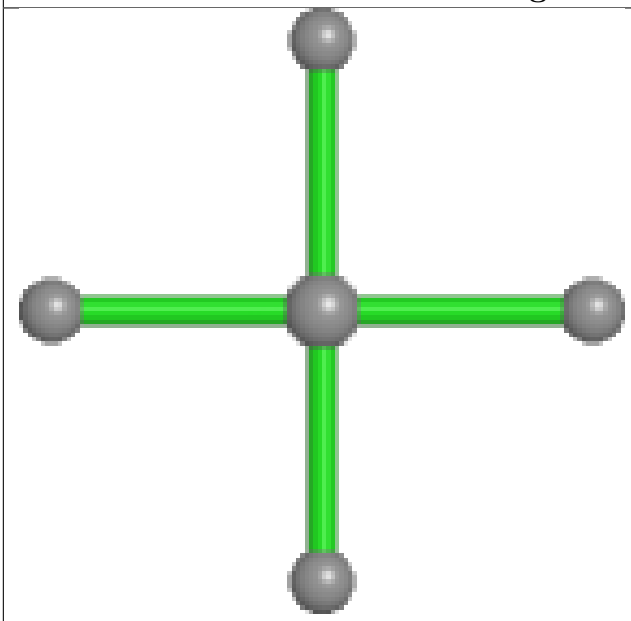


Torsions

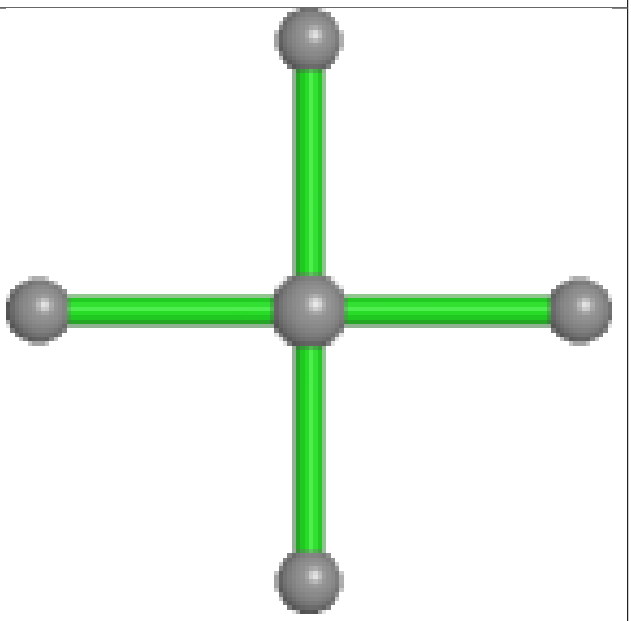


Rings

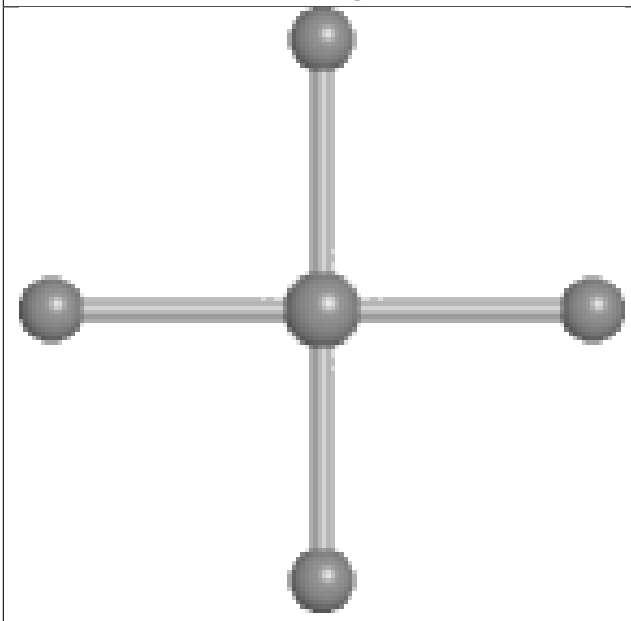
Ligand SO4 B 801



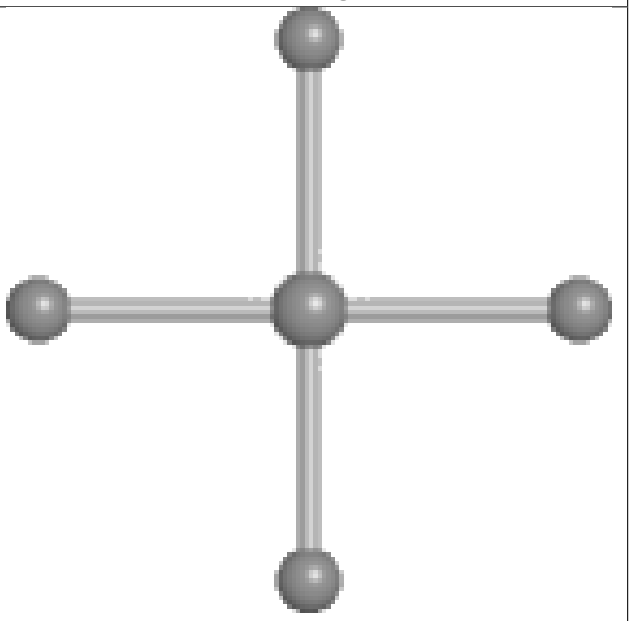
Bond lengths



Bond angles

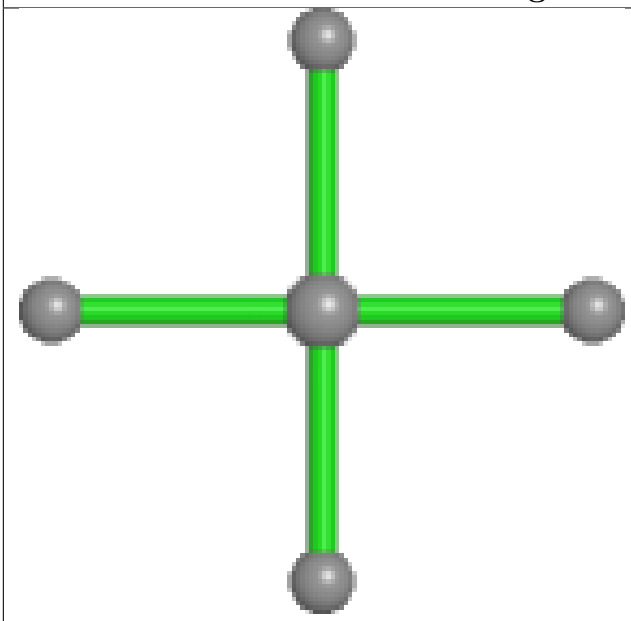


Torsions

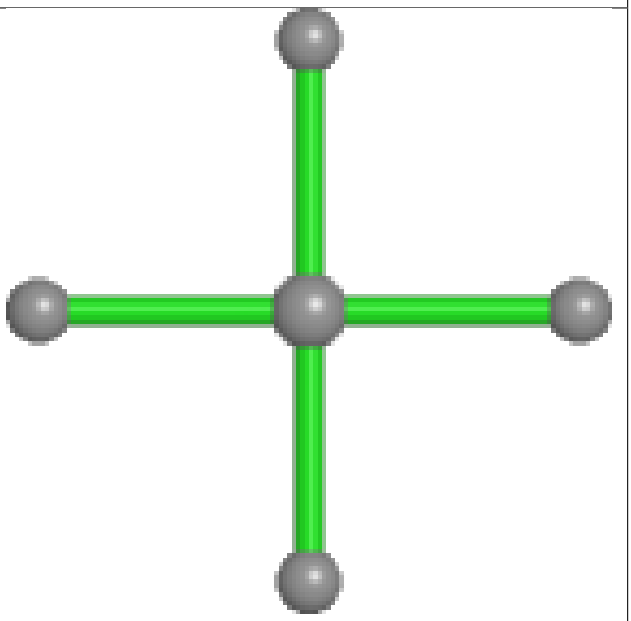


Rings

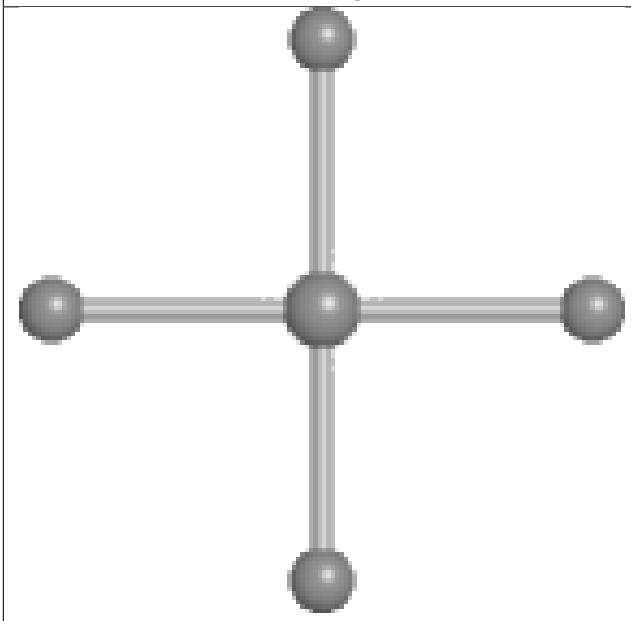
Ligand SO4 D 801



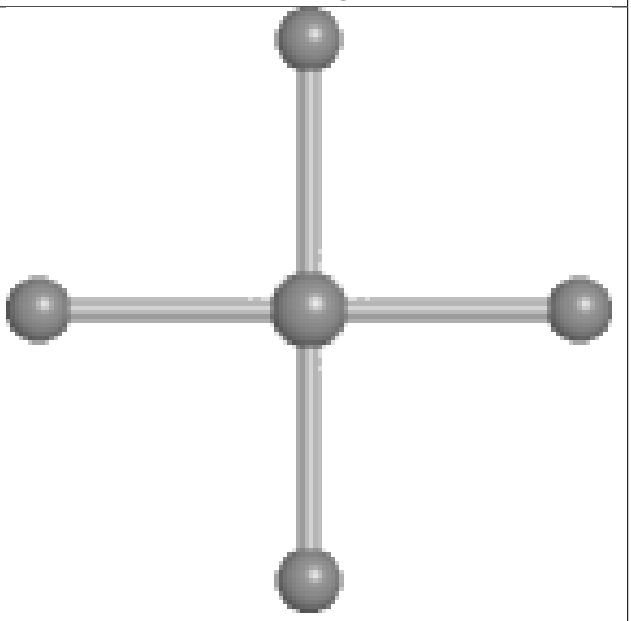
Bond lengths



Bond angles

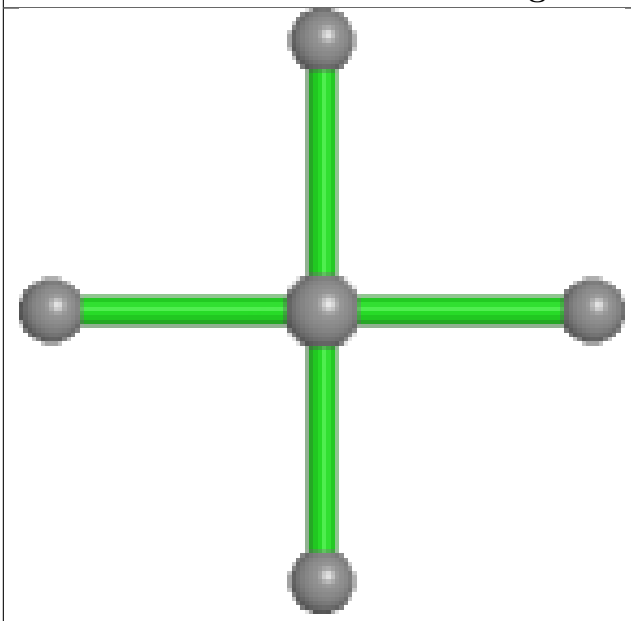


Torsions

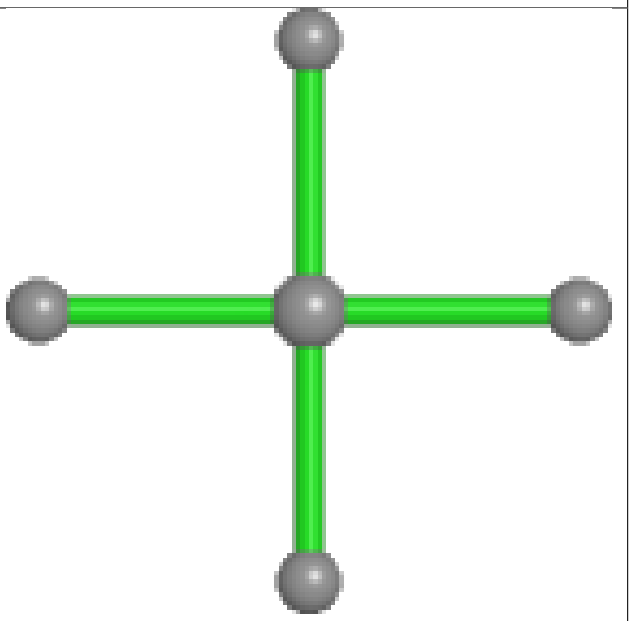


Rings

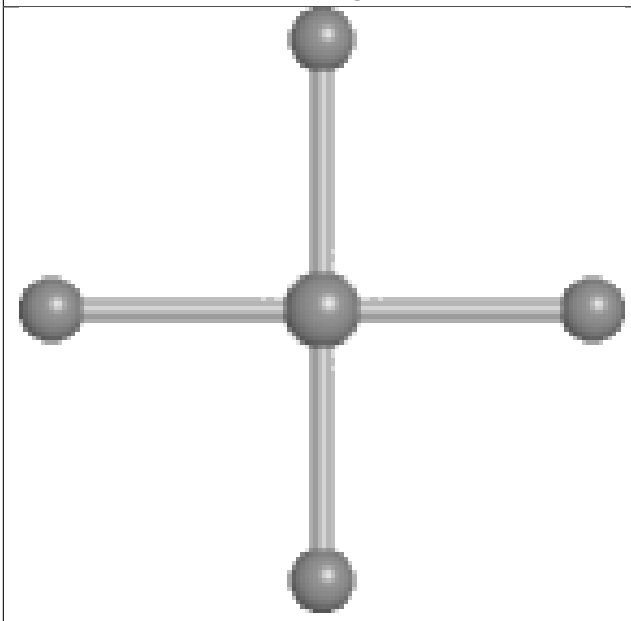
Ligand SO4 A 801



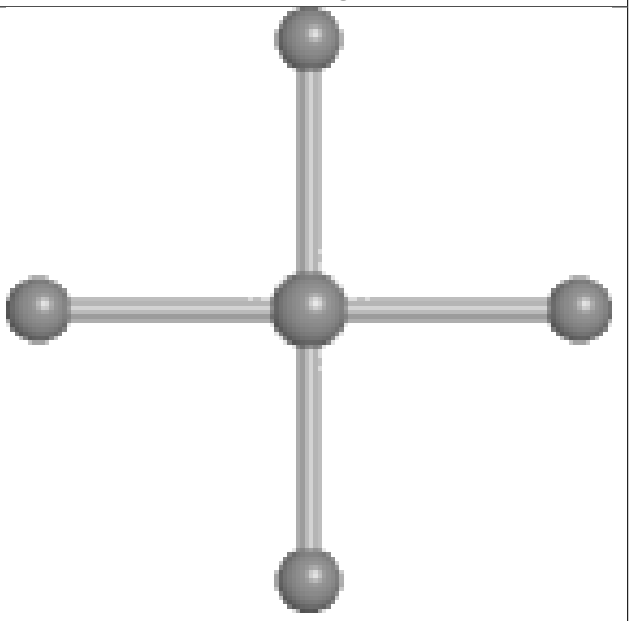
Bond lengths



Bond angles

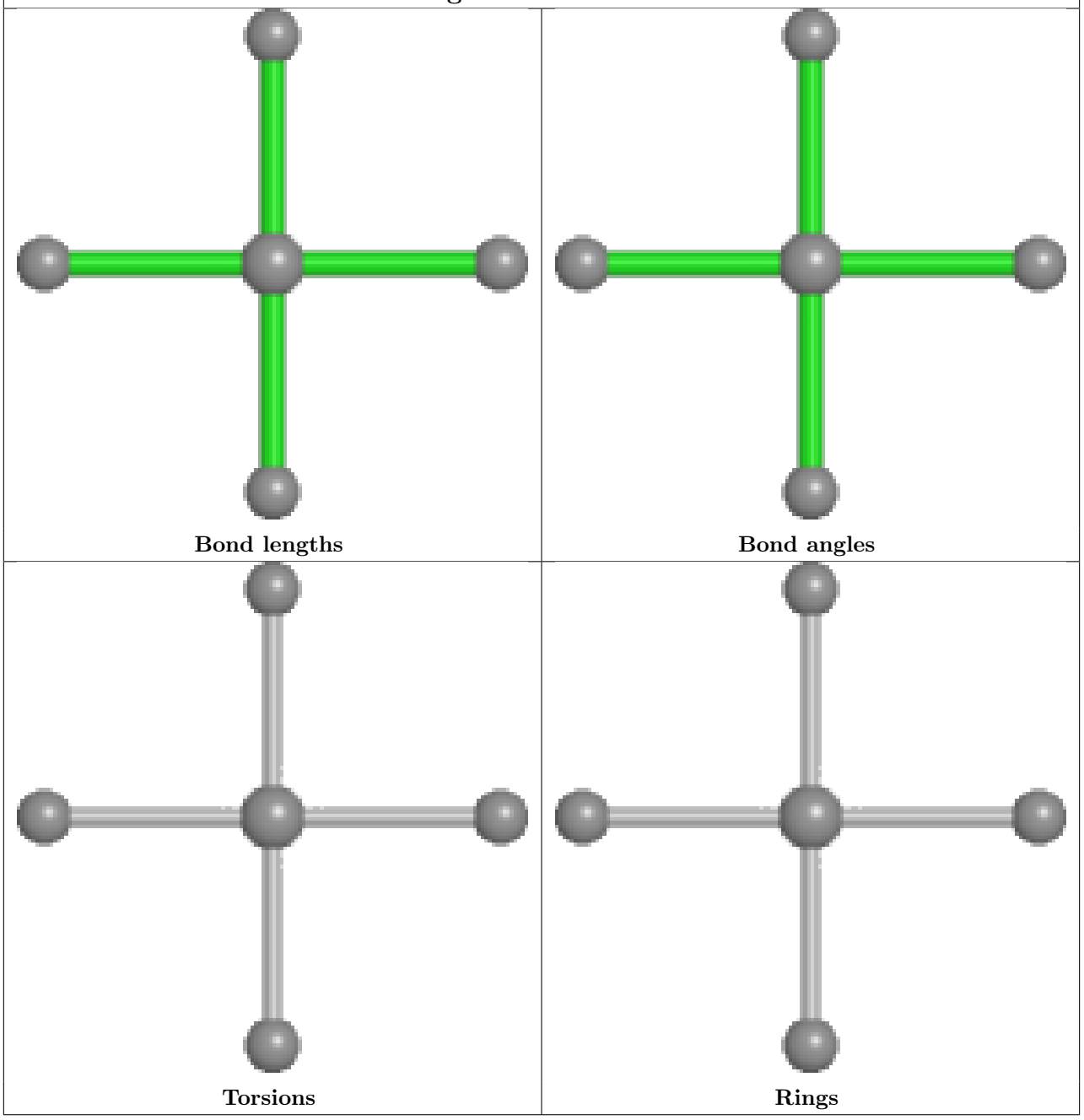


Torsions



Rings

Ligand SO4 C 801



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, 95^{th} 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%)	-0.06	6 (1%) 80 75	44, 74, 113, 185	0
1	B	498/593 (83%)	0.43	50 (10%) 7 4	45, 85, 197, 250	0
1	C	510/593 (86%)	0.70	77 (15%) 2 1	47, 109, 216, 272	0
1	D	530/593 (89%)	0.36	44 (8%) 11 6	45, 96, 172, 230	0
1	E	540/593 (91%)	0.30	39 (7%) 15 8	44, 80, 175, 214	0
1	F	527/593 (88%)	0.66	88 (16%) 1 1	47, 101, 215, 273	0
All	All	3145/3558 (88%)	0.39	304 (9%) 7 4	44, 89, 198, 273	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	379	TRP	9.7
1	F	443	LEU	9.5
1	F	380	THR	9.4
1	C	438	ASP	8.8
1	F	377	LEU	8.5
1	F	429	PHE	8.3
1	D	377	LEU	7.7
1	C	452	ASN	7.5
1	B	306	PHE	7.1
1	B	383	GLY	7.1
1	C	383	GLY	6.9
1	F	425	LEU	6.8
1	C	437	GLY	6.8
1	B	359	PHE	6.6
1	D	408	SER	6.5
1	F	358	PHE	6.4
1	E	451	TRP	6.3
1	C	644	ASN	6.2
1	B	360	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	467	VAL	6.1
1	D	359	PHE	6.1
1	E	392	ILE	5.9
1	C	465	SER	5.8
1	F	378	MET	5.6
1	B	469	GLY	5.6
1	F	442	VAL	5.6
1	E	425	LEU	5.6
1	C	369	ILE	5.5
1	C	464	TYR	5.5
1	F	409	GLY	5.4
1	C	442	VAL	5.2
1	B	470	VAL	5.2
1	F	360	SER	5.2
1	F	359	PHE	5.2
1	C	450	MET	5.1
1	B	472	THR	5.0
1	D	411	ASN	5.0
1	B	445	PRO	5.0
1	B	380	THR	4.9
1	F	428	PHE	4.9
1	B	446	ALA	4.9
1	F	376	ASP	4.9
1	A	426	MET	4.9
1	E	442	VAL	4.9
1	C	734	LEU	4.8
1	D	464	TYR	4.8
1	B	466	SER	4.8
1	C	440	LEU	4.8
1	C	446	ALA	4.7
1	C	441	ARG	4.7
1	F	438	ASP	4.7
1	B	379	TRP	4.7
1	E	380	THR	4.6
1	F	305	ASP	4.6
1	B	347	VAL	4.5
1	B	382	LYS	4.5
1	C	395	PRO	4.5
1	F	411	ASN	4.5
1	E	373	ILE	4.5
1	C	304	VAL	4.5
1	C	466	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	346	LEU	4.4
1	C	373	ILE	4.4
1	E	365	ASN	4.4
1	F	353	ASN	4.3
1	C	301	PHE	4.3
1	E	362	GLN	4.3
1	B	468	GLN	4.3
1	E	369	ILE	4.3
1	C	444	SER	4.3
1	F	392	ILE	4.3
1	B	394	MET	4.2
1	F	441	ARG	4.2
1	F	343	LEU	4.1
1	C	469	GLY	4.1
1	D	410	ILE	4.1
1	E	379	TRP	4.1
1	C	377	LEU	4.1
1	D	443	LEU	4.1
1	C	355	LYS	4.1
1	F	306	PHE	4.1
1	C	384	LEU	4.0
1	D	409	GLY	4.0
1	B	457	MET	4.0
1	E	376	ASP	4.0
1	F	708	LYS	4.0
1	D	747	GLU	4.0
1	F	375	ARG	4.0
1	C	372	ASN	4.0
1	E	443	LEU	3.9
1	F	557	TYR	3.9
1	B	384	LEU	3.9
1	F	371	CYS	3.8
1	F	340	ILE	3.8
1	F	355	LYS	3.8
1	F	383	GLY	3.8
1	C	439	ASN	3.7
1	C	468	GLN	3.7
1	B	405	SER	3.7
1	C	706	LEU	3.7
1	D	380	THR	3.7
1	F	696	THR	3.7
1	C	385	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	432	GLU	3.6
1	F	464	TYR	3.6
1	C	447	THR	3.6
1	B	304	VAL	3.6
1	C	397	THR	3.6
1	C	488	SER	3.6
1	C	713	GLY	3.6
1	E	343	LEU	3.6
1	F	410	ILE	3.5
1	C	382	LYS	3.5
1	D	744	GLY	3.5
1	D	743	VAL	3.5
1	F	408	SER	3.5
1	D	644	ASN	3.5
1	E	359	PHE	3.4
1	F	348	PHE	3.4
1	F	384	LEU	3.4
1	C	371	CYS	3.4
1	D	394	MET	3.4
1	C	712	LEU	3.4
1	D	449	ASN	3.4
1	B	377	LEU	3.3
1	C	399	THR	3.3
1	D	645	THR	3.3
1	F	398	PRO	3.3
1	D	358	PHE	3.3
1	C	645	THR	3.3
1	F	406	MET	3.3
1	C	473	SER	3.2
1	D	433	GLU	3.2
1	C	641	ILE	3.2
1	B	473	SER	3.2
1	F	368	VAL	3.2
1	D	383	GLY	3.2
1	B	479	ASN	3.2
1	C	368	VAL	3.2
1	E	377	LEU	3.2
1	D	451	TRP	3.2
1	E	429	PHE	3.2
1	F	467	VAL	3.1
1	B	370	ASN	3.1
1	E	384	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	369	ILE	3.1
1	C	467	VAL	3.1
1	B	305	ASP	3.1
1	B	401	PHE	3.1
1	C	353	ASN	3.1
1	C	449	ASN	3.1
1	D	456	THR	3.1
1	F	470	VAL	3.1
1	D	481	ALA	3.0
1	C	454	PHE	3.0
1	F	387	VAL	3.0
1	F	468	GLN	3.0
1	E	375	ARG	3.0
1	F	447	THR	3.0
1	F	712	LEU	3.0
1	C	489	ALA	3.0
1	E	456	THR	3.0
1	C	707	SER	3.0
1	C	274	GLY	3.0
1	F	394	MET	3.0
1	F	381	LYS	3.0
1	E	307	GLY	2.9
1	B	371	CYS	2.9
1	C	286	PHE	2.9
1	B	385	GLU	2.9
1	B	465	SER	2.9
1	D	641	ILE	2.9
1	C	443	LEU	2.9
1	F	346	LEU	2.9
1	E	387	VAL	2.9
1	F	347	VAL	2.9
1	F	349	PRO	2.9
1	B	363	ALA	2.9
1	B	481	ALA	2.9
1	A	354	GLU	2.9
1	E	410	ILE	2.9
1	B	387	VAL	2.9
1	B	449	ASN	2.9
1	F	372	ASN	2.9
1	F	700	ILE	2.9
1	B	393	ILE	2.8
1	E	393	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	366	LEU	2.8
1	D	356	ASP	2.8
1	D	426	MET	2.8
1	C	708	LYS	2.8
1	E	371	CYS	2.8
1	C	409	GLY	2.8
1	D	373	ILE	2.8
1	E	347	VAL	2.8
1	F	713	GLY	2.8
1	C	389	ARG	2.8
1	C	648	THR	2.8
1	F	462	GLU	2.8
1	E	454	PHE	2.8
1	E	460	ALA	2.8
1	F	365	ASN	2.7
1	E	430	GLY	2.7
1	F	389	ARG	2.7
1	C	396	GLU	2.7
1	F	439	ASN	2.7
1	A	237	ILE	2.7
1	F	352	PRO	2.7
1	F	430	GLY	2.7
1	F	707	SER	2.7
1	F	711	LYS	2.7
1	F	734	LEU	2.7
1	F	465	SER	2.6
1	B	378	MET	2.6
1	F	710	TYR	2.6
1	C	386	PHE	2.6
1	F	424	SER	2.6
1	C	303	TYR	2.6
1	D	440	LEU	2.6
1	C	431	GLY	2.6
1	F	373	ILE	2.6
1	B	358	PHE	2.6
1	D	430	GLY	2.6
1	F	444	SER	2.6
1	F	426	MET	2.6
1	B	454	PHE	2.6
1	D	468	GLN	2.5
1	D	454	PHE	2.5
1	C	410	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	375	ARG	2.5
1	F	457	MET	2.5
1	F	702	VAL	2.5
1	D	643	ASP	2.5
1	D	393	ILE	2.5
1	B	444	SER	2.4
1	B	390	LYS	2.4
1	D	642	ASP	2.4
1	C	445	PRO	2.4
1	C	640	SER	2.4
1	E	372	ASN	2.4
1	D	366	LEU	2.4
1	E	306	PHE	2.4
1	C	471	TYR	2.4
1	F	589	PRO	2.4
1	D	398	PRO	2.4
1	D	435	LYS	2.4
1	F	374	TYR	2.4
1	B	447	THR	2.4
1	F	463	THR	2.4
1	C	639	ARG	2.4
1	B	376	ASP	2.3
1	B	450	MET	2.3
1	D	360	SER	2.3
1	D	466	SER	2.3
1	F	706	LEU	2.3
1	F	432	GLU	2.3
1	C	704	PRO	2.3
1	B	400	MET	2.3
1	C	731	ARG	2.3
1	B	474	ALA	2.3
1	C	287	ILE	2.3
1	E	394	MET	2.3
1	E	406	MET	2.3
1	C	430	GLY	2.3
1	C	647	LYS	2.3
1	E	367	PHE	2.2
1	F	367	PHE	2.2
1	B	374	TYR	2.2
1	B	349	PRO	2.2
1	D	457	MET	2.2
1	F	386	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	709	LYS	2.2
1	F	385	GLU	2.2
1	F	427	GLU	2.2
1	C	429	PHE	2.2
1	F	474	ALA	2.2
1	A	449	ASN	2.2
1	C	642	ASP	2.2
1	C	387	VAL	2.2
1	B	348	PHE	2.1
1	F	445	PRO	2.1
1	E	374	TYR	2.1
1	F	435	LYS	2.1
1	C	344	ALA	2.1
1	D	407	ALA	2.1
1	E	396	GLU	2.1
1	E	553	THR	2.1
1	A	457	MET	2.1
1	F	704	PRO	2.1
1	C	341	PHE	2.1
1	A	645	THR	2.1
1	D	428	PHE	2.1
1	E	397	THR	2.1
1	C	709	LYS	2.1
1	D	422	VAL	2.1
1	F	337	SER	2.1
1	F	344	ALA	2.1
1	D	492	PHE	2.1
1	E	440	LEU	2.1
1	B	367	PHE	2.1
1	C	183	LEU	2.0
1	E	471	TYR	2.0
1	F	273	CYS	2.0
1	C	398	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

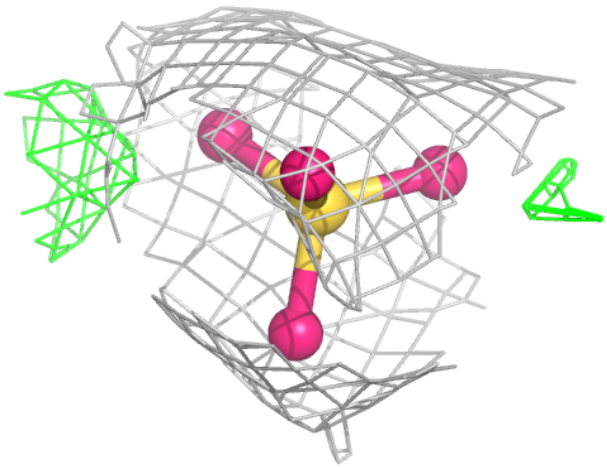
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

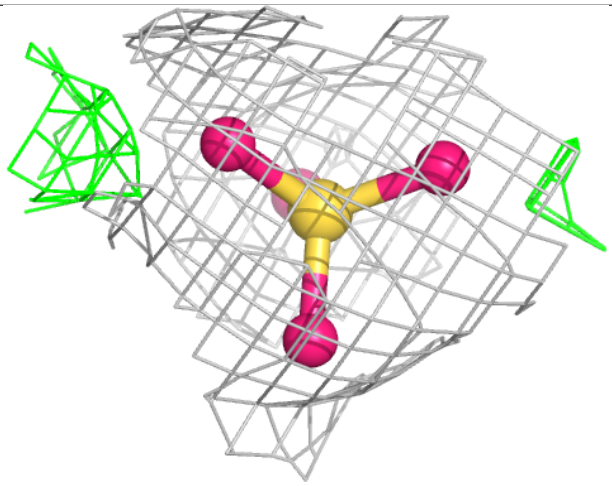
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	D	802	7/7	0.83	0.27	74,81,94,99	0
3	PEG	E	802	7/7	0.83	0.40	80,100,103,108	0
3	PEG	F	802	7/7	0.83	0.19	81,89,94,94	0
2	SO4	E	801	5/5	0.86	0.41	63,70,81,306	0
2	SO4	C	801	5/5	0.87	0.33	74,98,106,107	0
3	PEG	A	802	7/7	0.89	0.22	71,82,97,101	0
2	SO4	F	801	5/5	0.90	0.36	63,72,85,234	0
3	PEG	C	802	7/7	0.91	0.57	72,81,92,92	0
3	PEG	B	802	7/7	0.92	0.20	71,80,89,108	0
2	SO4	A	801	5/5	0.95	0.22	65,75,80,90	0
2	SO4	D	801	5/5	0.96	0.18	66,66,73,77	0
2	SO4	B	801	5/5	0.98	0.24	72,78,79,83	0

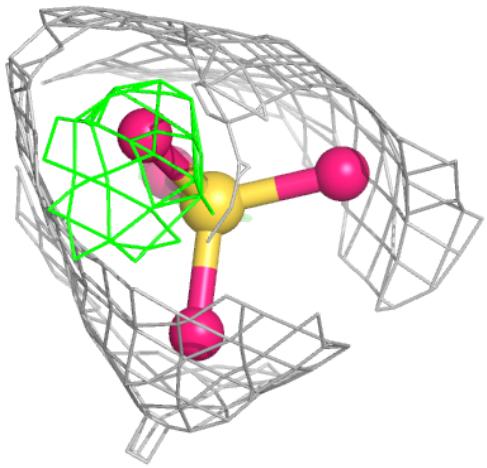
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SO4 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)

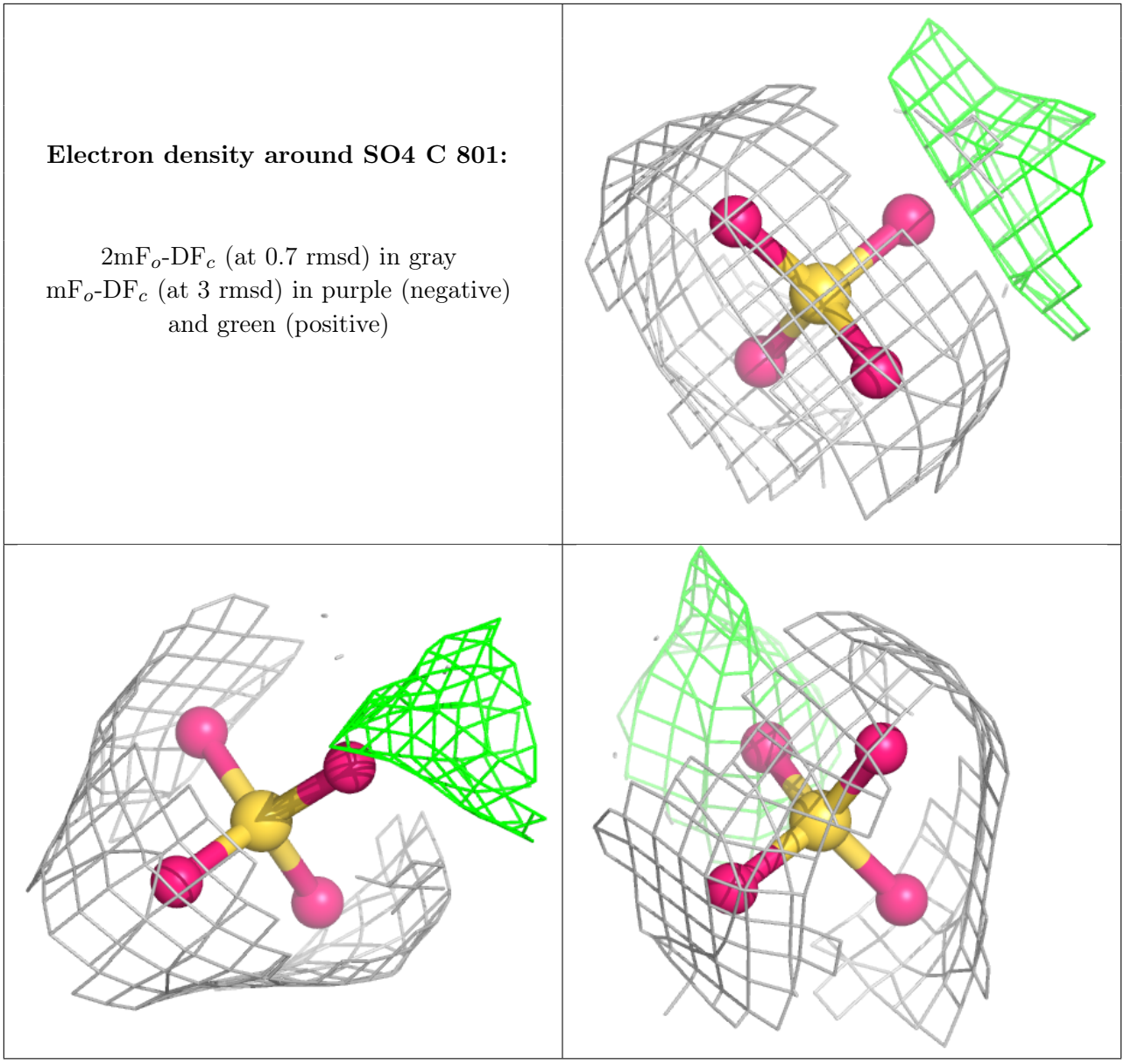






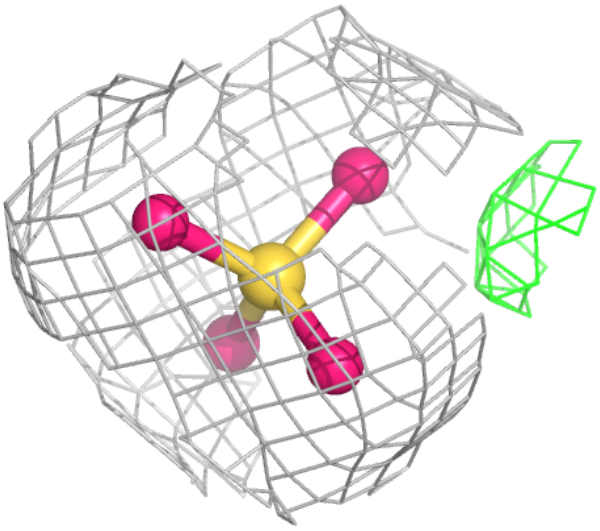
Electron density around SO4 C 801:

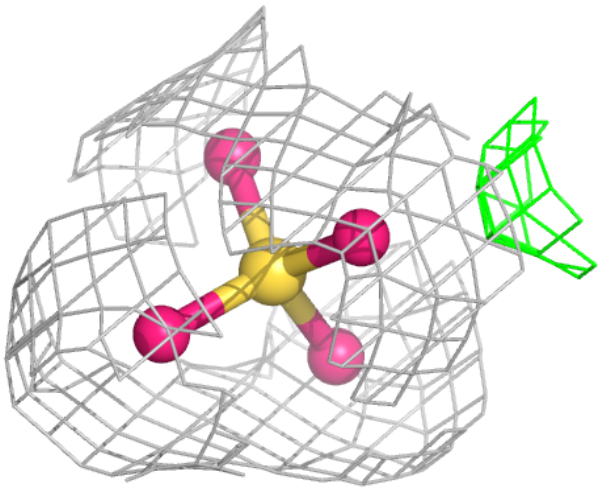
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

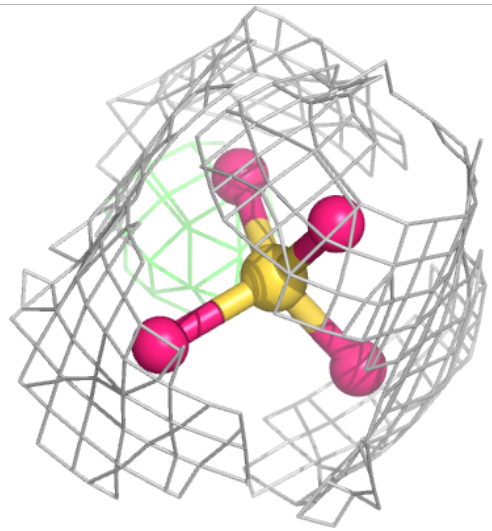


Electron density around SO4 F 801:

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

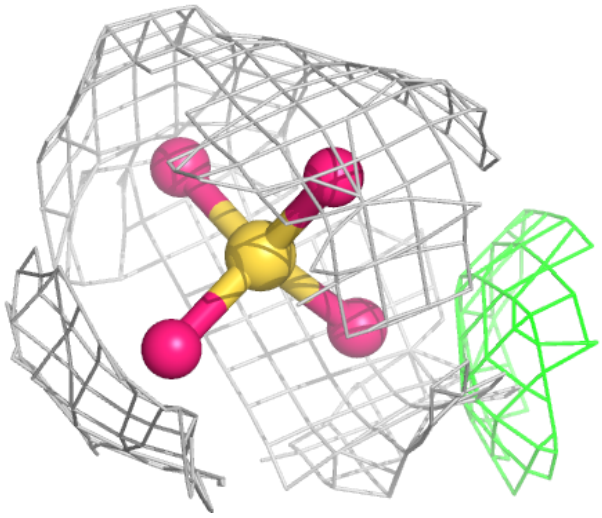


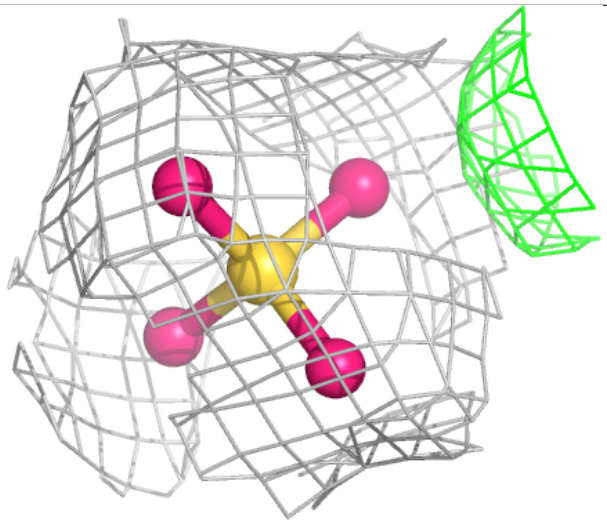


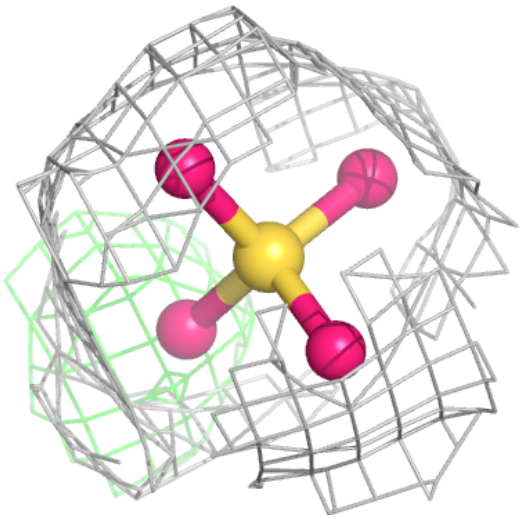


Electron density around SO4 A 801:

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

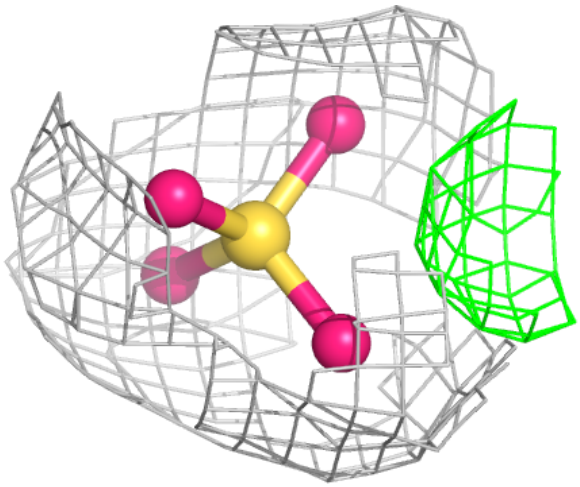


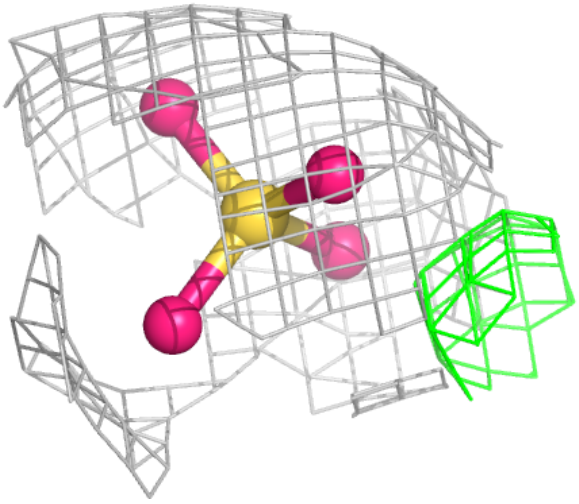


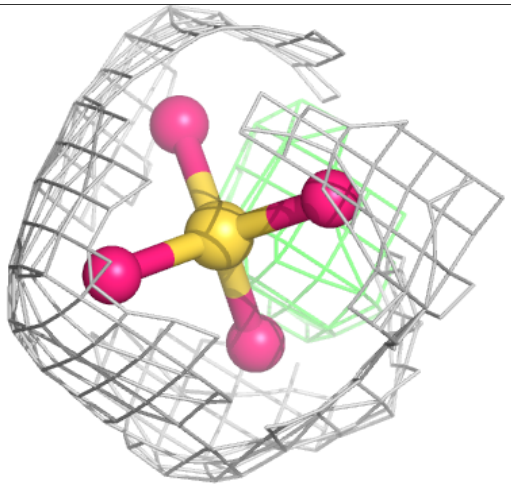


Electron density around SO4 D 801:

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

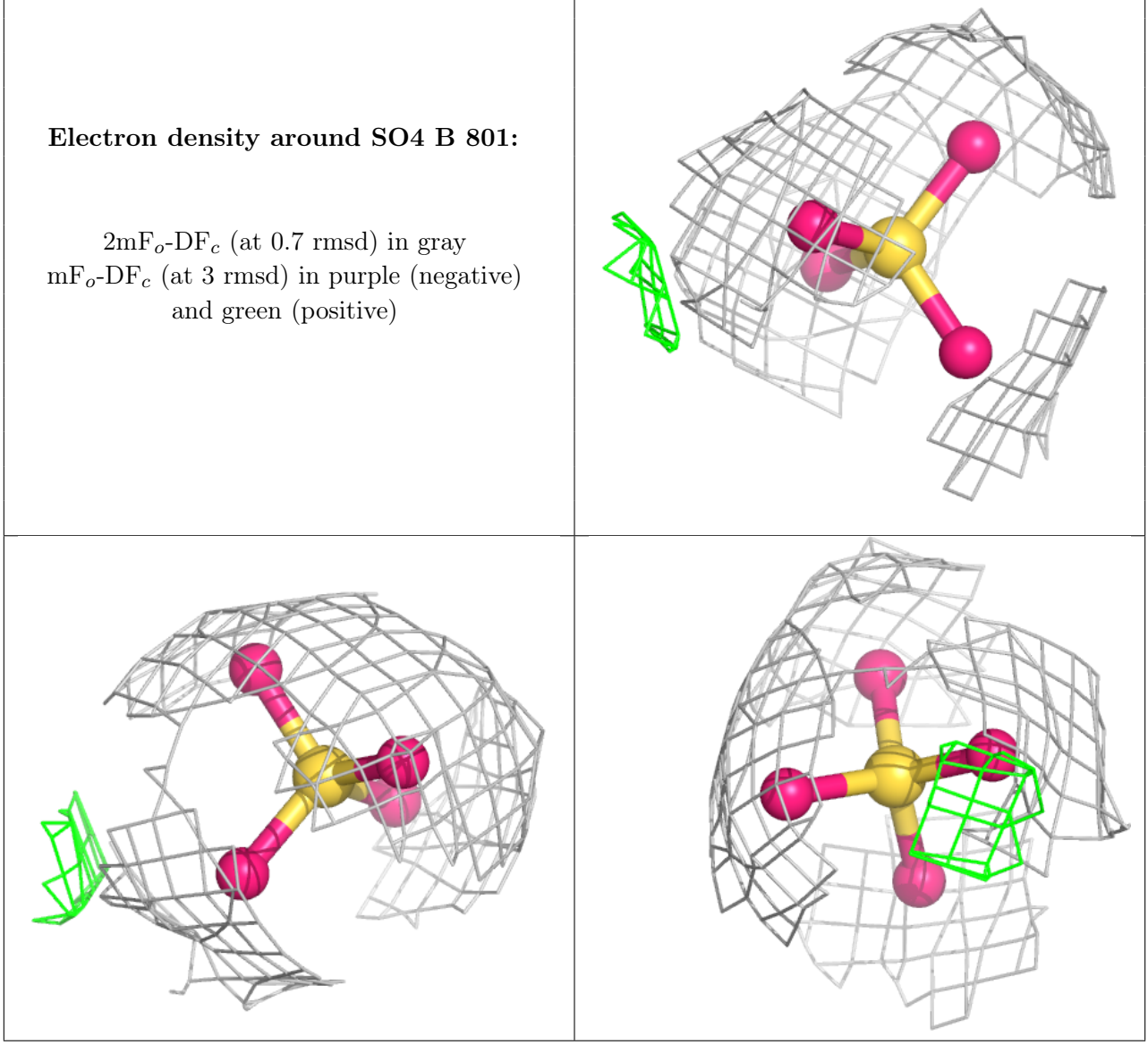






Electron density around SO4 B 801:

$2mF_o$-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

There are no such residues in this entry.