



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 11:26 PM EDT

PDB ID : 6TMO
Title : Structure determination of an enhanced affinity TCR, a24b17, in complex with HLA-A*02:01 presenting a MART-1 peptide, EAAGIGILTV
Authors : Rizkallah, P.J.; Cole, D.K.
Deposited on : 2019-12-05
Resolution : 2.10 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 : 2.37.1
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) : 2.37.1

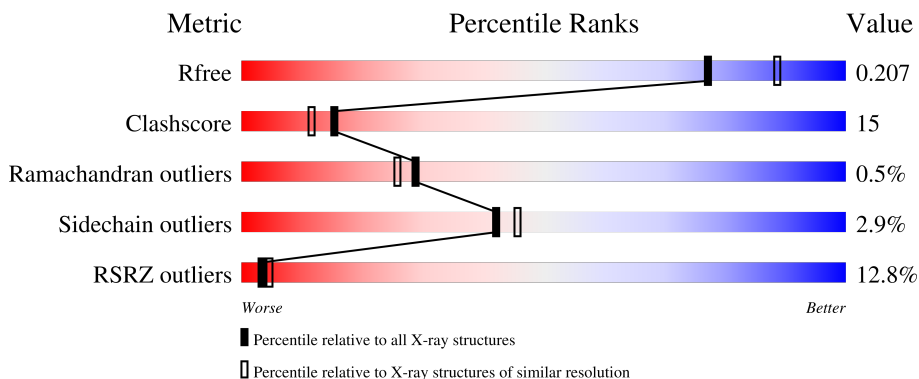
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



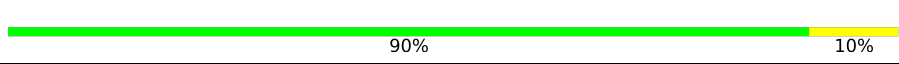


The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	
2	B	100	
3	C	10	
4	D	197	
5	E	244	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	302	-	-	X	-
6	GOL	A	303	-	-	X	-
6	GOL	D	201	-	-	X	-
6	GOL	E	301	-	-	X	-
8	SO4	E	304	-	-	-	X
9	TAM	A	310	-	-	X	-
9	TAM	E	305	-	-	X	-
9	TAM	E	306	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7167 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2253	1408	410	426	9	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called EAAGIGILTV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	10	66	42	10	14	0	0	0

- Molecule 4 is a protein called Alpha chain of engineered high affinity T-cell receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	197	1547	962	260	317	8	0	1	0

- Molecule 5 is a protein called Beta chain of high affinity engineered T-cell receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	244	1960	1247	338	369	6	0	2	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	E	1	Total C O 6 3 3	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



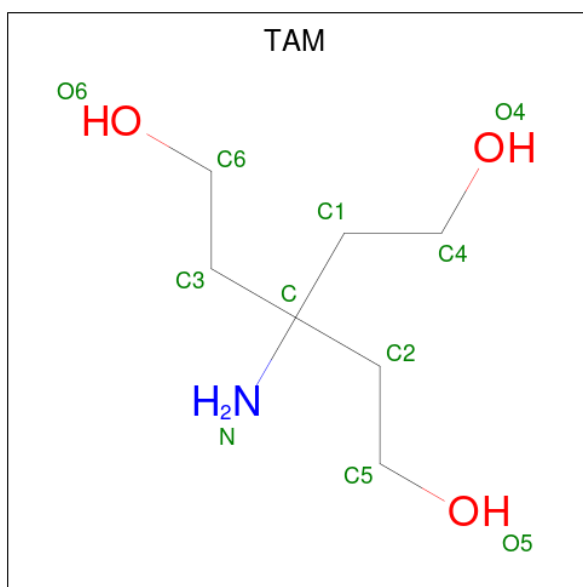
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C₇H₁₇NO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 11 7 1 3	0	0
9	E	1	Total C N O 11 7 1 3	0	0
9	E	1	Total C N O 11 7 1 3	0	0

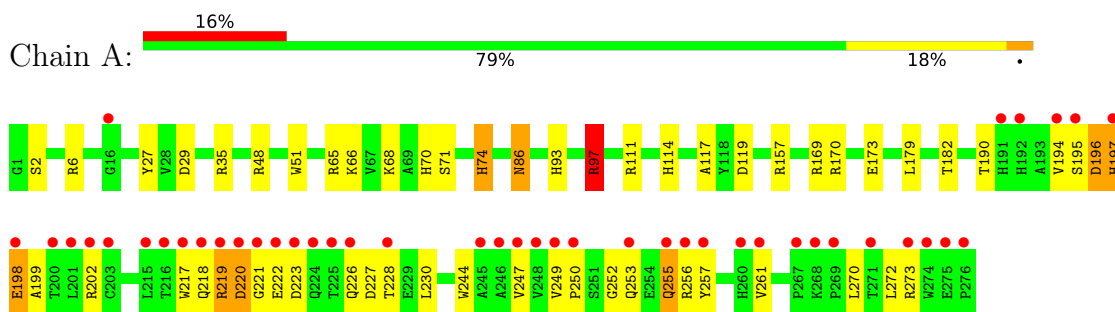
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	119	Total O 119 119	0	0
10	B	58	Total O 58 58	0	0
10	C	4	Total O 4 4	0	0
10	D	89	Total O 89 89	0	0
10	E	118	Total O 118 118	0	0

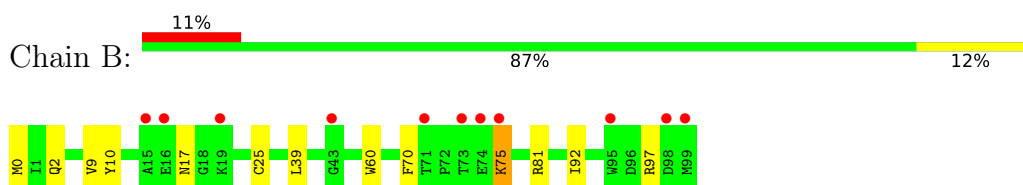
3 Residue-property plots [i](#)

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.

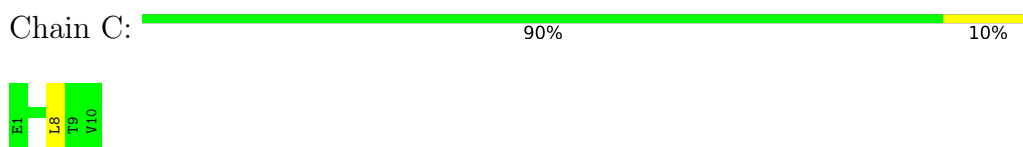
- Molecule 1: MHC class I antigen



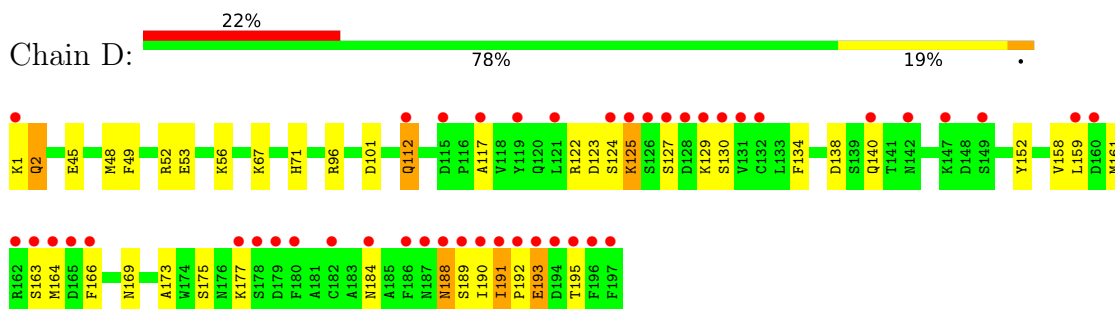
- Molecule 2: Beta-2-microglobulin



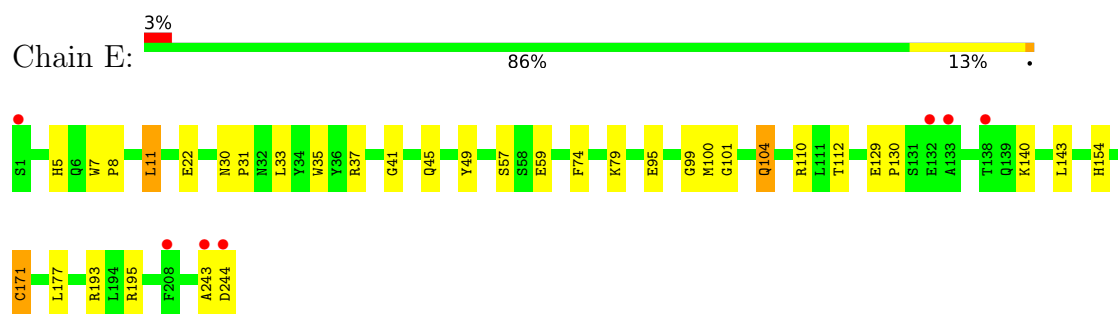
- Molecule 3: EAAGIGILTV



- Molecule 4: Alpha chain of engineered high affinity T-cell receptor



- Molecule 5: Beta chain of high affinity engineered T-cell receptor



4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	121.49Å 121.49Å 82.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.33 – 2.10 54.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.33-2.10) 99.4 (54.33-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.172 , 0.209 0.176 , 0.207	Depositor DCC
R_{free} test set	3532 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7167	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: GOL, EDO, SO4, TAM

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	0.74	0/2319	0.67	1/3149 (0.0%)
2	B	0.69	0/860	0.65	0/1162
3	C	0.87	0/65	0.67	0/86
4	D	0.80	1/1579 (0.1%)	0.71	0/2137
5	E	0.80	0/2022	0.71	1/2761 (0.0%)
All	All	0.77	1/6845 (0.0%)	0.69	2/9295 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	45	GLU	CB-CG	-5.68	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	11	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	97	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2253	0	2103	84	0
2	B	837	0	803	12	0
3	C	66	0	73	2	0
4	D	1547	0	1460	52	0
5	E	1960	0	1855	46	0
6	A	18	0	24	12	0
6	D	6	0	8	7	0
6	E	6	0	7	13	0
7	A	16	0	24	2	0
7	B	4	0	6	0	0
7	D	4	0	6	0	0
7	E	4	0	6	0	0
8	A	10	0	0	0	0
8	B	5	0	0	0	0
8	E	10	0	0	1	0
9	A	11	0	17	12	0
9	E	22	0	34	18	0
10	A	119	0	0	2	0
10	B	58	0	0	1	0
10	C	4	0	0	0	0
10	D	89	0	0	2	0
10	E	118	0	0	4	0
All	All	7167	0	6426	197	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 15.

All (197) 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)
5:E:99:GLY:HA3	6:E:301:GOL:C1	1.71	1.21
1:A:261:VAL:CG2	1:A:270:LEU:HB3	1.80	1.12
5:E:99:GLY:CA	6:E:301:GOL:H11	1.79	1.10
4:D:164:MET:HG3	4:D:166:PHE:HB2	1.38	1.05
1:A:157:ARG:NH2	9:A:310:TAM:H31	1.70	1.05
4:D:191:ILE:HD13	4:D:192:PRO:HD3	1.37	1.02
4:D:191:ILE:CD1	4:D:192:PRO:HD3	1.90	1.01
1:A:261:VAL:HG22	1:A:270:LEU:HB3	1.42	1.01
1:A:219:ARG:HG3	1:A:219:ARG:HH21	1.30	0.94
1:A:228:THR:HG22	1:A:247:VAL:HG12	1.51	0.92
4:D:188:ASN:H	4:D:188:ASN:ND2	1.67	0.92
1:A:157:ARG:NH2	9:A:310:TAM:C3	2.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:MET:HB2	6:D:201:GOL:H12	1.54	0.90
4:D:48:MET:CB	6:D:201:GOL:H12	2.04	0.88
4:D:188:ASN:H	4:D:188:ASN:HD22	0.87	0.87
4:D:164:MET:CG	4:D:166:PHE:HB2	2.06	0.86
2:B:75:LYS:HD3	2:B:75:LYS:H	1.40	0.85
1:A:190:THR:CG2	1:A:202:ARG:HB3	2.06	0.85
1:A:228:THR:HG22	1:A:247:VAL:CG1	2.07	0.84
1:A:219:ARG:O	1:A:221:GLY:N	2.09	0.84
5:E:99:GLY:CA	6:E:301:GOL:C1	2.45	0.84
1:A:29:ASP:O	6:A:303:GOL:H31	1.78	0.83
4:D:158:VAL:HG22	4:D:169:ASN:OD1	1.79	0.83
4:D:188:ASN:HD22	4:D:188:ASN:N	1.71	0.83
5:E:99:GLY:HA3	6:E:301:GOL:H11	0.87	0.81
5:E:95:GLU:OE1	6:E:301:GOL:O2	2.03	0.77
5:E:101:GLY:N	6:E:301:GOL:H31	1.98	0.76
5:E:101:GLY:H	6:E:301:GOL:H31	1.52	0.75
1:A:219:ARG:HG3	1:A:219:ARG:NH2	1.98	0.75
2:B:17:ASN:OD1	2:B:97:ARG:NH1	2.20	0.74
5:E:57:SER:HB2	9:E:306:TAM:C6	2.18	0.73
4:D:191:ILE:CG1	4:D:192:PRO:HD3	2.18	0.73
4:D:1:LYS:HD3	4:D:101:ASP:OD1	1.89	0.72
2:B:81:ARG:HG3	2:B:92:ILE:HD11	1.72	0.70
1:A:219:ARG:HD2	1:A:220:ASP:N	2.08	0.69
1:A:194:VAL:HG22	1:A:198:GLU:O	1.93	0.68
1:A:71:SER:CB	6:A:302:GOL:H32	2.25	0.67
1:A:249:VAL:CG1	1:A:250:PRO:HD2	2.24	0.67
1:A:93:HIS:HE1	10:A:454:HOH:O	1.77	0.67
4:D:53:GLU:OE2	4:D:67:LYS:HB2	1.96	0.66
1:A:29:ASP:O	6:A:303:GOL:C3	2.44	0.66
5:E:7[A]:TRP:CD2	5:E:8:PRO:HA	2.30	0.66
3:C:8:LEU:HD21	6:E:301:GOL:H2	1.78	0.65
1:A:217:TRP:CD1	1:A:247:VAL:HG13	2.32	0.65
1:A:249:VAL:HG13	1:A:250:PRO:HD2	1.79	0.65
2:B:81:ARG:HG3	2:B:92:ILE:CD1	2.27	0.65
4:D:163:SER:O	4:D:164:MET:HG2	1.97	0.64
4:D:161:MET:HE3	4:D:166:PHE:CD2	2.32	0.64
9:A:310:TAM:H51	9:A:310:TAM:C4	2.28	0.64
1:A:71:SER:OG	6:A:302:GOL:H32	1.98	0.64
9:A:310:TAM:H51	9:A:310:TAM:H42	1.79	0.64
1:A:27:TYR:HB3	6:A:303:GOL:H31	1.78	0.63
9:E:306:TAM:H51	9:E:306:TAM:H61	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD23	1:A:230:LEU:H	1.63	0.62
5:E:59:GLU:OE1	9:E:306:TAM:C6	2.47	0.62
5:E:110:ARG:HH12	9:E:305:TAM:C6	2.13	0.62
1:A:253:GLN:O	1:A:253:GLN:HG2	1.98	0.62
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.66	0.61
4:D:161:MET:HE1	5:E:195:ARG:HD3	1.82	0.61
1:A:157:ARG:HH21	9:A:310:TAM:C3	2.14	0.61
4:D:53:GLU:OE2	4:D:67:LYS:N	2.30	0.61
1:A:157:ARG:NH2	9:A:310:TAM:H32	2.15	0.61
1:A:261:VAL:CG2	1:A:270:LEU:CB	2.70	0.61
5:E:57:SER:HB2	9:E:306:TAM:C3	2.32	0.60
9:A:310:TAM:H32	4:D:52:ARG:HH12	1.67	0.60
1:A:93:HIS:HD2	1:A:119:ASP:OD1	1.84	0.60
1:A:190:THR:HG22	1:A:202:ARG:HB3	1.84	0.59
1:A:74:HIS:CE1	1:A:97:ARG:HH21	2.20	0.59
4:D:122:ARG:HH11	4:D:129:LYS:C	2.06	0.59
1:A:255:GLN:O	1:A:273:ARG:NH1	2.36	0.59
4:D:161:MET:CE	5:E:140:LYS:HD3	2.32	0.58
1:A:250:PRO:O	1:A:252:GLY:O	2.21	0.58
5:E:110:ARG:HH12	9:E:305:TAM:H62	1.69	0.58
1:A:227:ASP:OD2	1:A:227:ASP:O	2.21	0.58
4:D:161:MET:HE1	5:E:140:LYS:HD3	1.85	0.58
5:E:99:GLY:C	6:E:301:GOL:H12	2.25	0.57
4:D:191:ILE:HG12	4:D:192:PRO:HD3	1.86	0.57
5:E:99:GLY:CA	6:E:301:GOL:H12	2.33	0.57
1:A:249:VAL:HG13	1:A:257:TYR:CE1	2.40	0.57
5:E:57:SER:HB2	9:E:306:TAM:H62	1.87	0.56
4:D:191:ILE:HG12	4:D:192:PRO:CD	2.35	0.56
1:A:74:HIS:HE1	1:A:97:ARG:HH21	1.52	0.55
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.41	0.55
1:A:217:TRP:HD1	1:A:228:THR:HG21	1.72	0.54
1:A:157:ARG:HH22	9:A:310:TAM:C3	2.20	0.54
4:D:71:HIS:HD2	10:D:372:HOH:O	1.89	0.54
5:E:154:HIS:CE1	10:E:432:HOH:O	2.61	0.54
1:A:6:ARG:HD2	6:A:303:GOL:O2	2.08	0.54
1:A:35:ARG:HD3	1:A:48:ARG:NH1	2.23	0.53
1:A:219:ARG:HD2	1:A:219:ARG:C	2.29	0.53
6:A:301:GOL:H2	4:D:96:ARG:NH2	2.23	0.53
5:E:110:ARG:HH22	9:E:305:TAM:H21	1.72	0.53
4:D:123:ASP:CG	4:D:125:LYS:HE2	2.29	0.53
4:D:152:TYR:O	4:D:173:ALA:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7[B]:TRP:CZ2	5:E:22:GLU:OE1	2.61	0.53
1:A:51:TRP:CZ2	1:A:179:LEU:HD11	2.44	0.52
4:D:122:ARG:HD2	4:D:124:SER:HA	1.92	0.52
4:D:159:LEU:HB3	5:E:171:CYS:HB3	1.92	0.52
1:A:198:GLU:HA	1:A:250:PRO:HA	1.91	0.52
5:E:30:ASN:N	5:E:31:PRO:CD	2.73	0.52
1:A:261:VAL:O	1:A:261:VAL:HG23	2.09	0.51
1:A:157:ARG:HH22	9:A:310:TAM:H31	1.70	0.51
1:A:71:SER:HB3	6:A:302:GOL:H32	1.91	0.51
5:E:59:GLU:OE1	9:E:306:TAM:H61	2.11	0.51
4:D:1:LYS:HB3	10:D:356:HOH:O	2.10	0.51
1:A:65:ARG:HH11	9:E:306:TAM:H32	1.75	0.51
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.92	0.51
1:A:226:GLN:O	1:A:228:THR:HG23	2.11	0.50
2:B:75:LYS:H	2:B:75:LYS:CD	2.17	0.50
5:E:7[B]:TRP:CZ2	5:E:22:GLU:CD	2.84	0.50
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.46	0.50
4:D:122:ARG:HE	4:D:130:SER:HA	1.75	0.50
1:A:97:ARG:HD3	1:A:114:HIS:NE2	2.26	0.50
9:E:306:TAM:H61	9:E:306:TAM:C5	2.42	0.50
1:A:68:LYS:HG2	6:A:302:GOL:H12	1.94	0.49
1:A:261:VAL:HG21	1:A:270:LEU:HB3	1.86	0.49
5:E:100:MET:H	6:E:301:GOL:C3	2.26	0.49
1:A:71:SER:OG	6:A:302:GOL:C3	2.60	0.49
4:D:190:ILE:HG13	4:D:192:PRO:HD2	1.94	0.49
2:B:0:MET:HE3	2:B:2:GLN:HG2	1.94	0.49
3:C:8:LEU:CD2	6:E:301:GOL:H2	2.42	0.49
1:A:182:THR:O	1:A:182:THR:HG23	2.13	0.49
1:A:190:THR:HG23	1:A:202:ARG:HB3	1.92	0.49
1:A:219:ARG:HH21	1:A:219:ARG:CG	2.12	0.49
4:D:56:LYS:CE	6:D:201:GOL:H11	2.42	0.49
4:D:56:LYS:HE2	6:D:201:GOL:H11	1.95	0.48
4:D:122:ARG:HH11	4:D:130:SER:N	2.11	0.48
4:D:191:ILE:HD13	4:D:191:ILE:N	2.28	0.48
1:A:66:LYS:O	1:A:70:HIS:HD2	1.97	0.48
5:E:59:GLU:OE1	9:E:306:TAM:O6	2.29	0.48
5:E:45:GLN:NE2	10:E:406:HOH:O	2.47	0.47
5:E:57:SER:HB2	9:E:306:TAM:H31	1.96	0.47
4:D:138:ASP:OD2	4:D:140:GLN:HG2	2.14	0.47
4:D:193:GLU:OE1	4:D:195:THR:HG23	2.14	0.47
5:E:177:LEU:C	5:E:177:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:CD	9:A:310:TAM:H22	2.44	0.47
1:A:169:ARG:O	1:A:173:GLU:HG3	2.14	0.47
5:E:7[A]:TRP:CG	5:E:8:PRO:HA	2.50	0.47
4:D:161:MET:CE	4:D:166:PHE:CD2	2.98	0.47
1:A:170:ARG:HB2	7:A:304:EDO:H11	1.96	0.47
1:A:190:THR:HG22	1:A:202:ARG:O	2.15	0.46
5:E:41:GLY:H	9:E:305:TAM:C4	2.28	0.46
9:E:306:TAM:C6	9:E:306:TAM:H51	2.43	0.46
1:A:249:VAL:HG12	1:A:250:PRO:HD2	1.98	0.46
5:E:110:ARG:NH1	9:E:305:TAM:H62	2.30	0.46
5:E:110:ARG:HH12	9:E:305:TAM:H61	1.80	0.46
5:E:112:THR:OG1	5:E:154:HIS:NE2	2.36	0.45
5:E:33:LEU:HD13	5:E:74:PHE:HB2	1.98	0.45
2:B:81:ARG:HB2	2:B:92:ILE:CD1	2.47	0.45
1:A:182:THR:O	1:A:182:THR:CG2	2.65	0.44
1:A:27:TYR:CB	6:A:303:GOL:H31	2.47	0.44
4:D:48:MET:HB3	6:D:201:GOL:H12	1.94	0.44
5:E:37:ARG:NH1	10:E:406:HOH:O	2.46	0.43
4:D:117:ALA:CB	4:D:193:GLU:HB3	2.47	0.43
5:E:104:GLN:HG3	10:E:447:HOH:O	2.17	0.43
2:B:81:ARG:HA	2:B:92:ILE:HD13	2.00	0.43
1:A:221:GLY:O	1:A:223:ASP:N	2.52	0.43
1:A:255:GLN:N	1:A:255:GLN:OE1	2.52	0.43
1:A:272:LEU:HD12	1:A:272:LEU:N	2.34	0.43
4:D:122:ARG:HH21	4:D:124:SER:HA	1.84	0.43
4:D:122:ARG:NH1	4:D:127:SER:O	2.52	0.43
5:E:5[B]:HIS:CD2	5:E:7[B]:TRP:CE3	3.07	0.43
1:A:217:TRP:CD1	1:A:228:THR:HG21	2.52	0.43
1:A:218:GLN:NE2	1:A:221:GLY:HA2	2.33	0.42
1:A:261:VAL:HG21	1:A:270:LEU:HD23	2.01	0.42
4:D:159:LEU:C	4:D:159:LEU:HD12	2.39	0.42
1:A:194:VAL:CG2	1:A:197:HIS:CD2	3.02	0.42
4:D:49:PHE:C	4:D:49:PHE:CD2	2.92	0.42
4:D:48:MET:HB2	6:D:201:GOL:C1	2.36	0.42
9:E:306:TAM:H22	9:E:306:TAM:H41	1.90	0.42
4:D:112:GLN:HE21	4:D:112:GLN:C	2.23	0.42
1:A:195:SER:C	1:A:196:ASP:OD2	2.58	0.42
4:D:175:SER:OG	4:D:177:LYS:HG2	2.20	0.42
5:E:79:LYS:NZ	8:E:303:SO4:O3	2.53	0.42
1:A:157:ARG:HH21	9:A:310:TAM:H32	1.78	0.41
2:B:9:VAL:HG12	10:B:211:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:HB3	7:A:307:EDO:H11	2.01	0.41
1:A:157:ARG:HD2	9:A:310:TAM:H22	2.02	0.41
5:E:95:GLU:HB3	6:E:301:GOL:O2	2.20	0.41
5:E:129:GLU:HA	5:E:130:PRO:HD3	1.96	0.41
4:D:123:ASP:OD2	4:D:125:LYS:HD2	2.20	0.41
4:D:134:PHE:CZ	4:D:189:SER:HB2	2.56	0.41
5:E:143:LEU:HD12	5:E:143:LEU:N	2.35	0.41
1:A:219:ARG:C	1:A:221:GLY:N	2.73	0.41
1:A:199:ALA:N	1:A:249:VAL:O	2.39	0.41
4:D:56:LYS:NZ	6:D:201:GOL:H11	2.36	0.41
1:A:197:HIS:CD2	1:A:198:GLU:HG2	2.56	0.41
1:A:253:GLN:HG3	1:A:256:ARG:CD	2.51	0.41
5:E:35:TRP:CD1	5:E:74:PHE:CE2	3.09	0.41
1:A:190:THR:HG22	1:A:202:ARG:CB	2.51	0.40
1:A:86:ASN:ND2	10:A:414:HOH:O	2.55	0.40
1:A:71:SER:CB	6:A:302:GOL:C3	2.99	0.40
2:B:10:TYR:CD2	2:B:10:TYR:N	2.90	0.40
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.57	0.40
1:A:249:VAL:CG1	1:A:257:TYR:CE1	3.04	0.40
4:D:2:GLN:HE21	4:D:2:GLN:HA	1.87	0.40
5:E:243:ALA:O	5:E:244:ASP:C	2.59	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	274/276 (99%)	260 (95%)	10 (4%)	4 (2%)	10	5
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	196/197 (100%)	185 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	244/244 (100%)	239 (98%)	5 (2%)	0	100	100
All	All	820/827 (99%)	789 (96%)	27 (3%)	4 (0%)	29	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	222	GLU
1	A	220	ASP
1	A	198	GLU

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	232/232 (100%)	225 (97%)	7 (3%)	41	44
2	B	95/95 (100%)	93 (98%)	2 (2%)	53	59
3	C	6/6 (100%)	6 (100%)	0	100	100
4	D	176/175 (101%)	169 (96%)	7 (4%)	31	32
5	E	212/210 (101%)	207 (98%)	5 (2%)	49	53
All	All	721/718 (100%)	700 (97%)	21 (3%)	42	46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	86	ASN
1	A	97	ARG
1	A	111	ARG
1	A	196	ASP
1	A	219	ARG
1	A	255	GLN
2	B	70	PHE

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Mol	Chain	Res	Type
2	B	75	LYS
4	D	2	GLN
4	D	112	GLN
4	D	125	LYS
4	D	184	ASN
4	D	188	ASN
4	D	191	ILE
4	D	193	GLU
5	E	11	LEU
5	E	49	TYR
5	E	104	GLN
5	E	171	CYS
5	E	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	70	HIS
1	A	74	HIS
1	A	93	HIS
1	A	141	GLN
1	A	174	ASN
1	A	197	HIS
1	A	218	GLN
1	A	224	GLN
2	B	2	GLN
2	B	89	GLN
4	D	2	GLN
4	D	64	GLN
4	D	110	ASN
4	D	112	GLN
4	D	184	ASN
4	D	188	ASN
5	E	119	ASN
5	E	139	GLN
5	E	184	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
8	SO4	A	308	-	4,4,4	0.17	0	6,6,6	0.41	0
9	TAM	E	305	-	7,10,10	1.08	0	9,12,12	5.33	6 (66%)
9	TAM	A	310	-	7,10,10	0.92	0	9,12,12	0.83	0
6	GOL	A	301	-	5,5,5	0.54	0	5,5,5	0.55	0
7	EDO	D	202	-	3,3,3	0.53	0	2,2,2	0.20	0
6	GOL	E	301	-	5,5,5	1.87	1 (20%)	5,5,5	1.64	1 (20%)
7	EDO	A	306	-	3,3,3	0.50	0	2,2,2	0.10	0
6	GOL	A	303	-	5,5,5	0.62	0	5,5,5	0.40	0
7	EDO	A	305	-	3,3,3	0.38	0	2,2,2	0.56	0
6	GOL	D	201	-	5,5,5	0.88	0	5,5,5	0.74	0
7	EDO	B	101	-	3,3,3	0.61	0	2,2,2	0.13	0
7	EDO	A	307	-	3,3,3	0.36	0	2,2,2	0.55	0
6	GOL	A	302	-	5,5,5	0.60	0	5,5,5	1.01	0
7	EDO	E	302	-	3,3,3	0.62	0	2,2,2	0.39	0
8	SO4	A	309	-	4,4,4	0.27	0	6,6,6	0.23	0
7	EDO	A	304	-	3,3,3	0.35	0	2,2,2	0.36	0
8	SO4	B	102	-	4,4,4	0.17	0	6,6,6	0.06	0
9	TAM	E	306	-	7,10,10	1.09	0	9,12,12	5.35	6 (66%)
8	SO4	E	303	-	4,4,4	0.11	0	6,6,6	0.12	0
8	SO4	E	304	-	4,4,4	0.21	0	6,6,6	0.16	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	303	-	-	2/4/4/4	-
7	EDO	A	305	-	-	1/1/1/1	-
7	EDO	A	307	-	-	1/1/1/1	-
9	TAM	A	310	-	-	6/12/12/12	-
6	GOL	D	201	-	-	2/4/4/4	-
6	GOL	A	301	-	-	2/4/4/4	-
7	EDO	D	202	-	-	0/1/1/1	-
6	GOL	A	302	-	-	2/4/4/4	-
9	TAM	E	305	-	-	7/12/12/12	-
9	TAM	E	306	-	-	6/12/12/12	-
7	EDO	B	101	-	-	1/1/1/1	-
6	GOL	E	301	-	-	0/4/4/4	-
7	EDO	A	306	-	-	0/1/1/1	-
7	EDO	E	302	-	-	0/1/1/1	-
7	EDO	A	304	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	301	GOL	O2-C2	-3.99	1.31	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	306	TAM	C1-C-N	-8.66	83.42	108.09
9	E	305	TAM	C3-C-N	-8.27	84.51	108.09
9	E	306	TAM	C3-C-C1	7.54	123.80	110.50
9	E	305	TAM	C1-C-N	-7.47	86.80	108.09
9	E	306	TAM	C3-C-N	-7.09	87.88	108.09
9	E	305	TAM	C2-C-N	-6.98	88.20	108.09
9	E	305	TAM	C3-C-C1	6.08	121.23	110.50
9	E	306	TAM	C2-C-N	-6.02	90.93	108.09
9	E	305	TAM	C3-C-C2	5.29	119.83	110.50
9	E	306	TAM	C2-C-C1	4.32	118.13	110.50
9	E	305	TAM	C2-C-C1	4.15	117.83	110.50
9	E	306	TAM	C3-C-C2	3.92	117.42	110.50
6	E	301	GOL	C3-C2-C1	2.47	121.33	111.70

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	GOL	O1-C1-C2-O2
6	A	301	GOL	O1-C1-C2-C3
6	A	303	GOL	O1-C1-C2-C3
6	D	201	GOL	C1-C2-C3-O3
9	A	310	TAM	C2-C-C1-C4
9	A	310	TAM	N-C-C1-C4
9	A	310	TAM	N-C-C2-C5
9	E	305	TAM	C3-C-C1-C4
9	E	305	TAM	N-C-C1-C4
9	E	305	TAM	N-C-C2-C5
9	E	305	TAM	C2-C-C3-C6
9	E	306	TAM	C3-C-C1-C4
9	E	306	TAM	N-C-C1-C4
9	E	306	TAM	C1-C-C2-C5
9	E	306	TAM	N-C-C2-C5
9	E	306	TAM	C1-C-C3-C6
9	E	306	TAM	C2-C-C3-C6
6	A	302	GOL	O1-C1-C2-O2
6	A	302	GOL	O1-C1-C2-C3
6	A	303	GOL	O1-C1-C2-O2
7	A	304	EDO	O1-C1-C2-O2
7	A	305	EDO	O1-C1-C2-O2
9	A	310	TAM	C3-C-C1-C4
9	E	305	TAM	C1-C-C2-C5
6	D	201	GOL	O2-C2-C3-O3
9	E	305	TAM	C-C3-C6-O6
7	A	307	EDO	O1-C1-C2-O2
9	A	310	TAM	C1-C-C2-C5
7	B	101	EDO	O1-C1-C2-O2
9	A	310	TAM	C-C2-C5-O5
9	E	305	TAM	C1-C-C3-C6

There are no ring outliers.

11 monomers are involved in 65 short contacts:

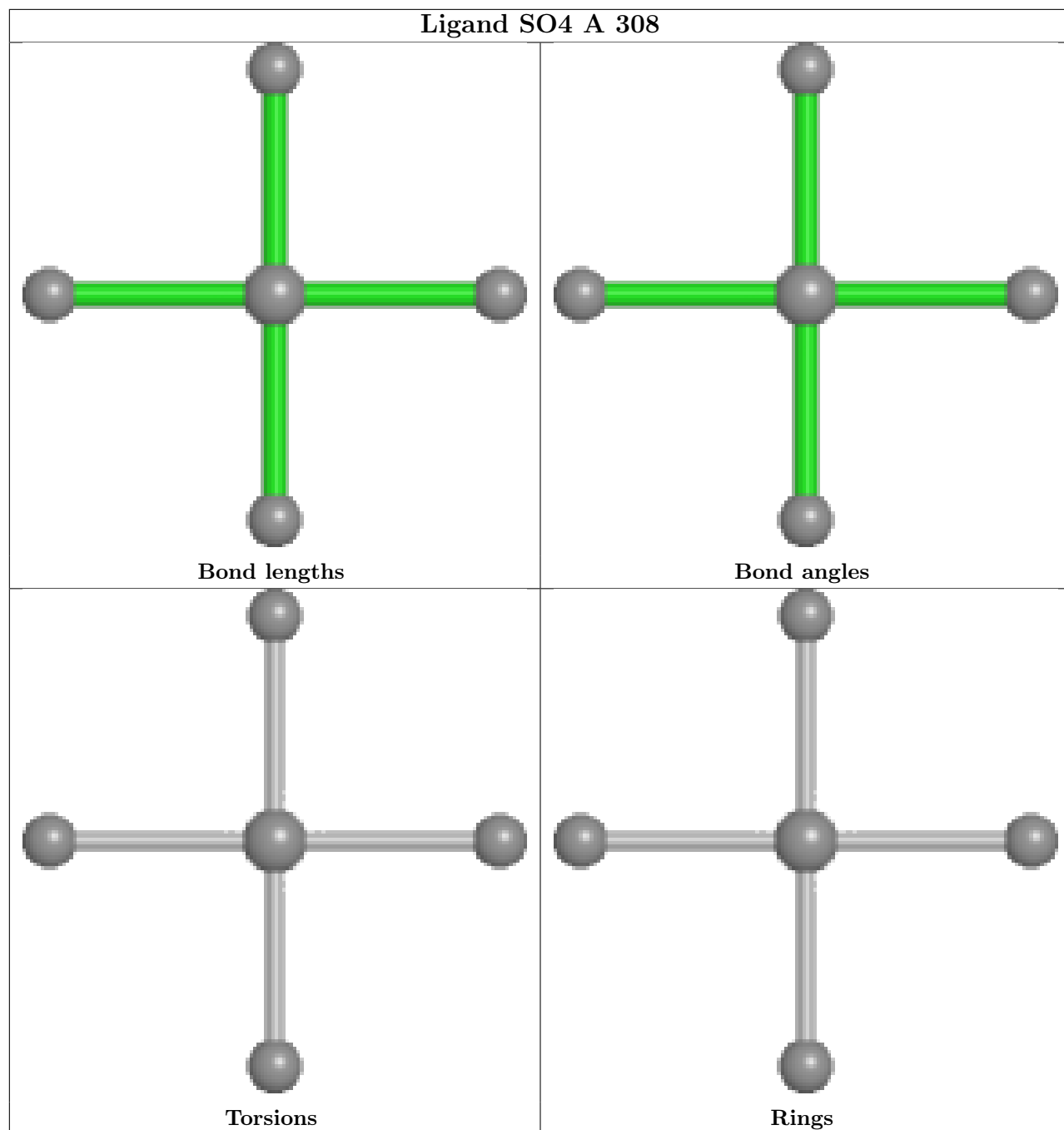
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	305	TAM	6	0
9	A	310	TAM	12	0
6	A	301	GOL	1	0
6	E	301	GOL	13	0

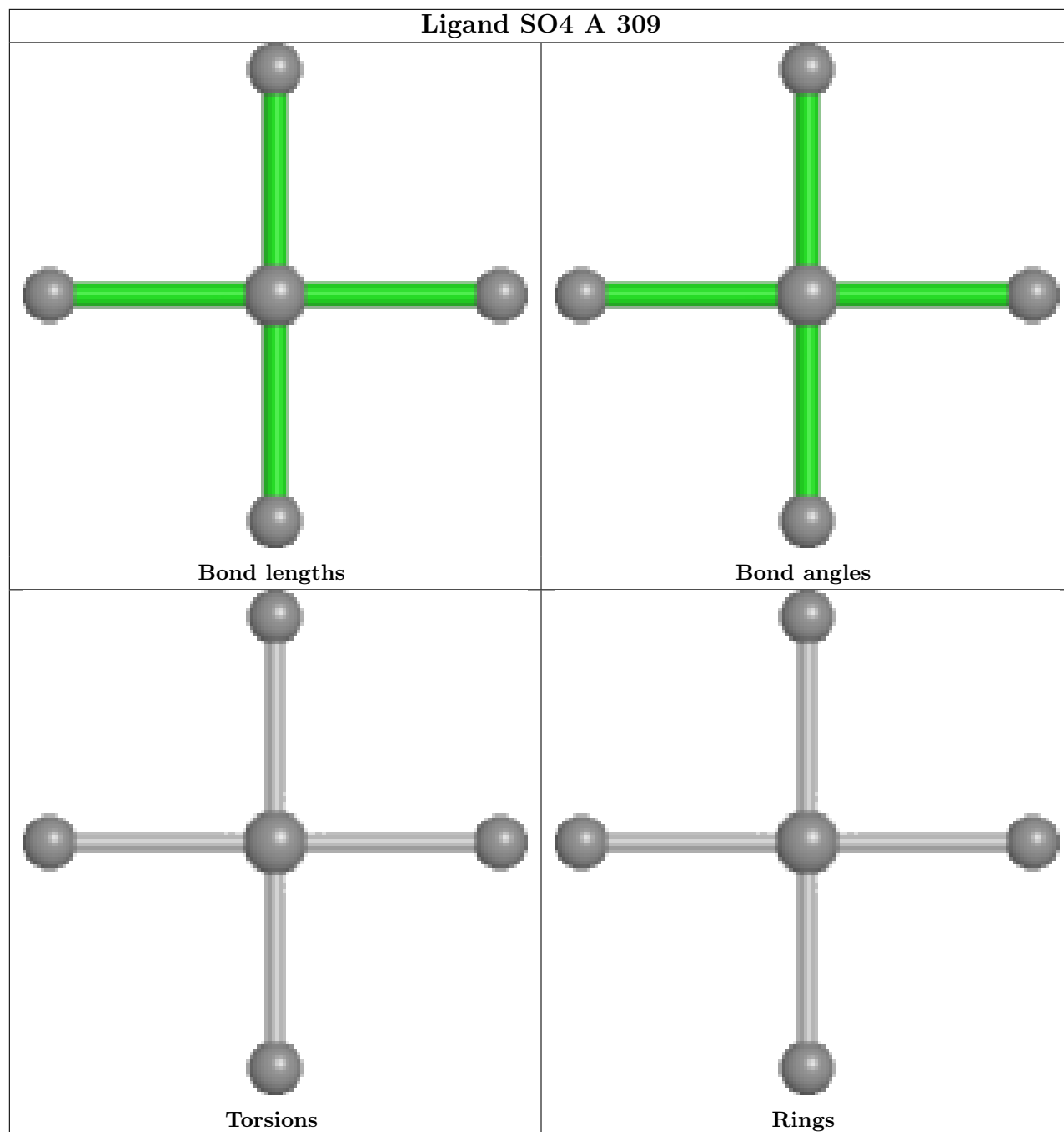
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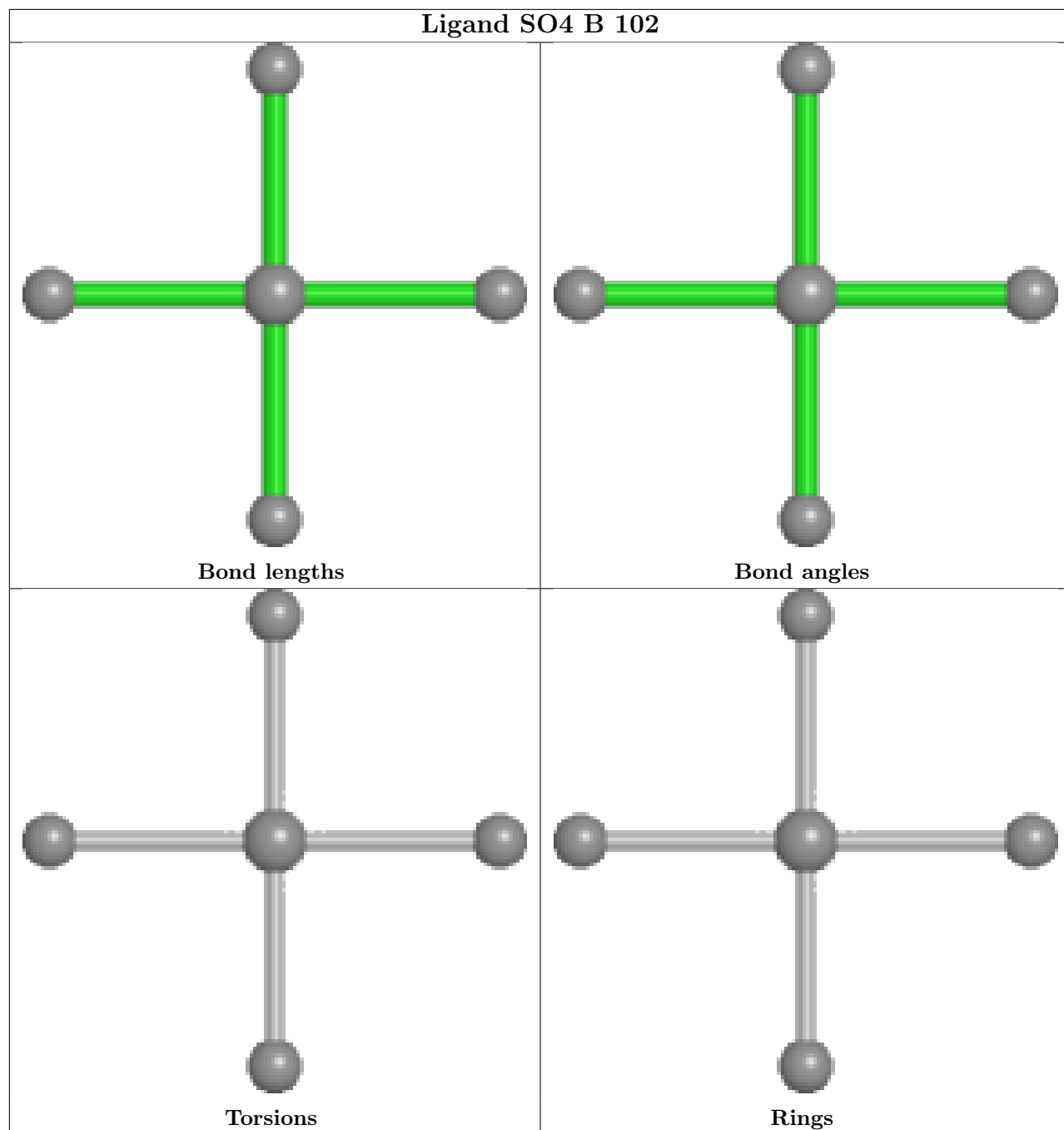
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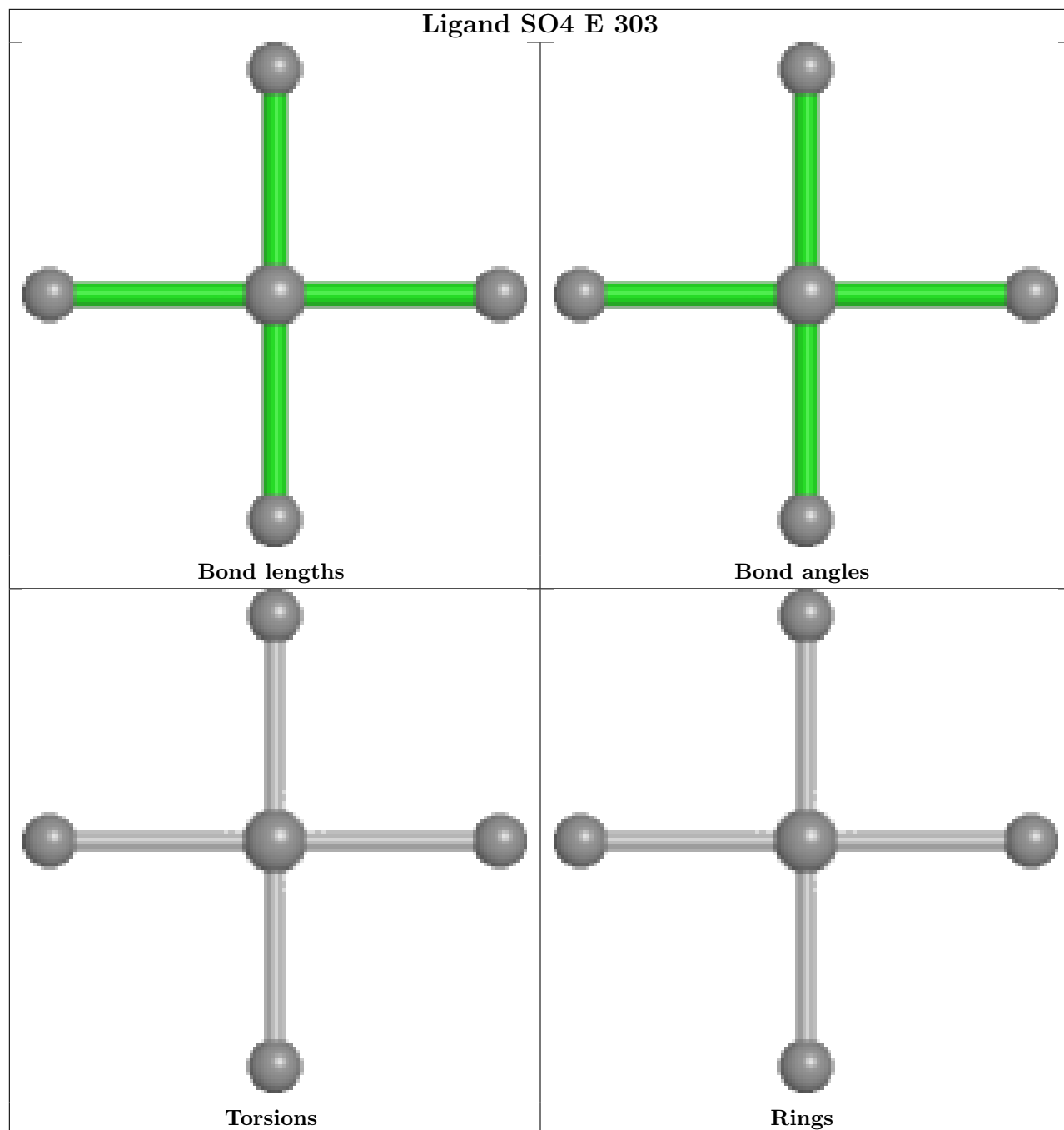
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	303	GOL	5	0
6	D	201	GOL	7	0
7	A	307	EDO	1	0
6	A	302	GOL	6	0
7	A	304	EDO	1	0
9	E	306	TAM	12	0
8	E	303	SO4	1	0

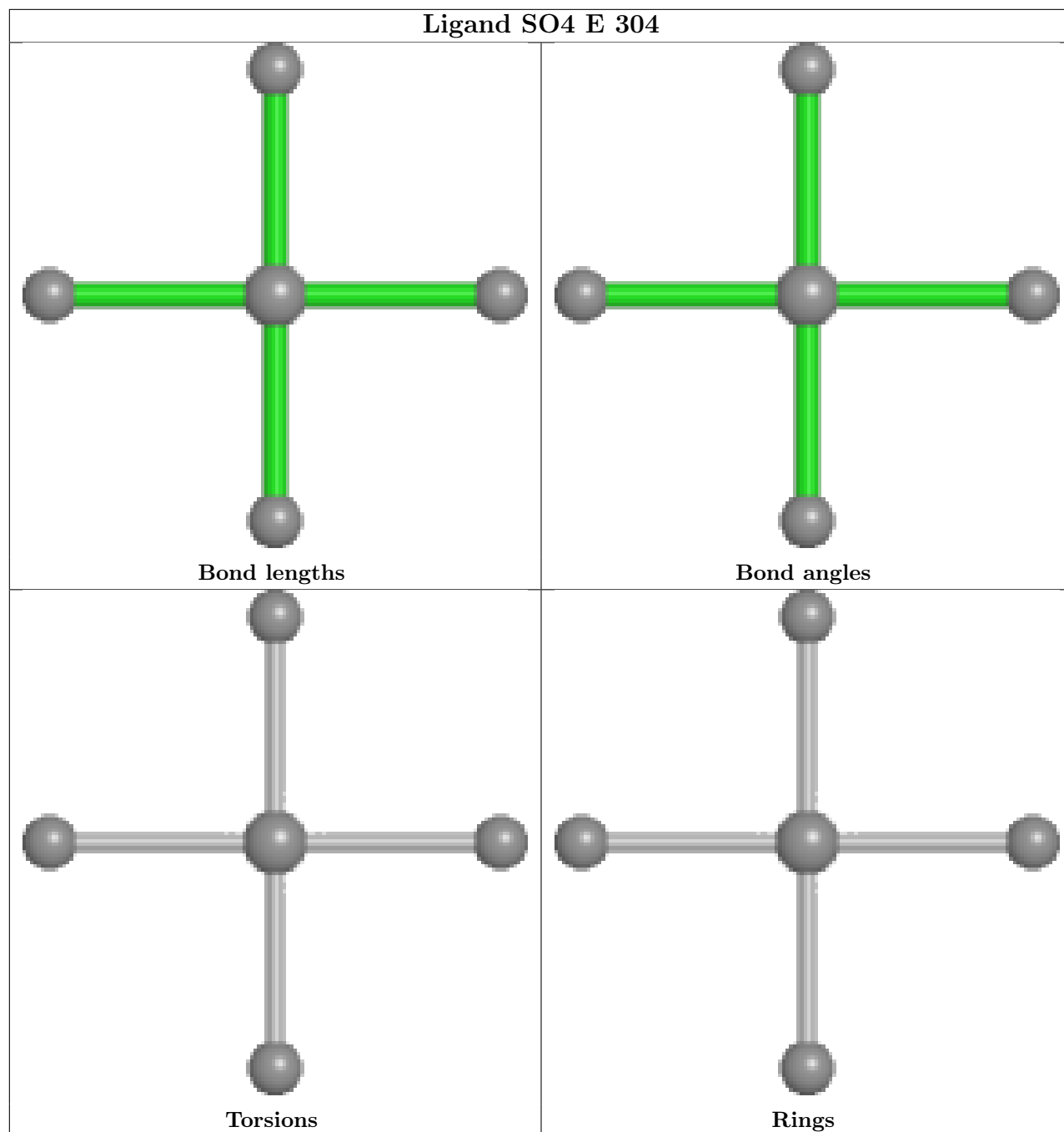
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	276/276 (100%)	0.80	44 (15%) 1 2	20, 38, 136, 163	0
2	B	100/100 (100%)	0.68	11 (11%) 5 7	21, 47, 100, 117	0
3	C	10/10 (100%)	0.23	0 100 100	19, 21, 27, 30	0
4	D	197/197 (100%)	1.28	44 (22%) 0 0	16, 36, 107, 144	0
5	E	244/244 (100%)	0.29	7 (2%) 51 57	18, 35, 89, 126	0
All	All	827/827 (100%)	0.74	106 (12%) 3 4	16, 37, 110, 163	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	190	ILE	9.2
4	D	197	PHE	8.8
1	A	224	GLN	8.7
1	A	225	THR	8.0
4	D	126	SER	7.5
1	A	222	GLU	7.1
1	A	228	THR	7.1
4	D	128	ASP	7.1
4	D	164	MET	6.8
4	D	180	PHE	6.8
1	A	195	SER	6.4
1	A	276	PRO	6.2
1	A	194	VAL	6.0
4	D	191	ILE	5.9
1	A	247	VAL	5.6
1	A	216	THR	5.4
1	A	223	ASP	5.4
4	D	196	PHE	5.3
1	A	197	HIS	5.3
5	E	244	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
4	D	179	ASP	5.2
1	A	201	LEU	5.2
4	D	166	PHE	4.8
4	D	188	ASN	4.7
1	A	260	HIS	4.7
4	D	127	SER	4.6
4	D	182	CYS	4.5
4	D	124	SER	4.4
1	A	275	GLU	4.4
4	D	192	PRO	4.3
4	D	162	ARG	4.3
4	D	159	LEU	4.3
4	D	130	SER	4.1
4	D	189	SER	3.9
4	D	147	LYS	3.9
4	D	129	LYS	3.9
1	A	261	VAL	3.9
1	A	220	ASP	3.9
1	A	248	VAL	3.8
1	A	217	TRP	3.6
1	A	226	GLN	3.6
1	A	218	GLN	3.6
1	A	268	LYS	3.6
1	A	198	GLU	3.6
4	D	132	CYS	3.5
4	D	119	TYR	3.5
4	D	177	LYS	3.5
2	B	19	LYS	3.4
1	A	221	GLY	3.4
4	D	178	SER	3.3
1	A	249	VAL	3.3
4	D	149	SER	3.3
1	A	257	TYR	3.3
4	D	121	LEU	3.3
4	D	163	SER	3.2
5	E	132	GLU	3.2
4	D	160	ASP	3.2
1	A	256	ARG	3.2
1	A	245	ALA	3.1
4	D	112	GLN	3.1
1	A	202	ARG	3.1
5	E	1	SER	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	165	ASP	3.0
4	D	125	LYS	2.9
4	D	140	GLN	2.8
5	E	208	PHE	2.8
1	A	253	GLN	2.8
1	A	274	TRP	2.8
5	E	133	ALA	2.8
2	B	99	MET	2.8
4	D	187	ASN	2.7
1	A	200	THR	2.7
1	A	191	HIS	2.6
4	D	142	ASN	2.6
2	B	15	ALA	2.6
2	B	71	THR	2.6
4	D	131	VAL	2.6
2	B	16	GLU	2.5
1	A	219	ARG	2.5
2	B	73	THR	2.5
4	D	117	ALA	2.5
1	A	255	GLN	2.5
5	E	243	ALA	2.5
4	D	184	ASN	2.4
5	E	138	THR	2.4
4	D	115	ASP	2.4
1	A	271	THR	2.4
1	A	269	PRO	2.3
2	B	43	GLY	2.3
4	D	194	ASP	2.3
2	B	75	LYS	2.3
1	A	267	PRO	2.3
2	B	95	TRP	2.3
2	B	98	ASP	2.3
4	D	186	PHE	2.2
4	D	1	LYS	2.2
1	A	246	ALA	2.2
4	D	195	THR	2.2
1	A	215	LEU	2.2
1	A	192	HIS	2.2
1	A	203	CYS	2.2
1	A	250	PRO	2.1
1	A	273	ARG	2.1
1	A	16	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	74	GLU	2.1
4	D	193	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

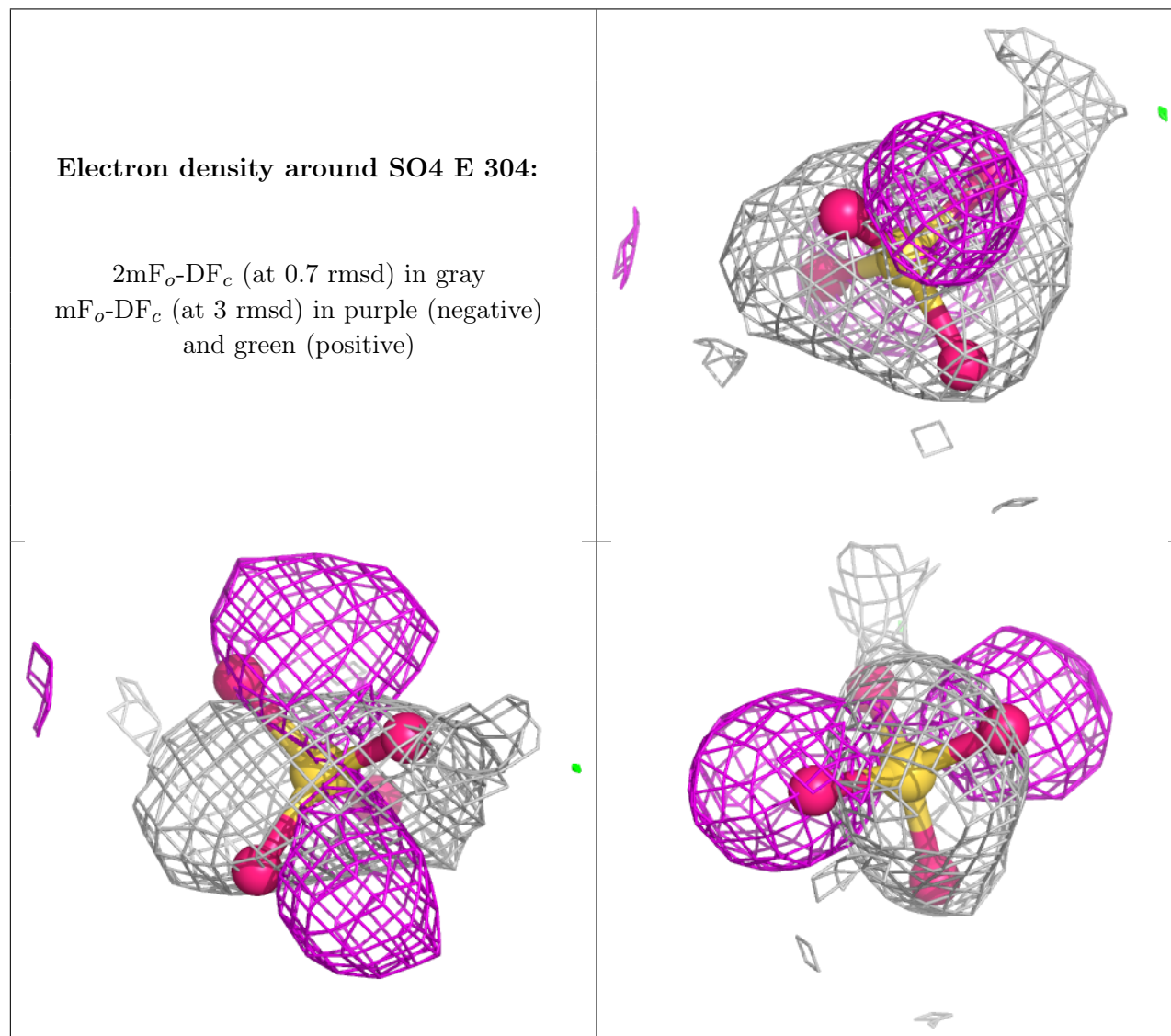
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

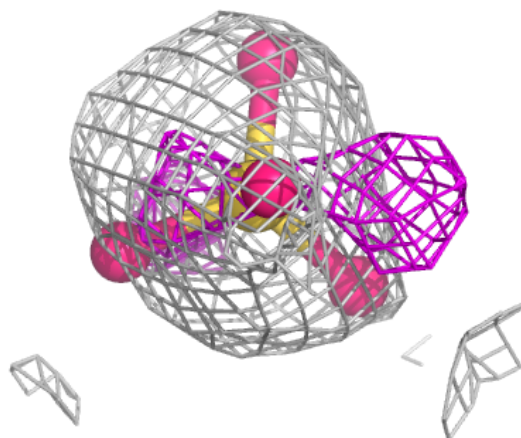
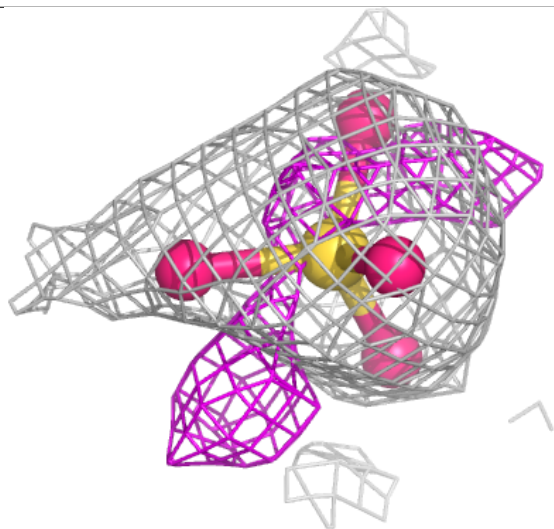
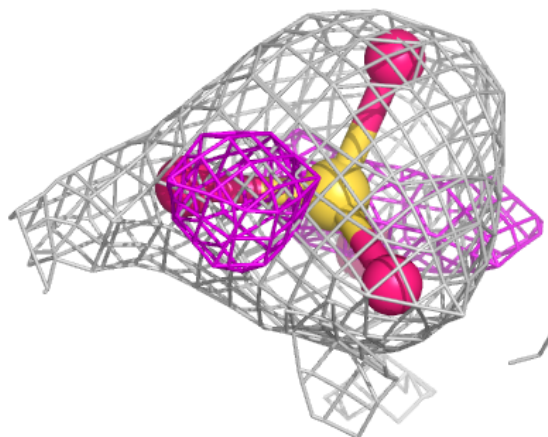
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	TAM	E	305	11/11	0.64	0.30	56,63,65,66	0
6	GOL	A	303	6/6	0.67	0.28	40,54,56,58	0
6	GOL	A	302	6/6	0.69	0.39	41,50,52,53	0
9	TAM	A	310	11/11	0.72	0.22	46,59,62,64	0
7	EDO	A	304	4/4	0.74	0.23	54,54,56,58	0
8	SO4	E	304	5/5	0.77	0.52	100,100,100,100	0
9	TAM	E	306	11/11	0.77	0.22	38,47,52,53	0
6	GOL	D	201	6/6	0.79	0.38	28,37,45,50	0
6	GOL	A	301	6/6	0.83	0.39	26,43,46,46	0
8	SO4	E	303	5/5	0.88	0.34	88,89,90,93	0
6	GOL	E	301	6/6	0.92	0.24	21,29,34,41	0
8	SO4	A	309	5/5	0.93	0.38	68,69,74,76	0
7	EDO	B	101	4/4	0.93	0.15	50,50,52,54	0
7	EDO	E	302	4/4	0.94	0.12	29,34,39,40	0
7	EDO	A	307	4/4	0.94	0.28	46,55,58,63	0
8	SO4	B	102	5/5	0.94	0.20	59,61,64,64	0
7	EDO	D	202	4/4	0.94	0.17	43,44,44,47	0
7	EDO	A	306	4/4	0.95	0.15	34,37,38,41	0
8	SO4	A	308	5/5	0.95	0.15	61,61,62,65	0
7	EDO	A	305	4/4	0.95	0.17	57,58,60,60	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.



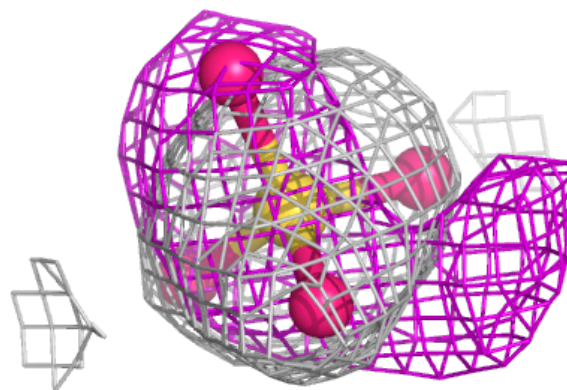
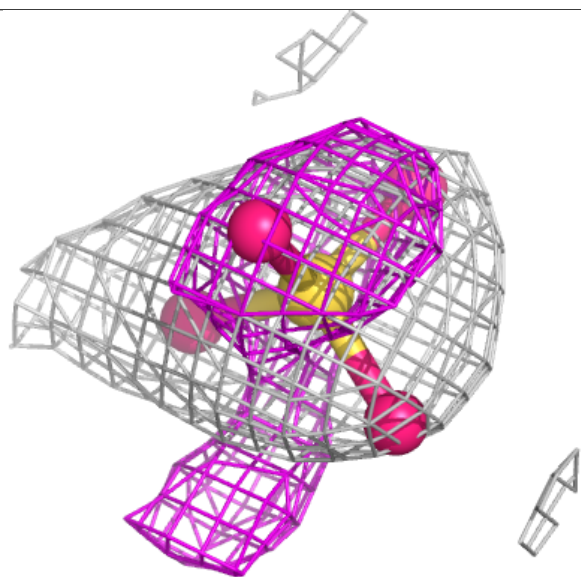
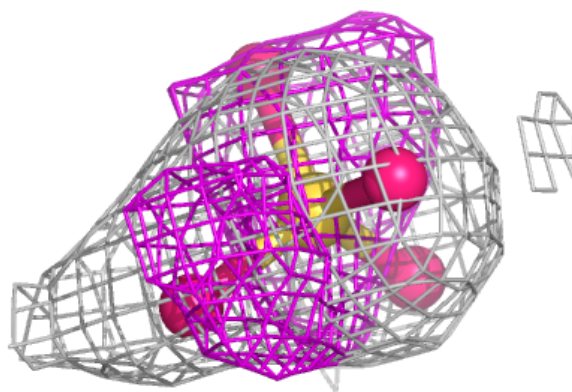
Electron density around SO4 E 303:

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



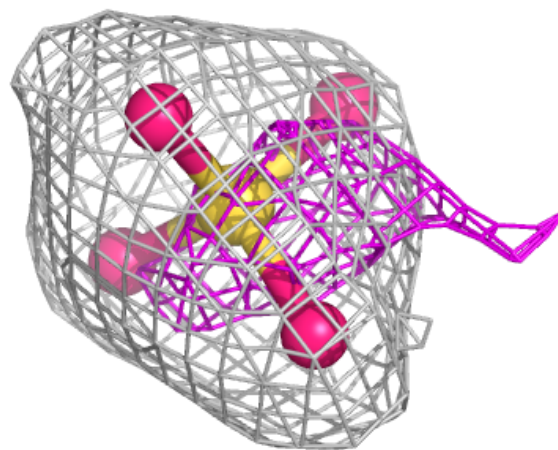
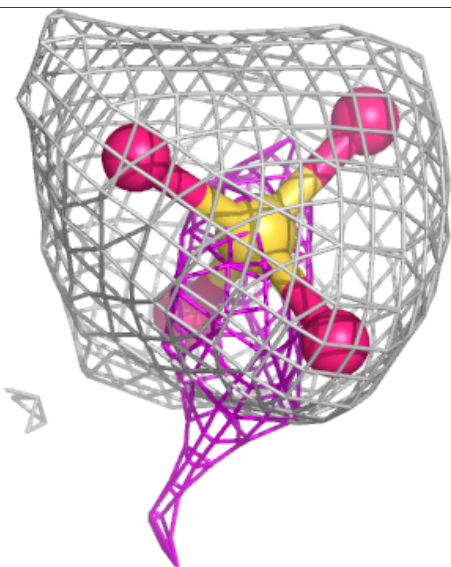
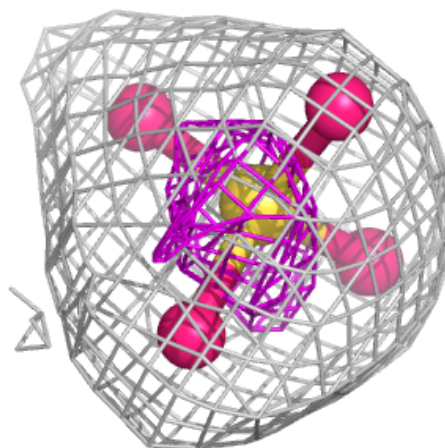
Electron density around SO4 A 309:

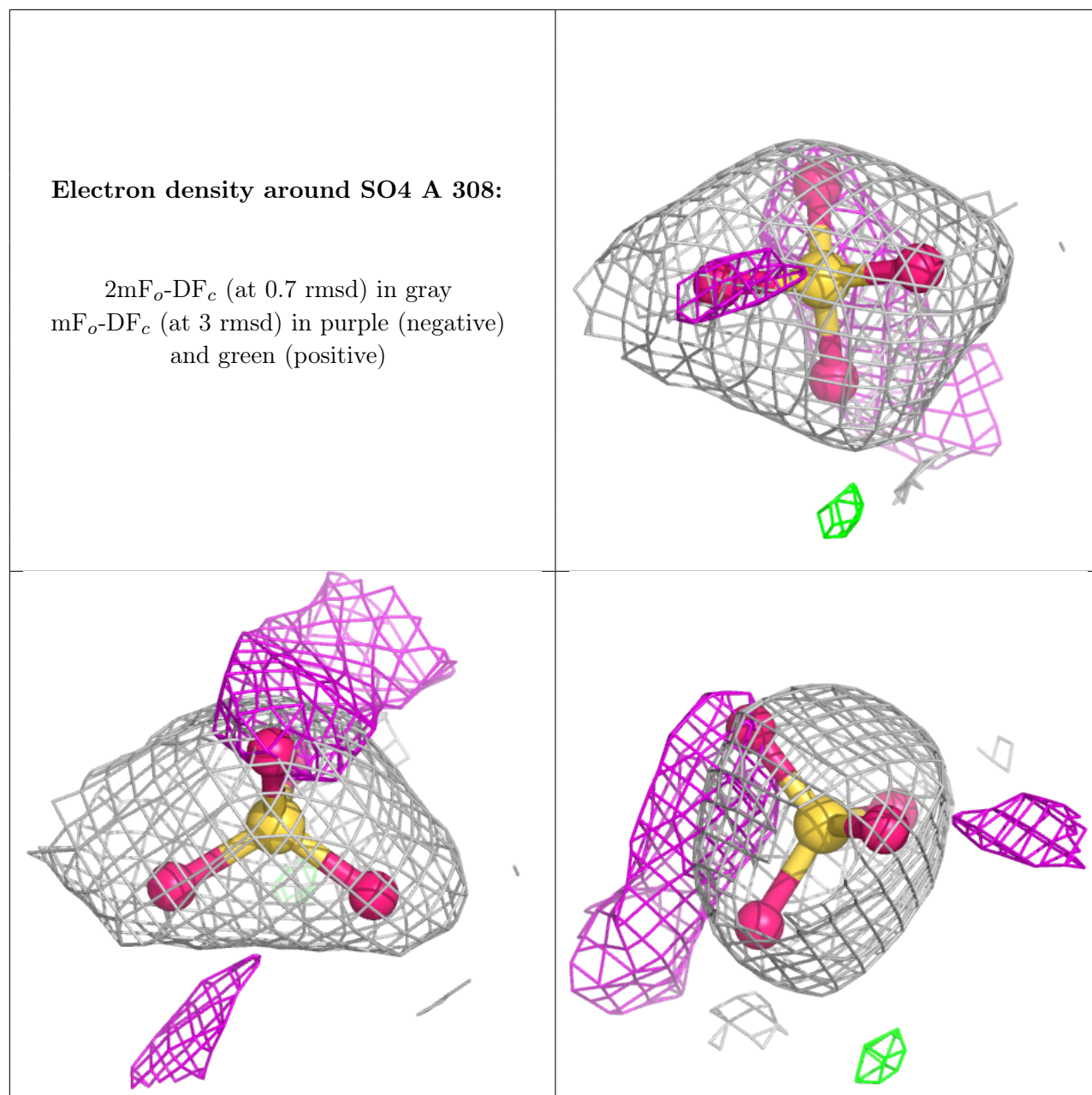
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 B 102:

$2mF_o-DF_c$ (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.