Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 12:45 PM EST

PDB ID	:	9DL1
Title	:	Crystal Structure of HLA-A*02:01/NY-ESO-1 (SLLMWITQV) and a target specific TRACeR-I
Authors	:	Mallik, L.; Du, H.; Huang, P.; Sgourakis, N.G.
Deposited on	:	2024-09-10
Resolution	:	2.30 Å(reported)

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

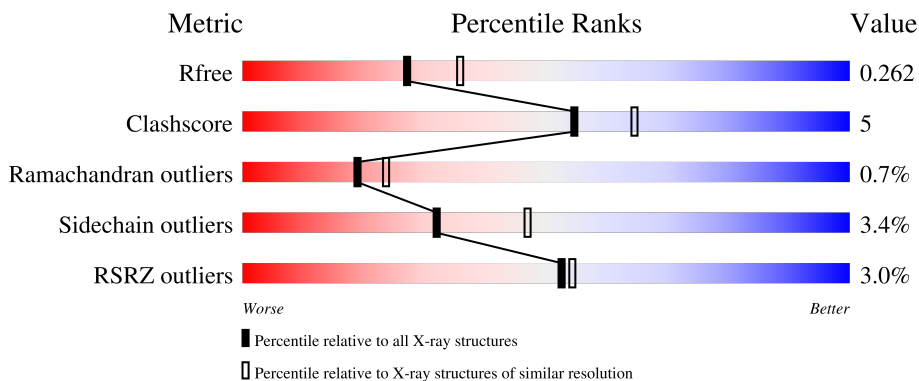|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 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.
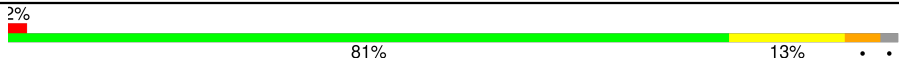
Metric	Percentile Ranks	Value
Rfree		0.262
Clashscore		5
Ramachandran outliers		0.7%
Sidechain outliers		3.4%
RSRZ outliers		3.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	132	3% 77% 13% 11%
1	D	132	5% 76% 14% 5% 6%
2	B	276	3% 87% 12%
2	F	276	3% 87% 12% •
3	C	100	% 86% 12% ••

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Mol	Chain	Length	Quality of chain
3	G	100	2% 81% 13%
4	E	9	89% 11%
4	H	9	89% 11%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8899 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 TRACeR-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			1011	652	172	181	6			
1	D	124	Total	C	N	O	S	0	0	0
			1059	682	177	194	6			

- Molecule 2 is a protein called MHC class I antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
2	F	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP A0A5B8RNS7
F	0	MET	-	initiating methionine	UNP A0A5B8RNS7

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
3	G	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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• Molecule 4 is a protein called Cancer/testis antigen 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	9	Total 76	C 51	N 11	O 13	S 1	0	0	0
4	H	9	Total 76	C 51	N 11	O 13	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	9	VAL	-	expression tag	UNP P78358
H	9	VAL	-	expression tag	UNP P78358

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).
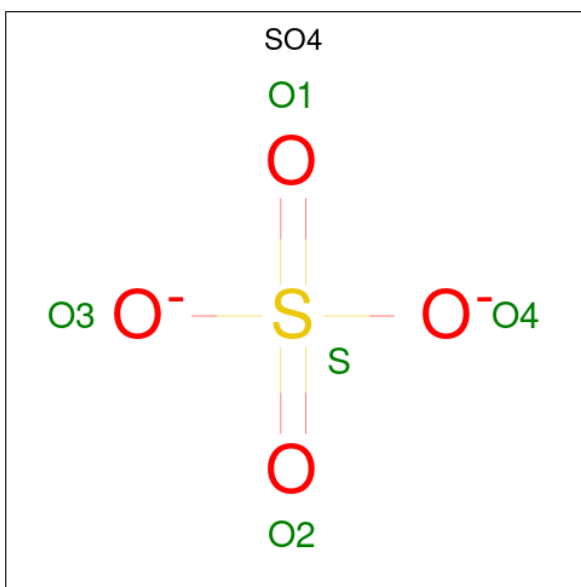
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	D	1	Total 5	O 4	S 1	0	0

• Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total 57	O 57	0	0
6	B	154	Total 154	O 154	0	0
6	C	64	Total 64	O 64	0	0
6	D	72	Total 72	O 72	0	0
6	E	5	Total 5	O 5	0	0
6	F	116	Total 116	O 116	0	0
6	G	47	Total 47	O 47	0	0
6	H	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

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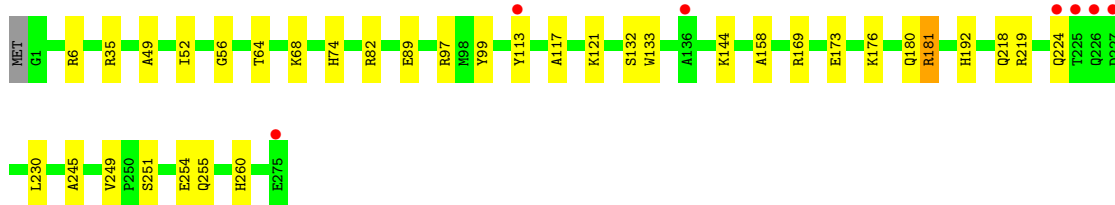
- Molecule 1: TRACeR-I
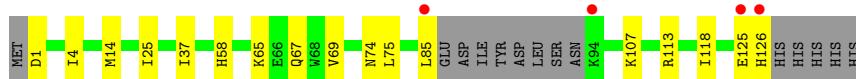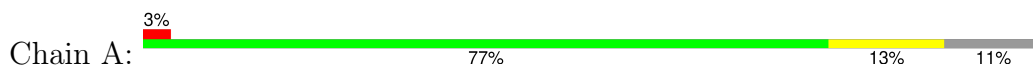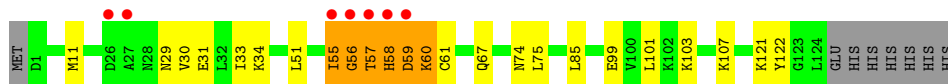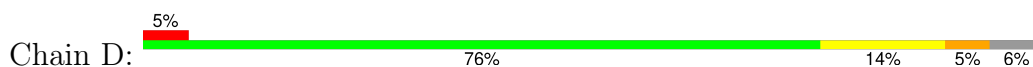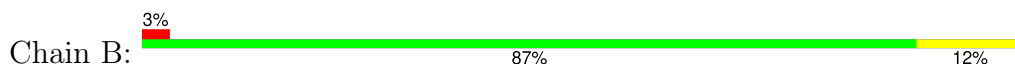
Chain A:

- Molecule 1: TRACeR-I

Chain D:

- Molecule 2: MHC class I antigen, A-2 alpha chain

Chain B:

- Molecule 2: MHC class I antigen, A-2 alpha chain

Chain F:

- Molecule 3: Beta-2-microglobulin

Chain C:

86%　　　12%

M0 N21 F22 C25 L39 K48 H51 W60 L65 E69 F70 K75 K91 R97 D98 MET

• Molecule 3: Beta-2-microglobulin

Chain G:

81%　　　13%

MET I1 Q2 I7 N24 C25 P32 L39 L40 R45 I46 K58 D59 W60 L65 F70 K75 K91 R97 D98 MET

• Molecule 4: Cancer/testis antigen 1

Chain E:

89%　　　11%

S1 L2 L3 V9

• Molecule 4: Cancer/testis antigen 1

Chain H:

89%　　　11%

S1 L2 L3 V9
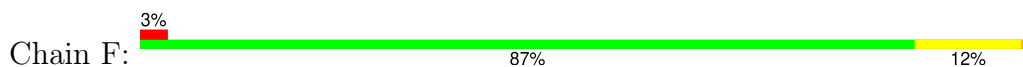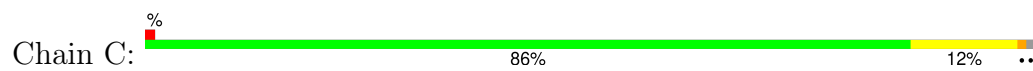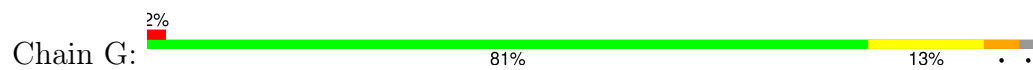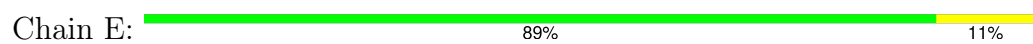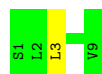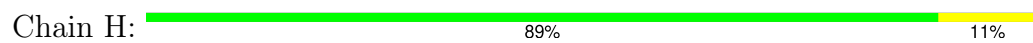
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.42Å 95.61Å 259.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.73 – 2.30 89.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (89.73-2.30) 98.8 (89.73-2.30)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???), BUSTER	Depositor
R, R_{free}	0.196 , 0.265 0.198 , 0.262	Depositor DCC
R_{free} test set	53926 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8899	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: 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	0.42	0/1032	0.56	0/1385
1	D	0.42	0/1081	0.57	0/1454
2	B	0.41	0/2311	0.61	0/3137
2	F	0.40	0/2311	0.64	0/3137
3	C	0.42	0/851	0.59	0/1152
3	G	0.41	0/843	0.59	0/1142
4	E	0.43	0/77	0.64	0/103
4	H	0.39	0/77	0.64	0/103
All	All	0.41	0/8583	0.60	0/11613

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	181	ARG	Sidechain
2	B	6	ARG	Sidechain

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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	1011	0	996	11	0
1	D	1059	0	1040	17	0
2	B	2246	0	2096	19	0
2	F	2246	0	2096	19	0
3	C	828	0	794	8	0
3	G	820	0	785	11	0
4	E	76	0	83	2	0
4	H	76	0	83	2	0
5	B	10	0	0	0	0
5	D	5	0	0	0	0
6	A	57	0	0	2	0
6	B	154	0	0	1	0
6	C	64	0	0	1	0
6	D	72	0	0	1	0
6	E	5	0	0	0	0
6	F	116	0	0	0	0
6	G	47	0	0	0	0
6	H	7	0	0	0	0
All	All	8899	0	7973	77	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 5.

All (77) 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:A:1:ASP:HB3	1:A:4:ILE:HD12	1.55	0.89
2:F:204:TRP:HZ2	3:G:98:ASP:HB2	1.51	0.74
2:B:219:ARG:HB2	2:B:224:GLN:HE22	1.56	0.70
2:B:218:GLN:OE1	2:B:260:HIS:NE2	2.26	0.69
1:D:30:VAL:HG12	1:D:34:LYS:HE2	1.75	0.67
2:B:82:ARG:CZ	2:B:89:GLU:HG3	2.28	0.64
1:D:55:ILE:O	1:D:57:THR:N	2.32	0.62
1:D:74:ASN:HB3	1:D:85:LEU:HD21	1.82	0.60
1:A:118:ILE:HG12	1:D:51:LEU:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:24:ASN:HB3	3:G:65:LEU:HD11	1.87	0.56
2:F:218:GLN:NE2	2:F:223:ASP:OD1	2.39	0.54
2:B:117:ALA:HB2	3:C:60:TRP:CE2	2.43	0.53
2:B:249:VAL:HG21	2:B:254:GLU:HG3	1.89	0.53
3:G:39:LEU:HB3	3:G:46:ILE:HD12	1.90	0.53
2:F:99:TYR:CE2	4:H:3:LEU:HD12	2.44	0.53
2:F:224:GLN:O	2:F:228:THR:HG23	2.08	0.53
2:B:169:ARG:O	2:B:173:GLU:HG3	2.09	0.52
1:D:58:HIS:O	1:D:60:LYS:N	2.43	0.52
1:A:113:ARG:NH1	6:A:203:HOH:O	2.43	0.52
2:B:176:LYS:HG3	2:B:180:GLN:OE1	2.10	0.51
2:B:82:ARG:NH2	2:B:89:GLU:HG3	2.26	0.51
2:B:219:ARG:HB2	2:B:224:GLN:NE2	2.23	0.51
1:A:67:GLN:HG3	6:A:204:HOH:O	2.12	0.50
2:F:117:ALA:HB2	3:G:60:TRP:CE2	2.46	0.50
2:F:108:ARG:HG2	2:F:108:ARG:HH11	1.76	0.50
3:C:91:LYS:NZ	6:C:102:HOH:O	2.44	0.50
2:B:64:THR:HG22	2:B:68:LYS:HD2	1.94	0.49
2:B:133:TRP:HB2	2:B:144:LYS:HD2	1.94	0.49
1:D:55:ILE:O	1:D:55:ILE:HG22	2.11	0.49
2:F:224:GLN:C	2:F:226:GLN:H	2.16	0.49
2:B:255:GLN:H	2:B:255:GLN:CD	2.16	0.49
1:D:121:LYS:HD3	1:D:122:TYR:CZ	2.48	0.48
1:D:59:ASP:O	1:D:61:CYS:N	2.40	0.47
1:D:31:GLU:HA	1:D:34:LYS:HE3	1.96	0.47
1:D:61:CYS:HB2	6:D:362:HOH:O	2.14	0.47
2:F:22:PHE:CD2	2:F:71:SER:HB2	2.50	0.47
2:B:99:TYR:CE2	4:E:3:LEU:HD12	2.50	0.47
1:D:29:ASN:O	1:D:33:ILE:HG13	2.15	0.47
2:F:49:ALA:O	2:F:52:ILE:HG22	2.15	0.47
3:G:75:LYS:H	3:G:75:LYS:HG3	1.65	0.46
1:A:25:ILE:HG23	1:D:101:LEU:HD21	1.97	0.46
3:G:97:ARG:H	3:G:97:ARG:HG3	1.55	0.46
3:G:2:GLN:HG2	3:G:32:PRO:HD3	1.98	0.45
2:B:99:TYR:CZ	4:E:3:LEU:HD12	2.51	0.45
2:F:106:ASP:OD2	2:F:108:ARG:HG3	2.16	0.45
1:D:60:LYS:H	1:D:60:LYS:HG3	1.56	0.44
2:F:127:LYS:HD3	2:F:132:SER:HB2	1.98	0.44
1:A:74:ASN:OD1	1:A:85:LEU:HD21	2.17	0.44
2:F:6:ARG:HG2	2:F:113:TYR:HE1	1.82	0.44
2:F:258:THR:HG22	2:F:273:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:39:LEU:HD12	3:G:39:LEU:HA	1.88	0.44
3:G:25:CYS:HB2	3:G:39:LEU:HD11	1.99	0.44
2:F:20:PRO:HD2	2:F:75:ARG:HD2	2.00	0.44
2:F:194:VAL:HG23	2:F:195:SER:H	1.84	0.43
3:G:7:ILE:HD12	3:G:91:LYS:HD2	2.00	0.43
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.82	0.43
2:B:74:HIS:CE1	2:B:97:ARG:HH21	2.36	0.43
2:B:230:LEU:HD12	2:B:245:ALA:HB2	2.00	0.43
3:C:22:PHE:CZ	3:C:69:GLU:HG2	2.53	0.43
2:F:121:LYS:HB3	2:F:121:LYS:HE2	1.85	0.43
1:A:37:ILE:HG23	1:D:107:LYS:HG2	1.99	0.43
1:D:99:GLU:HG3	1:D:103:LYS:NZ	2.34	0.43
3:C:51:HIS:HA	3:C:65:LEU:O	2.18	0.42
1:A:14:MET:SD	1:D:11:MET:HE1	2.60	0.42
3:C:22:PHE:CE2	3:C:69:GLU:HG2	2.54	0.42
1:A:69:VAL:HG22	2:B:158:ALA:HA	2.01	0.42
2:B:49:ALA:O	2:B:52:ILE:HG22	2.19	0.42
2:F:142:THR:O	2:F:146:LYS:HG3	2.19	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB2	1.69	0.41
3:C:21:ASN:HB3	3:C:70:PHE:CE1	2.55	0.41
1:D:56:GLY:O	1:D:57:THR:HB	2.21	0.41
2:F:214:THR:HB	2:F:262:GLN:HB2	2.02	0.41
2:F:99:TYR:CZ	4:H:3:LEU:HD12	2.56	0.40
3:C:25:CYS:HB2	3:C:39:LEU:HD21	2.03	0.40
3:G:40:LEU:HD23	3:G:45:ARG:HA	2.03	0.40
2:B:56:GLY:HA3	6:B:549:HOH:O	2.21	0.40
3:C:97:ARG:H	3:C:97:ARG:HG3	1.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	114/132 (86%)	112 (98%)	2 (2%)	0	100	100
1	D	122/132 (92%)	113 (93%)	3 (2%)	6 (5%)	2	1
2	B	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
2	F	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	30	39
3	C	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
3	G	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
4	E	7/9 (78%)	7 (100%)	0	0	100	100
4	H	7/9 (78%)	7 (100%)	0	0	100	100
All	All	989/1034 (96%)	958 (97%)	24 (2%)	7 (1%)	19	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	57	THR
1	D	59	ASP
1	D	56	GLY
1	D	60	LYS
1	D	58	HIS
2	F	225	THR
1	D	55	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/124 (89%)	106 (96%)	4 (4%)	30	44
1	D	116/124 (94%)	114 (98%)	2 (2%)	56	72
2	B	231/232 (100%)	224 (97%)	7 (3%)	36	52
2	F	231/232 (100%)	223 (96%)	8 (4%)	31	46
3	C	94/95 (99%)	91 (97%)	3 (3%)	34	50
3	G	93/95 (98%)	87 (94%)	6 (6%)	14	20
4	E	9/9 (100%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	9/9 (100%)	9 (100%)	0	100	100
All	All	893/920 (97%)	863 (97%)	30 (3%)	32	47

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	65	LYS
1	A	125	GLU
1	A	126	HIS
2	B	35	ARG
2	B	113	TYR
2	B	121	LYS
2	B	132	SER
2	B	181	ARG
2	B	192	HIS
2	B	251	SER
3	C	0	MET
3	C	70	PHE
3	C	75	LYS
1	D	67	GLN
1	D	75	LEU
2	F	34	VAL
2	F	67	VAL
2	F	75	ARG
2	F	113	TYR
2	F	128	GLU
2	F	182	THR
2	F	195	SER
2	F	264	GLU
3	G	39	LEU
3	G	45	ARG
3	G	58	LYS
3	G	70	PHE
3	G	75	LYS
3	G	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS

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Mol	Chain	Res	Type
2	B	224	GLN
3	G	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	$\#|Z| > 2$
5	SO4	B	302	-	4,4,4	0.28	0	6,6,6	0.23	0
5	SO4	D	201	-	4,4,4	0.27	0	6,6,6	0.45	0
5	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.41	0

There are no bond length outliers.

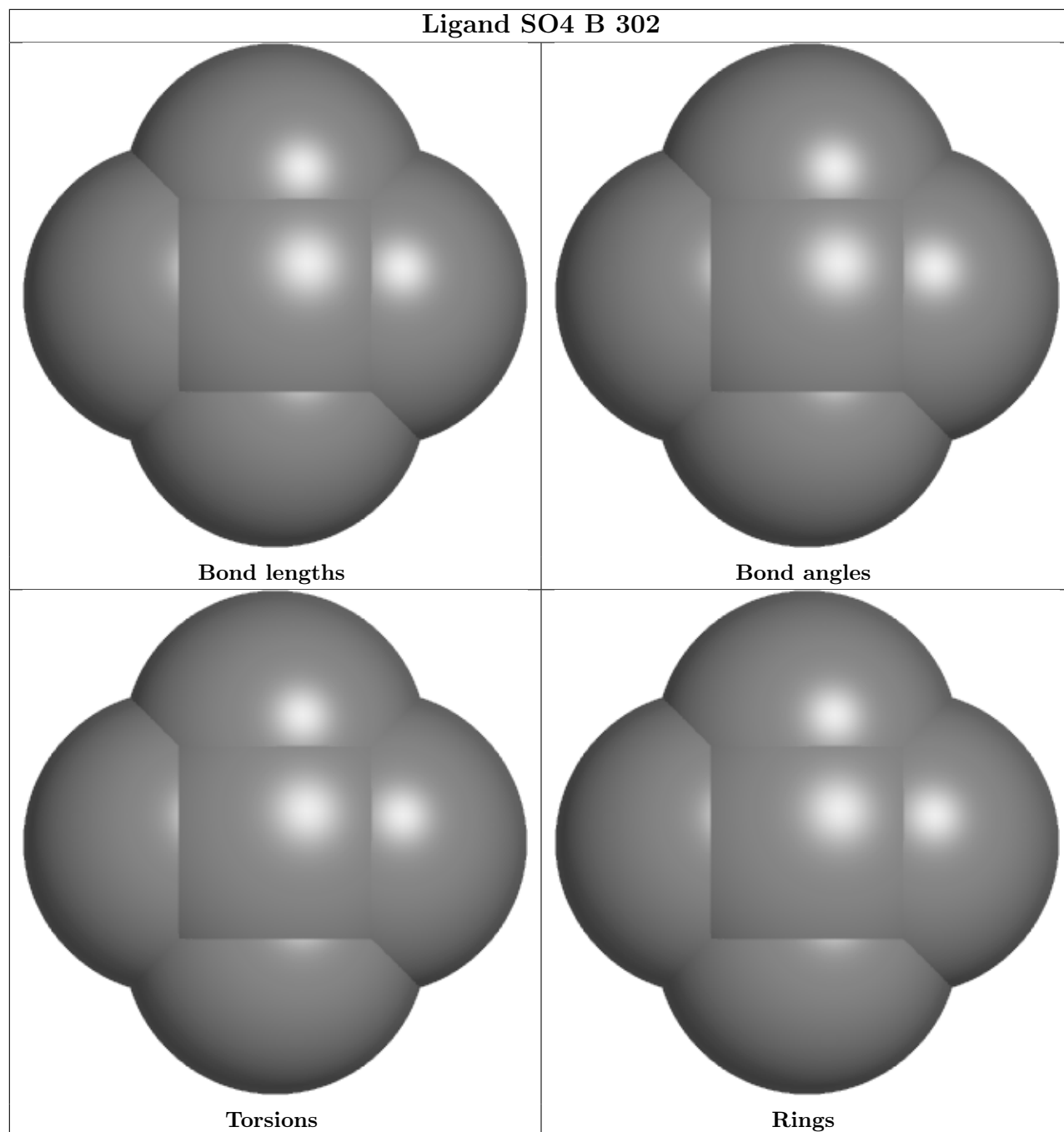There are no bond angle outliers.
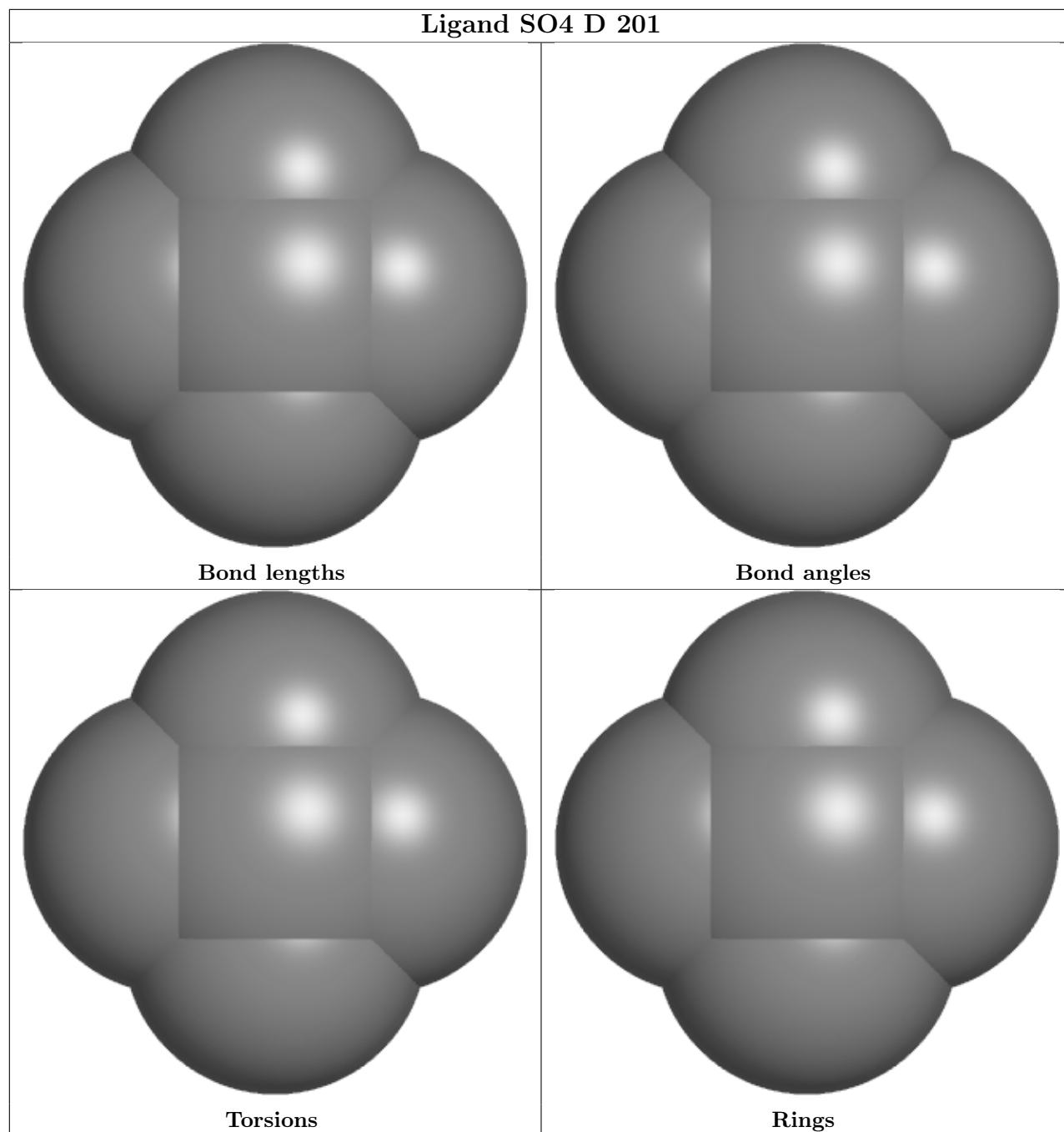
There are no chirality outliers.
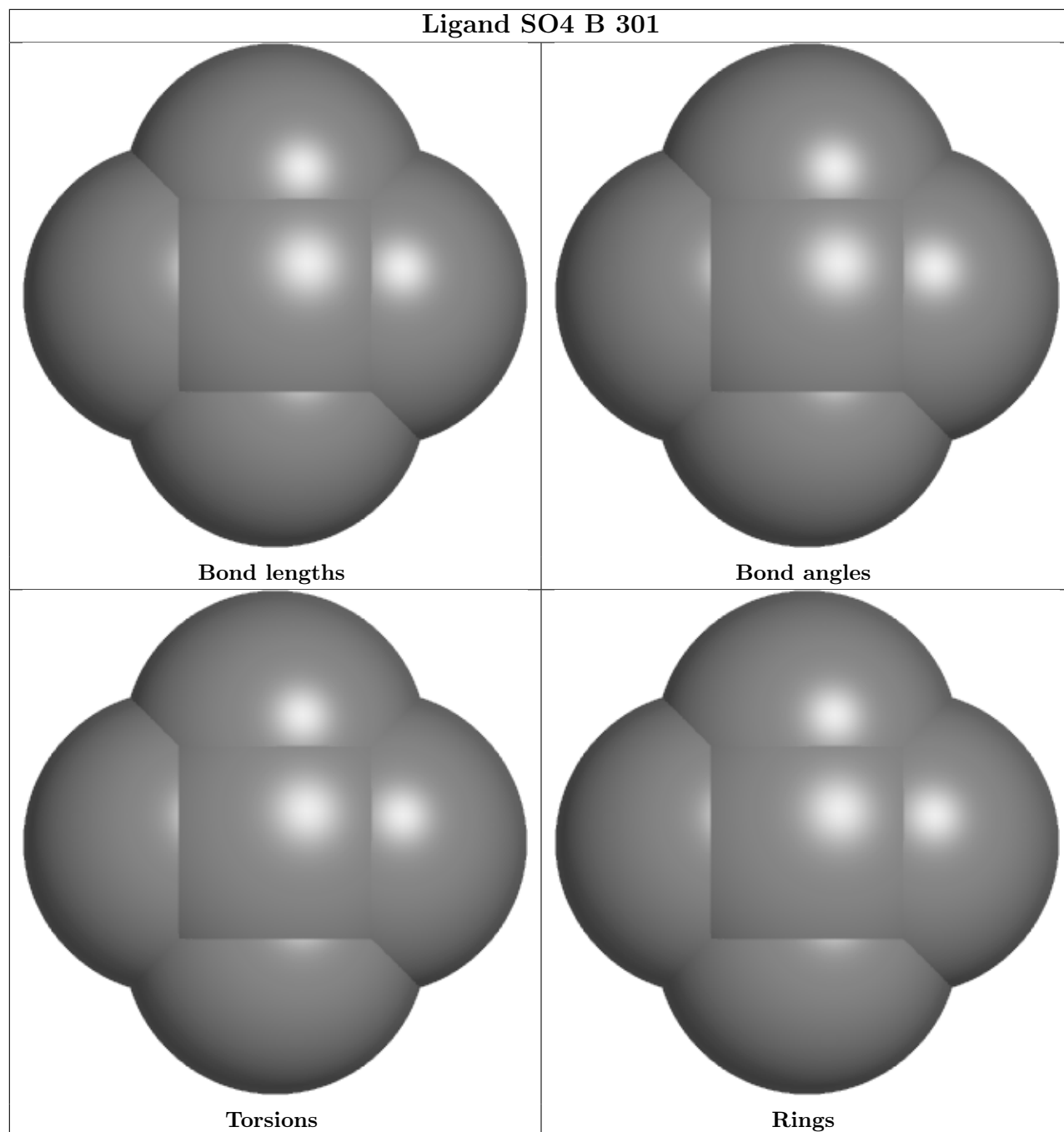
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 B 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	118/132 (89%)	-0.11	4 (3%)	48	50	20, 29, 61, 77	0
1	D	124/132 (93%)	0.07	7 (5%)	31	33	19, 33, 68, 82	0
2	B	275/276 (99%)	-0.18	7 (2%)	58	59	18, 29, 55, 68	0
2	F	275/276 (99%)	0.03	9 (3%)	49	51	22, 35, 59, 80	0
3	C	99/100 (99%)	-0.16	1 (1%)	79	79	21, 31, 52, 60	0
3	G	98/100 (98%)	-0.05	2 (2%)	64	66	23, 32, 52, 65	0
4	E	9/9 (100%)	-0.77	0	100	100	20, 21, 23, 25	0
4	H	9/9 (100%)	-0.55	0	100	100	22, 23, 26, 27	0
All	All	1007/1034 (97%)	-0.08	30 (2%)	52	54	18, 32, 58, 82	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	THR	5.4
1	D	56	GLY	4.5
1	D	55	ILE	4.3
2	B	227	ASP	4.0
3	G	1	ILE	3.7
1	D	58	HIS	3.5
1	A	94	LYS	3.3
1	A	125	GLU	3.0
2	B	224	GLN	3.0
2	F	225	THR	3.0
1	D	26	ASP	3.0
2	F	197	HIS	3.0
1	A	126	HIS	2.9
1	D	27	ALA	2.8
2	F	227	ASP	2.6
2	B	226	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	226	GLN	2.4
1	A	85	LEU	2.4
3	G	98	ASP	2.4
2	F	51	TRP	2.3
2	F	113	TYR	2.3
3	C	48	LYS	2.2
2	B	225	THR	2.2
2	F	192	HIS	2.1
2	F	6	ARG	2.1
2	B	136	ALA	2.1
2	B	275	GLU	2.0
2	B	113	TYR	2.0
2	F	195	SER	2.0
1	D	59	ASP	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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
5	SO4	B	302	5/5	0.88	0.14	50,56,63,66	0
5	SO4	D	201	5/5	0.89	0.12	47,53,59,67	0
5	SO4	B	301	5/5	0.94	0.10	40,42,44,49	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.
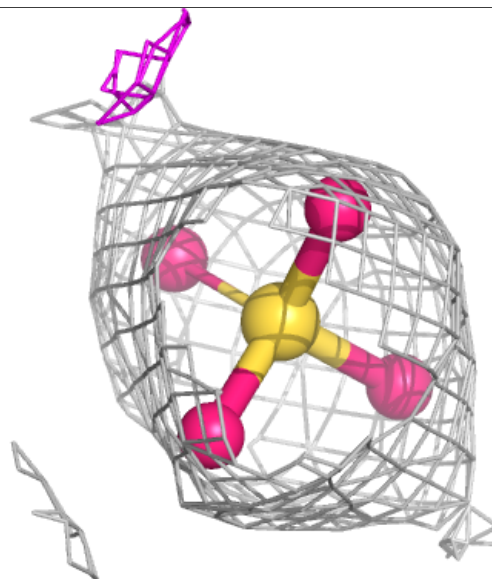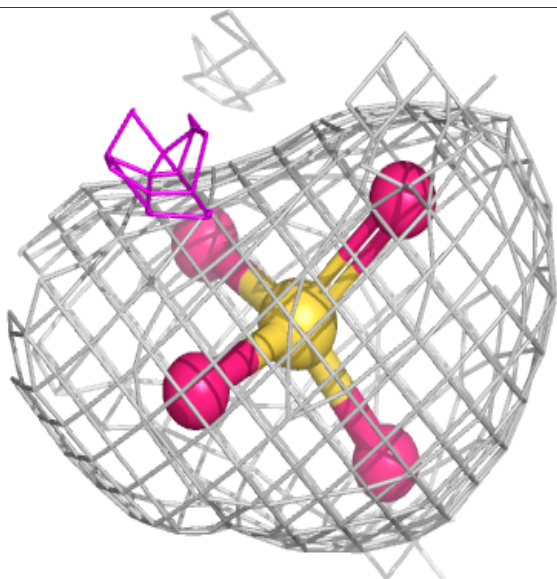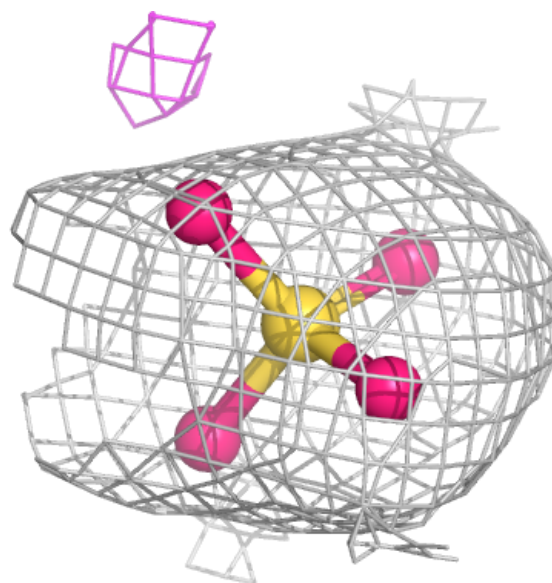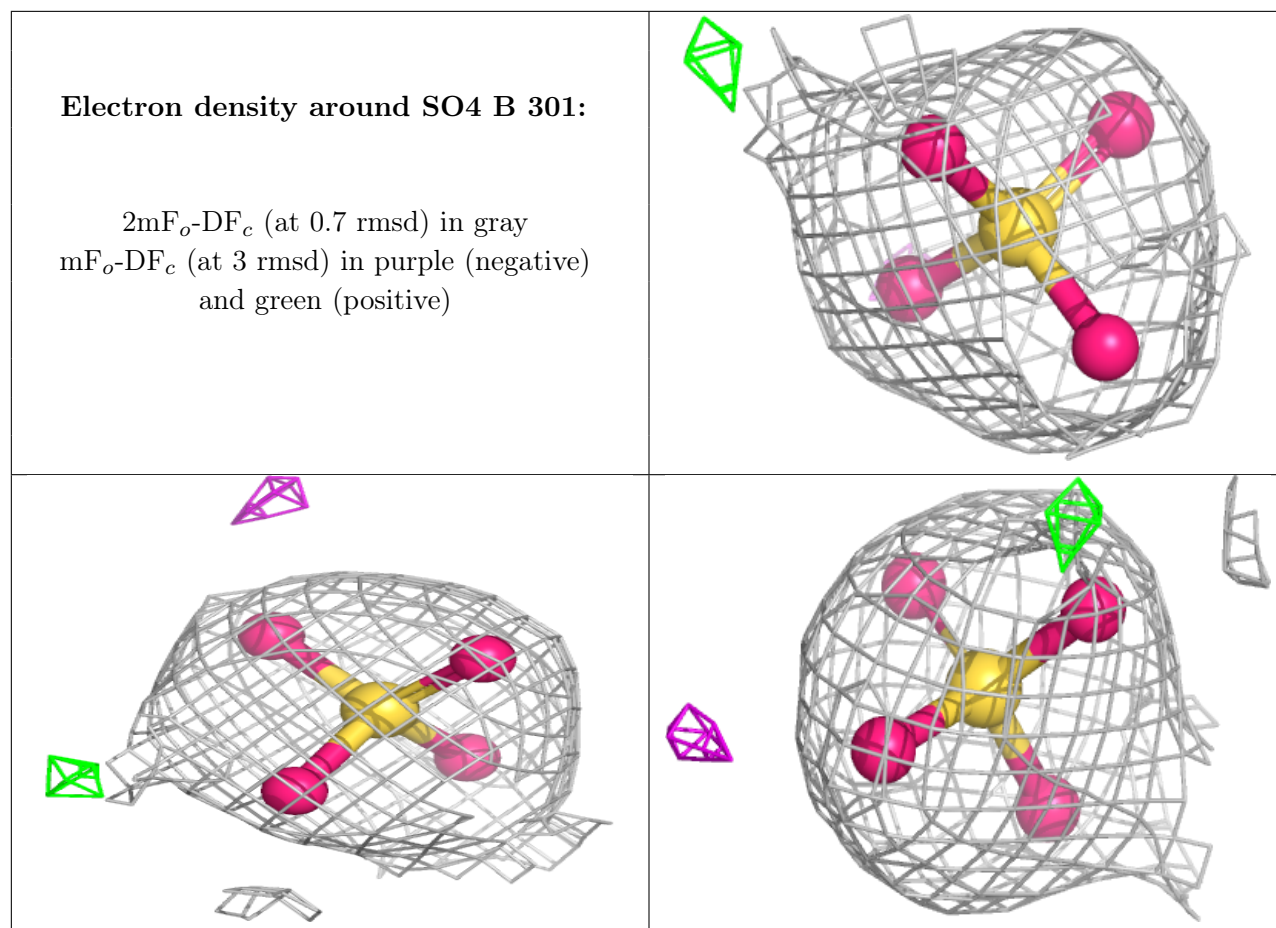
Electron density around SO4 B 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
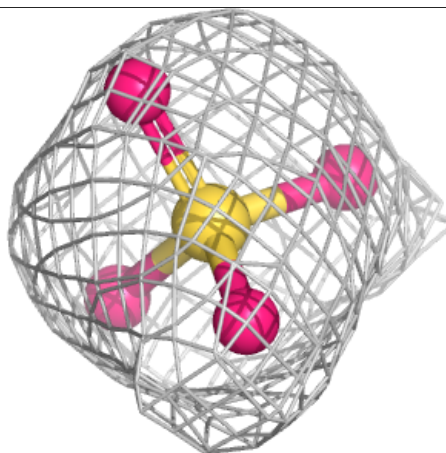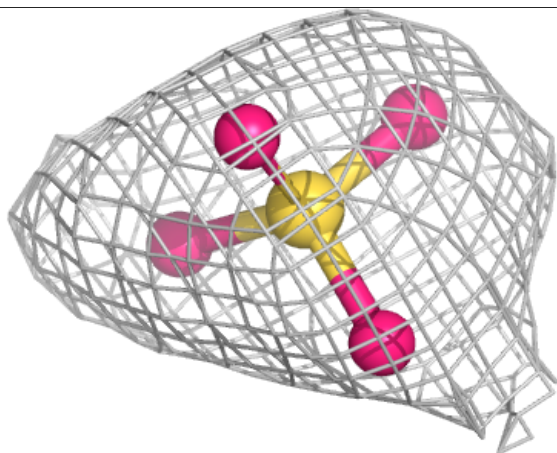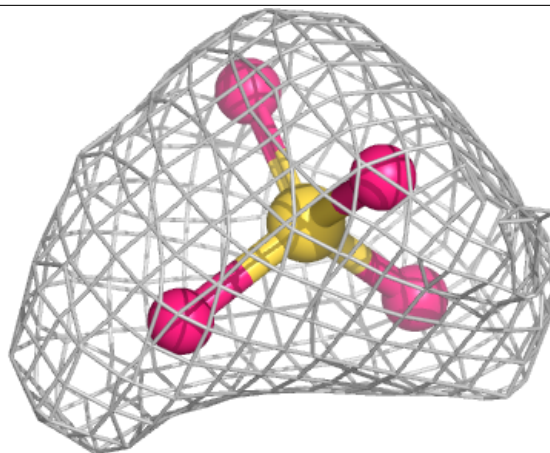
Electron density around SO4 D 201:

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

Electron density around SO4 B 301:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.