



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:42 AM UTC

PDB ID : 7Q2W / pdb_00007q2w
Title : Mutant T91S of uridine phosphorylase from *Shewanella oneidensis*
Authors : Polyakov, K.; Safonova, T.
Deposited on : 2021-10-26
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

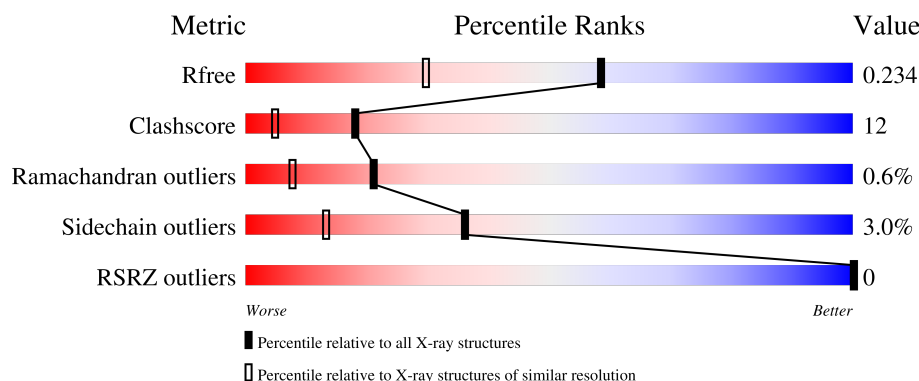
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	AAA	251	63% 29% 6% .
1	BBB	251	58% 31% 6% .
1	CCC	251	64% 28% 7%
1	DDD	251	60% 32% 8%
1	EEE	251	65% 26% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FFF	251	63% 27% 8%

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
2	SO4	EEE	301	-	-	X	-
2	SO4	FFF	303	-	-	X	-
3	GOL	DDD	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22765 atoms, of which 10920 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	DDD	251	Total	C	H	N	O	S	87	2	0
			3718	1169	1851	322	362	14			
1	FFF	244	Total	C	H	N	O	S	86	3	0
			3649	1146	1824	315	351	13			
1	AAA	245	Total	C	H	N	O	S	85	2	0
			3643	1145	1818	316	350	14			
1	CCC	250	Total	C	H	N	O	S	86	2	0
			3711	1166	1851	321	358	15			
1	EEE	242	Total	C	H	N	O	S	83	1	0
			3583	1126	1789	311	344	13			
1	BBB	240	Total	C	H	N	O	S	83	0	0
			3542	1114	1767	307	341	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DDD	91	SER	THR	engineered mutation	UNP Q8E9X9
FFF	91	SER	THR	engineered mutation	UNP Q8E9X9
AAA	91	SER	THR	engineered mutation	UNP Q8E9X9
CCC	91	SER	THR	engineered mutation	UNP Q8E9X9
EEE	91	SER	THR	engineered mutation	UNP Q8E9X9
BBB	91	SER	THR	engineered mutation	UNP Q8E9X9

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



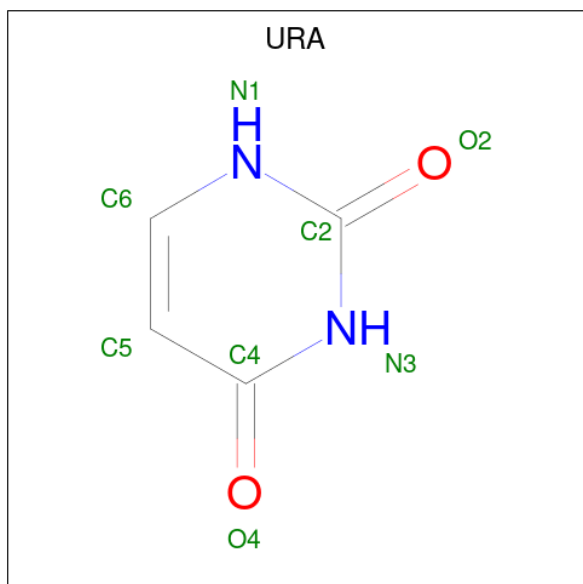
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	DDD	1	Total	O	S	0	0
			5	4	1		
2	FFF	1	Total	O	S	0	1
			5	4	1		
2	FFF	1	Total	O	S	0	0
			5	4	1		
2	AAA	1	Total	O	S	0	0
			5	4	1		
2	EEE	1	Total	O	S	0	0
			5	4	1		
2	BBB	1	Total	O	S	0	1
			10	8	2		
2	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	DDD	1	Total	C	H	O	2	0
			14	3	8	3		
3	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 4 is URACIL (CCD ID: URA) (formula: $C_4H_4N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	FFF	1	Total	C	H	N	O	0	0
			12	4	4	2	2		

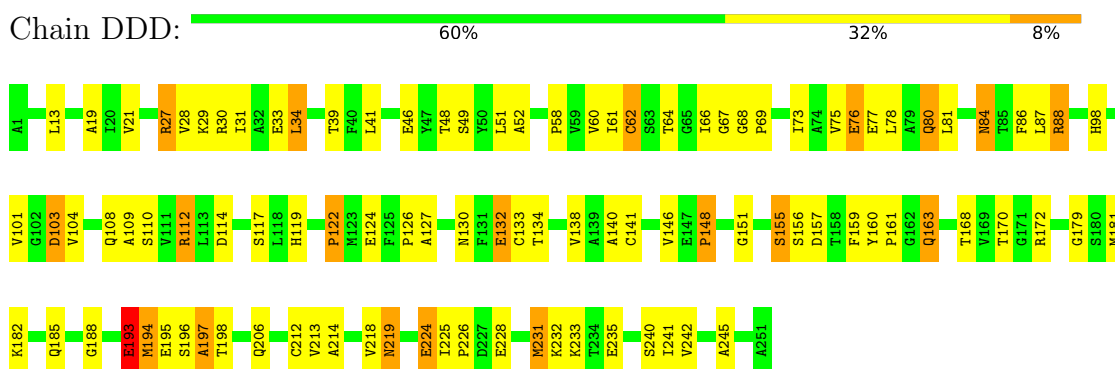
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	DDD	150	Total 150	O 150	0	0
5	FFF	123	Total 123	O 123	0	0
5	AAA	156	Total 156	O 156	0	0
5	CCC	152	Total 152	O 152	0	0
5	EEE	126	Total 126	O 126	0	0
5	BBB	132	Total 132	O 132	0	0

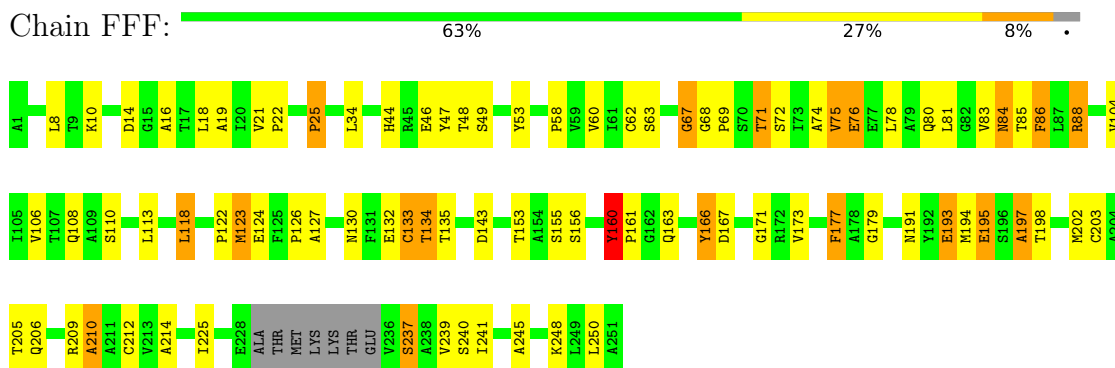
3 Residue-property plots [i](#)

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.

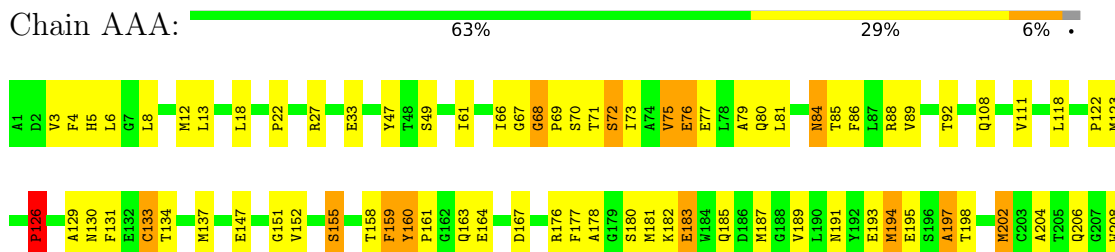
• Molecule 1: Uridine phosphorylase

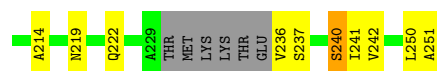


• Molecule 1: Uridine phosphorylase



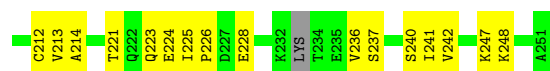
• Molecule 1: Uridine phosphorylase





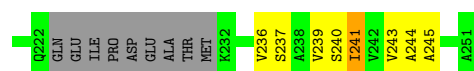
- Molecule 1: Uridine phosphorylase

Chain CCC: 64% 28% 7%



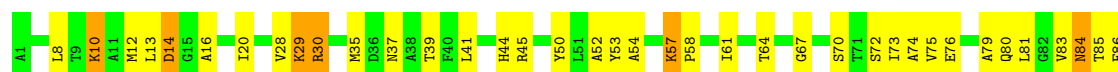
- Molecule 1: Uridine phosphorylase

Chain EEE: 65% 26% 6%



- Molecule 1: Uridine phosphorylase

Chain BBB: 58% 31% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.40Å 95.49Å 91.41Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	25.00 – 1.65 25.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.3 (25.00-1.65) 98.3 (25.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.232 0.192 , 0.234	Depositor DCC
R_{free} test set	7780 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	1.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 26.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.338 for -h-l,k,h 0.338 for l,k,-h-l 0.310 for l,-k,h 0.370 for h,-k,-h-l 0.308 for -h-l,-k,l	Xtriage
Reported twinning fraction	0.082 for H, K, L 0.449 for -L, -K, -H 0.136 for -H-L, -K, L 0.040 for L, K, -H-L 0.208 for -H-L, K, H 0.084 for -H, -K, H+L	Depositor
Outliers	0 of 159146 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22765	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	AAA	1.50	20/1866 (1.1%)	1.74	22/2536 (0.9%)
1	BBB	1.56	23/1806 (1.3%)	1.78	27/2455 (1.1%)
1	CCC	1.61	29/1902 (1.5%)	1.74	26/2585 (1.0%)
1	DDD	1.60	31/1907 (1.6%)	1.77	37/2593 (1.4%)
1	EEE	1.51	27/1830 (1.5%)	1.78	22/2488 (0.9%)
1	FFF	1.57	26/1869 (1.4%)	1.72	19/2542 (0.7%)
All	All	1.56	156/11180 (1.4%)	1.75	153/15199 (1.0%)

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
1	BBB	0	1
1	CCC	0	2
1	DDD	0	1
1	EEE	0	3
All	All	0	7

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	80	GLN	C-O	9.62	1.36	1.24
1	CCC	189	VAL	C-O	9.44	1.33	1.24
1	FFF	198	THR	C-O	8.81	1.34	1.24
1	CCC	105	ILE	C-O	-8.72	1.14	1.24
1	FFF	133	CYS	C-O	-8.40	1.13	1.24
1	DDD	196	SER	C-O	8.39	1.34	1.24
1	FFF	67	GLY	C-O	-8.26	1.14	1.23
1	EEE	130	ASN	C-O	8.08	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	189	VAL	C-O	7.66	1.31	1.24
1	FFF	104	VAL	C-O	7.65	1.32	1.24
1	DDD	198	THR	C-O	7.64	1.32	1.24
1	BBB	119	HIS	C-O	7.56	1.34	1.24
1	BBB	198	THR	C-O	7.51	1.32	1.24
1	BBB	130	ASN	C-O	7.45	1.32	1.23
1	AAA	189	VAL	C-O	7.43	1.32	1.24
1	CCC	184	TRP	C-O	-7.35	1.15	1.24
1	EEE	194	MET	C-O	-7.31	1.14	1.24
1	FFF	134[A]	THR	N-CA	7.23	1.54	1.46
1	FFF	134[B]	THR	N-CA	7.23	1.54	1.46
1	DDD	126	PRO	C-O	7.18	1.31	1.23
1	BBB	155	SER	C-O	7.13	1.32	1.23
1	DDD	224	GLU	C-O	7.09	1.32	1.24
1	CCC	193	GLU	C-O	7.08	1.31	1.24
1	EEE	159	PHE	C-O	6.99	1.32	1.24
1	BBB	193	GLU	C-O	6.96	1.31	1.24
1	CCC	214	ALA	C-O	-6.94	1.15	1.23
1	DDD	62	CYS	C-O	6.93	1.31	1.23
1	DDD	140	ALA	C-O	-6.93	1.15	1.24
1	EEE	169	VAL	C-O	6.91	1.31	1.24
1	FFF	67	GLY	C-N	-6.89	1.29	1.34
1	DDD	49[A]	SER	C-O	6.88	1.31	1.24
1	DDD	49[B]	SER	C-O	6.88	1.31	1.24
1	FFF	126	PRO	C-O	6.80	1.31	1.23
1	DDD	193	GLU	C-O	6.71	1.30	1.24
1	CCC	111	VAL	C-O	6.70	1.30	1.24
1	BBB	72	SER	C-O	6.69	1.31	1.24
1	EEE	195	GLU	C-O	6.69	1.32	1.24
1	CCC	83	VAL	C-O	6.60	1.31	1.24
1	BBB	151	GLY	C-O	6.59	1.32	1.23
1	AAA	204	ALA	C-O	6.56	1.31	1.24
1	CCC	223	GLN	C-O	6.55	1.31	1.23
1	CCC	203	CYS	C-O	6.53	1.31	1.24
1	CCC	240	SER	C-O	6.52	1.31	1.24
1	EEE	245	ALA	C-O	-6.51	1.16	1.24
1	FFF	108	GLN	C-O	6.51	1.31	1.24
1	AAA	202	MET	C-O	6.44	1.32	1.24
1	CCC	86	PHE	C-O	-6.44	1.16	1.24
1	EEE	151	GLY	C-O	6.40	1.29	1.23
1	DDD	156	SER	C-O	6.38	1.31	1.24
1	DDD	195	GLU	C-O	6.38	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	FFF	179	GLY	C-O	6.37	1.32	1.24
1	BBB	152	VAL	C-O	6.37	1.31	1.24
1	CCC	167	ASP	C-O	6.37	1.31	1.23
1	CCC	134	THR	C-O	6.34	1.31	1.24
1	FFF	209	ARG	C-O	-6.33	1.16	1.23
1	AAA	6	LEU	C-O	6.33	1.32	1.24
1	CCC	221	THR	C-O	6.33	1.32	1.24
1	EEE	198	THR	C-O	6.32	1.31	1.24
1	AAA	198	THR	C-O	6.32	1.31	1.24
1	BBB	80	GLN	C-O	6.30	1.32	1.24
1	FFF	156	SER	C-O	6.27	1.31	1.24
1	FFF	25	PRO	C-O	-6.27	1.16	1.24
1	CCC	195	GLU	N-CA	6.26	1.54	1.46
1	DDD	155	SER	C-O	6.25	1.31	1.24
1	FFF	210	ALA	C-O	-6.25	1.16	1.23
1	AAA	152	VAL	C-O	6.25	1.31	1.24
1	AAA	76	GLU	C-O	6.22	1.31	1.24
1	FFF	166	TYR	C-O	6.21	1.32	1.24
1	DDD	161	PRO	C-O	-6.20	1.15	1.24
1	CCC	50	TYR	C-O	6.19	1.31	1.23
1	CCC	198	THR	C-O	6.17	1.31	1.24
1	DDD	87	LEU	C-O	6.14	1.31	1.23
1	BBB	194	MET	C-O	-6.11	1.15	1.24
1	EEE	112	ARG	C-O	6.10	1.30	1.23
1	DDD	69	PRO	C-O	6.09	1.32	1.24
1	CCC	202	MET	C-O	6.08	1.31	1.24
1	DDD	179	GLY	C-O	6.02	1.32	1.24
1	EEE	116	ALA	C-O	5.98	1.31	1.24
1	DDD	213	VAL	C-O	5.97	1.29	1.24
1	EEE	204	ALA	C-O	5.96	1.30	1.24
1	FFF	106	VAL	C-O	5.95	1.30	1.24
1	CCC	195	GLU	C-O	5.93	1.31	1.24
1	FFF	123	MET	C-O	5.92	1.31	1.24
1	DDD	241	ILE	C-O	-5.89	1.17	1.24
1	CCC	80	GLN	N-CA	5.88	1.54	1.46
1	DDD	157	ASP	C-O	-5.88	1.16	1.24
1	EEE	72	SER	C-O	5.87	1.31	1.24
1	EEE	108	GLN	C-O	5.86	1.31	1.24
1	EEE	111	VAL	C-O	5.85	1.30	1.24
1	BBB	119	HIS	CE1-NE2	5.83	1.38	1.32
1	CCC	60	VAL	C-O	5.83	1.32	1.24
1	DDD	78	LEU	C-O	-5.81	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	156	SER	CA-CB	5.77	1.62	1.53
1	EEE	203	CYS	C-O	5.76	1.31	1.24
1	EEE	202	MET	C-O	5.75	1.31	1.24
1	AAA	164	GLU	C-O	5.72	1.31	1.23
1	FFF	153	THR	C-O	-5.72	1.16	1.24
1	BBB	74	ALA	C-O	5.71	1.30	1.24
1	EEE	58	PRO	C-O	5.66	1.30	1.23
1	CCC	75	VAL	C-O	-5.66	1.17	1.24
1	EEE	243	VAL	C-O	5.66	1.30	1.24
1	BBB	187	MET	C-O	5.64	1.33	1.24
1	BBB	161	PRO	C-O	-5.63	1.17	1.24
1	DDD	80	GLN	C-O	5.62	1.31	1.24
1	DDD	119	HIS	CE1-NE2	5.62	1.38	1.32
1	FFF	205	THR	C-O	5.61	1.31	1.24
1	EEE	161	PRO	C-O	-5.57	1.17	1.24
1	EEE	210	ALA	C-O	5.56	1.30	1.23
1	AAA	111	VAL	C-O	5.56	1.30	1.24
1	DDD	195	GLU	N-CA	5.55	1.53	1.46
1	AAA	155	SER	C-O	5.54	1.30	1.24
1	FFF	173	VAL	C-O	-5.53	1.18	1.24
1	CCC	61	ILE	C-O	-5.53	1.18	1.24
1	FFF	127	ALA	C-O	5.53	1.31	1.23
1	AAA	208	TRP	C-O	-5.51	1.16	1.23
1	AAA	195	GLU	N-CA	5.50	1.53	1.46
1	BBB	156	SER	C-O	5.50	1.30	1.24
1	AAA	89	VAL	C-O	5.49	1.29	1.23
1	EEE	195	GLU	N-CA	5.48	1.53	1.46
1	AAA	134	THR	C-O	5.47	1.30	1.24
1	CCC	109	ALA	C-O	5.46	1.30	1.23
1	FFF	195	GLU	C-O	5.43	1.31	1.24
1	CCC	182	LYS	C-O	5.43	1.30	1.24
1	EEE	239	VAL	C-O	5.43	1.31	1.24
1	BBB	116	ALA	C-O	5.42	1.30	1.24
1	CCC	213	VAL	C-O	-5.42	1.17	1.24
1	FFF	76	GLU	C-O	5.41	1.30	1.24
1	DDD	194	MET	C-O	-5.41	1.16	1.24
1	EEE	124	GLU	CD-OE2	5.40	1.35	1.25
1	EEE	137	MET	C-O	-5.39	1.18	1.24
1	BBB	201	THR	C-O	5.38	1.30	1.24
1	DDD	68	GLY	N-CA	5.33	1.49	1.45
1	AAA	181	MET	C-O	-5.33	1.17	1.24
1	DDD	109	ALA	C-O	5.32	1.29	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	76	GLU	C-O	5.32	1.30	1.24
1	FFF	240	SER	C-O	5.31	1.30	1.24
1	DDD	157	ASP	CG-OD2	-5.30	1.15	1.25
1	AAA	194[A]	MET	C-O	-5.27	1.16	1.24
1	AAA	194[B]	MET	C-O	-5.27	1.16	1.24
1	CCC	108	GLN	C-O	5.27	1.31	1.24
1	BBB	164	GLU	C-O	5.25	1.29	1.23
1	EEE	208	TRP	C-O	-5.24	1.17	1.23
1	EEE	119	HIS	CE1-NE2	5.23	1.37	1.32
1	DDD	52	ALA	C-O	5.16	1.30	1.23
1	BBB	35	MET	C-O	5.15	1.30	1.23
1	BBB	198	THR	N-CA	5.15	1.52	1.46
1	AAA	79	ALA	C-O	-5.14	1.18	1.24
1	AAA	33	GLU	C-O	5.13	1.30	1.24
1	AAA	72	SER	C-O	5.11	1.30	1.24
1	BBB	52	ALA	C-O	5.10	1.29	1.23
1	DDD	156	SER	N-CA	5.08	1.52	1.46
1	DDD	172	ARG	C-O	5.07	1.30	1.24
1	EEE	18	LEU	C-O	5.06	1.29	1.24
1	FFF	71	THR	N-CA	5.04	1.52	1.46
1	BBB	70	SER	C-O	5.04	1.30	1.24
1	FFF	110	SER	C-O	-5.02	1.18	1.24

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	67	GLY	CA-C-O	-9.92	114.25	122.29
1	FFF	133	CYS	N-CA-C	-9.21	100.36	111.69
1	DDD	86	PHE	CA-C-O	-8.51	109.85	120.57
1	CCC	67	GLY	CA-C-O	-8.43	115.86	122.52
1	BBB	10	LYS	N-CA-C	-8.13	102.50	111.36
1	CCC	177	PHE	CA-CB-CG	-8.11	105.69	113.80
1	FFF	67	GLY	CA-C-O	-8.06	116.15	122.52
1	FFF	68	GLY	CA-C-O	-7.94	114.33	119.65
1	AAA	126	PRO	CB-CA-C	7.91	122.00	110.85
1	DDD	197	ALA	N-CA-C	-7.85	102.81	111.36
1	EEE	67	GLY	CA-C-O	-7.80	116.36	122.52
1	EEE	132	GLU	CA-C-O	-7.57	112.87	120.82
1	BBB	67	GLY	CA-C-O	-7.38	116.13	121.88
1	DDD	245	ALA	N-CA-C	-7.35	103.35	111.36
1	CCC	55	ASP	CA-CB-CG	7.27	119.87	112.60
1	AAA	133	CYS	N-CA-C	-7.22	103.49	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	103	ASP	N-CA-C	-7.19	101.57	110.41
1	CCC	79	ALA	N-CA-C	-7.13	104.05	112.89
1	BBB	194	MET	CA-C-O	-7.09	111.61	119.34
1	AAA	70	SER	CA-C-N	7.05	129.60	120.44
1	AAA	70	SER	C-N-CA	7.05	129.60	120.44
1	BBB	132	GLU	CA-C-O	-7.00	113.47	120.82
1	BBB	157	ASP	CA-CB-CG	-7.00	105.60	112.60
1	EEE	163	GLN	N-CA-C	-6.96	103.37	112.41
1	EEE	241	ILE	N-CA-C	-6.93	104.02	110.53
1	FFF	163	GLN	N-CA-C	-6.90	104.85	112.72
1	EEE	208	TRP	N-CA-C	-6.82	98.94	109.24
1	DDD	81	LEU	CA-C-N	6.76	131.12	122.00
1	DDD	81	LEU	C-N-CA	6.76	131.12	122.00
1	BBB	20	ILE	CB-CA-C	6.71	120.51	111.19
1	CCC	75	VAL	N-CA-C	-6.67	103.73	111.00
1	AAA	75	VAL	N-CA-C	-6.61	104.31	110.53
1	FFF	214	ALA	O-C-N	6.61	130.88	123.48
1	FFF	86	PHE	CA-C-O	-6.58	113.22	120.33
1	DDD	148	PRO	CB-CA-C	-6.53	102.40	110.95
1	DDD	112	ARG	CB-CA-C	6.51	122.24	111.83
1	AAA	79	ALA	N-CA-C	-6.48	104.30	111.36
1	BBB	245	ALA	N-CA-C	-6.43	104.19	111.07
1	CCC	137	MET	N-CA-C	-6.42	104.20	111.07
1	FFF	75	VAL	N-CA-C	-6.39	104.04	111.00
1	BBB	44	HIS	CA-CB-CG	-6.36	107.44	113.80
1	AAA	197	ALA	N-CA-C	-6.30	104.33	111.07
1	BBB	162	GLY	CA-C-N	6.29	132.06	122.37
1	BBB	162	GLY	C-N-CA	6.29	132.06	122.37
1	CCC	133	CYS	N-CA-C	-6.29	104.53	111.82
1	DDD	77	GLU	CB-CG-CD	6.28	123.27	112.60
1	DDD	68	GLY	CA-C-O	-6.25	115.75	119.69
1	AAA	159	PHE	N-CA-C	-6.25	104.72	112.90
1	CCC	86	PHE	CA-C-O	-6.18	113.66	120.33
1	BBB	14	ASP	CA-CB-CG	6.16	118.76	112.60
1	BBB	122	PRO	N-CA-CB	6.15	109.17	103.39
1	DDD	163	GLN	N-CA-C	-6.12	105.12	112.59
1	BBB	75	VAL	CA-C-O	-6.12	114.74	121.29
1	CCC	81	LEU	CA-C-N	6.08	131.41	122.10
1	CCC	81	LEU	C-N-CA	6.08	131.41	122.10
1	FFF	113	LEU	CB-CA-C	6.08	118.69	111.22
1	DDD	170	THR	CA-CB-OG1	-6.07	100.49	109.60
1	EEE	137	MET	CA-C-O	-6.04	114.48	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	133	CYS	N-CA-C	-6.01	104.65	112.23
1	EEE	121	ALA	O-C-N	5.99	128.21	121.32
1	AAA	67	GLY	CA-C-O	-5.98	117.21	121.88
1	FFF	118	LEU	N-CA-C	-5.98	105.48	112.89
1	EEE	244	ALA	CA-C-N	5.96	128.75	120.29
1	EEE	244	ALA	C-N-CA	5.96	128.75	120.29
1	AAA	163	GLN	N-CA-C	-5.93	105.23	112.88
1	BBB	175	ARG	O-C-N	-5.92	114.72	122.59
1	BBB	103	ASP	N-CA-C	-5.91	101.78	110.52
1	AAA	68	GLY	O-C-N	-5.90	118.94	121.07
1	FFF	68	GLY	O-C-N	5.90	123.19	121.07
1	DDD	66	ILE	CA-C-N	5.87	132.02	121.92
1	DDD	66	ILE	C-N-CA	5.87	132.02	121.92
1	DDD	75	VAL	N-CA-C	-5.81	105.19	110.82
1	BBB	105	ILE	O-C-N	5.81	129.28	123.18
1	CCC	75	VAL	CA-C-O	-5.80	114.50	120.71
1	DDD	67	GLY	O-C-N	5.76	129.57	122.78
1	BBB	28	VAL	CA-C-O	-5.72	115.46	121.41
1	EEE	143	ASP	CA-CB-CG	5.70	118.30	112.60
1	DDD	66	ILE	O-C-N	5.70	128.88	122.67
1	AAA	122	PRO	N-CA-C	-5.70	102.86	111.41
1	BBB	79	ALA	CA-C-O	-5.69	114.52	120.55
1	DDD	58	PRO	CB-CA-C	-5.69	103.64	111.21
1	CCC	214	ALA	CA-C-O	-5.68	114.64	120.89
1	FFF	245	ALA	N-CA-C	-5.66	105.25	111.82
1	EEE	19	ALA	CA-C-O	-5.65	114.26	120.36
1	EEE	245	ALA	N-CA-C	-5.64	105.21	111.36
1	EEE	70	SER	CA-C-N	5.62	127.81	120.28
1	EEE	70	SER	C-N-CA	5.62	127.81	120.28
1	FFF	177	PHE	CA-CB-CG	-5.62	108.18	113.80
1	FFF	225	ILE	CB-CA-C	5.62	116.48	110.53
1	CCC	223	GLN	O-C-N	5.61	129.97	123.41
1	DDD	242	VAL	CA-C-O	-5.60	115.13	120.95
1	CCC	55	ASP	N-CA-C	-5.59	103.67	111.39
1	CCC	223	GLN	CA-C-O	-5.58	113.68	120.54
1	CCC	132	GLU	CA-C-O	-5.58	114.94	121.07
1	DDD	134	THR	CA-C-N	5.56	128.51	120.79
1	DDD	134	THR	C-N-CA	5.56	128.51	120.79
1	DDD	241	ILE	N-CA-C	-5.54	105.32	110.53
1	BBB	117	SER	CA-C-O	-5.54	114.65	120.63
1	BBB	163	GLN	N-CA-C	-5.54	105.13	112.94
1	DDD	214	ALA	CA-C-O	-5.53	113.91	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	214	ALA	CA-C-O	-5.53	113.91	120.43
1	CCC	89	VAL	O-C-N	-5.52	117.23	123.03
1	AAA	86	PHE	CA-C-O	-5.52	114.37	120.33
1	EEE	208	TRP	CA-C-O	-5.50	115.18	121.40
1	CCC	214	ALA	O-C-N	5.49	129.63	123.48
1	CCC	71	THR	N-CA-C	-5.48	105.21	111.07
1	BBB	76	GLU	CB-CG-CD	5.47	121.90	112.60
1	CCC	57	LYS	CA-C-O	5.47	123.37	119.32
1	AAA	214	ALA	O-C-N	5.44	129.69	123.48
1	BBB	112	ARG	CB-CA-C	5.43	120.50	112.03
1	DDD	168	THR	CA-CB-OG1	-5.42	101.47	109.60
1	DDD	27	ARG	N-CA-C	-5.41	106.52	113.23
1	DDD	122	PRO	CB-CA-C	5.40	118.08	111.12
1	DDD	103	ASP	N-CA-C	-5.39	103.41	110.53
1	DDD	170	THR	CA-C-N	5.39	128.24	120.11
1	DDD	170	THR	C-N-CA	5.39	128.24	120.11
1	FFF	197	ALA	N-CA-C	-5.38	105.33	111.14
1	AAA	183	GLU	CA-C-O	-5.36	115.16	120.90
1	EEE	133	CYS	N-CA-C	-5.36	105.61	111.82
1	CCC	208	TRP	N-CA-C	-5.32	101.09	109.50
1	EEE	198	THR	N-CA-C	-5.30	105.42	111.14
1	AAA	147	GLU	CA-C-O	5.29	122.73	119.29
1	FFF	127	ALA	CA-C-O	-5.25	115.85	122.63
1	EEE	78	LEU	CA-C-O	-5.24	115.29	120.90
1	DDD	34	LEU	N-CA-C	-5.22	106.68	113.16
1	CCC	213	VAL	O-C-N	-5.22	117.56	122.98
1	FFF	160	TYR	CB-CA-C	5.21	120.44	110.17
1	BBB	163	GLN	O-C-N	5.19	128.47	122.19
1	CCC	66	ILE	O-C-N	5.18	128.56	122.81
1	CCC	75	VAL	N-CA-CB	5.18	119.21	110.56
1	CCC	116	ALA	O-C-N	-5.17	115.91	122.27
1	BBB	105	ILE	CA-C-O	-5.15	115.02	120.48
1	EEE	186	ASP	CA-CB-CG	-5.13	107.47	112.60
1	AAA	167	ASP	CA-C-O	-5.13	115.57	122.44
1	DDD	188	GLY	CA-C-N	5.12	127.44	120.63
1	DDD	188	GLY	C-N-CA	5.12	127.44	120.63
1	AAA	241	ILE	N-CA-C	-5.11	105.56	110.72
1	DDD	110	SER	N-CA-C	5.11	117.39	108.76
1	DDD	132	GLU	CA-C-O	-5.11	115.14	120.55
1	DDD	219	ASN	CA-C-N	5.09	128.74	120.60
1	DDD	219	ASN	C-N-CA	5.09	128.74	120.60
1	DDD	28	VAL	CA-C-O	-5.08	115.98	121.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	28	VAL	O-C-N	5.08	127.45	121.96
1	EEE	236	VAL	CA-C-N	5.06	127.02	120.44
1	EEE	236	VAL	C-N-CA	5.06	127.02	120.44
1	FFF	203	CYS	CA-C-N	5.06	128.41	120.82
1	FFF	203	CYS	C-N-CA	5.06	128.41	120.82
1	AAA	73	ILE	CA-C-N	5.04	127.00	120.44
1	AAA	73	ILE	C-N-CA	5.04	127.00	120.44
1	FFF	191	ASN	O-C-N	5.04	128.33	123.29
1	AAA	219	ASN	CB-CA-C	5.02	118.41	109.72
1	BBB	167	ASP	CA-CB-CG	5.02	117.62	112.60
1	EEE	143	ASP	CA-C-O	-5.02	114.43	120.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	214	ALA	Mainchain
1	CCC	194	MET	Mainchain
1	CCC	209	ARG	Mainchain
1	DDD	232	LYS	Peptide
1	EEE	203	CYS	Mainchain
1	EEE	44	HIS	Mainchain
1	EEE	60	VAL	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1825	1818	1807	48	0
1	BBB	1775	1767	1758	43	1
1	CCC	1860	1851	1836	47	1
1	DDD	1867	1851	1839	56	0
1	EEE	1794	1789	1777	31	0
1	FFF	1825	1824	1810	51	0
2	AAA	5	0	0	0	0
2	BBB	15	0	0	1	0
2	DDD	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EEE	5	0	0	2	0
2	FFF	10	0	0	5	0
3	AAA	6	8	8	1	0
3	DDD	6	8	8	6	0
4	FFF	8	4	3	1	0
5	AAA	156	0	0	8	0
5	BBB	132	0	0	11	0
5	CCC	152	0	0	9	0
5	DDD	150	0	0	14	0
5	EEE	126	0	0	3	0
5	FFF	123	0	0	4	0
All	All	11845	10920	10846	267	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (267) 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)
2:EEE:301:SO4:S	5:EEE:402:HOH:O	2.17	0.99
1:FFF:130:ASN:O	1:FFF:134[B]:THR:HG23	1.63	0.98
1:CCC:123:MET:HE3	5:CCC:370:HOH:O	1.62	0.97
1:CCC:123:MET:CE	5:CCC:370:HOH:O	2.21	0.86
1:BBB:132:GLU:OE2	1:BBB:209:ARG:NH1	2.10	0.84
1:FFF:25:PRO:O	1:FFF:48[B]:THR:HG21	1.79	0.82
1:FFF:71:THR:O	1:FFF:75:VAL:HG23	1.81	0.81
1:AAA:155:SER:HB3	1:AAA:197:ALA:HB2	1.63	0.81
1:AAA:222:GLN:NE2	5:AAA:402:HOH:O	2.15	0.79
1:CCC:155:SER:HB3	1:CCC:197:ALA:HB2	1.64	0.78
1:CCC:195:GLU:OE1	5:CCC:303:HOH:O	2.03	0.77
1:DDD:130:ASN:HD22	1:DDD:133:CYS:H	1.34	0.76
1:BBB:81:LEU:O	5:BBB:403:HOH:O	2.03	0.76
1:FFF:195:GLU:OE1	2:FFF:303:SO4:O2	2.05	0.75
1:FFF:14:ASP:OD1	1:FFF:53:TYR:OH	2.05	0.74
1:DDD:138:VAL:O	5:DDD:402:HOH:O	2.05	0.74
1:CCC:130:ASN:HD22	1:CCC:133:CYS:H	1.37	0.72
1:CCC:194:MET:N	5:CCC:303:HOH:O	2.23	0.72
1:FFF:84:ASN:ND2	1:FFF:85:THR:OG1	2.22	0.72
1:BBB:143:ASP:OD2	1:BBB:248:LYS:NZ	2.23	0.71
1:BBB:175:ARG:NH1	2:BBB:301[A]:SO4:O2	2.23	0.71
1:FFF:88[A]:ARG:HG2	1:FFF:212:CYS:SG	2.31	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:202:MET:O	1:AAA:206:GLN:HG2	1.89	0.70
1:BBB:130:ASN:HD22	1:BBB:133:CYS:H	1.39	0.69
1:DDD:104:VAL:CG2	1:DDD:146:VAL:HG11	2.23	0.69
1:EEE:237:SER:O	1:EEE:240:SER:OG	2.10	0.69
1:DDD:155:SER:HB3	1:DDD:197:ALA:HB2	1.74	0.68
1:DDD:101:VAL:HB	1:DDD:231:MET:HE2	1.76	0.68
1:CCC:88[A]:ARG:HG2	1:CCC:212:CYS:SG	2.34	0.68
1:FFF:202:MET:O	1:FFF:206:GLN:HG2	1.94	0.67
1:CCC:19:ALA:HA	1:CCC:60:VAL:O	1.94	0.67
1:AAA:185:GLN:NE2	5:AAA:409:HOH:O	2.26	0.66
1:BBB:155:SER:HB3	1:BBB:197:ALA:HB2	1.76	0.66
1:BBB:41:LEU:O	5:BBB:404:HOH:O	2.13	0.66
1:BBB:30:ARG:HG3	5:BBB:432:HOH:O	1.95	0.66
5:DDD:406:HOH:O	1:AAA:123:MET:HG2	1.94	0.66
1:DDD:240:SER:O	5:DDD:403:HOH:O	2.14	0.65
2:EEE:301:SO4:O1	5:EEE:402:HOH:O	2.04	0.65
1:DDD:194:MET:HG3	3:DDD:302:GOL:O1	1.96	0.64
1:CCC:55:ASP:OD1	5:CCC:304:HOH:O	2.15	0.64
1:EEE:130:ASN:HD22	1:EEE:133:CYS:H	1.46	0.64
1:DDD:122:PRO:HB2	1:DDD:124:GLU:OE1	1.97	0.64
1:CCC:108:GLN:HE21	1:CCC:151:GLY:HA2	1.61	0.64
1:CCC:3:VAL:HG13	1:CCC:81:LEU:HD21	1.80	0.63
1:AAA:129:ALA:HB3	5:AAA:403:HOH:O	1.98	0.63
1:DDD:224:GLU:OE2	5:DDD:404:HOH:O	2.14	0.63
1:EEE:159:PHE:O	1:EEE:165[B]:ARG:HD2	1.99	0.63
1:CCC:202:MET:O	1:CCC:206:GLN:HG2	1.99	0.62
1:BBB:206:GLN:HG3	5:BBB:439:HOH:O	1.99	0.62
1:DDD:182:LYS:NZ	5:DDD:408:HOH:O	2.33	0.61
1:DDD:84:ASN:C	1:DDD:84:ASN:HD22	2.07	0.61
1:CCC:84:ASN:C	1:CCC:84:ASN:HD22	2.08	0.61
1:EEE:93:GLY:HA2	1:EEE:218:VAL:O	2.01	0.60
1:DDD:19:ALA:HA	1:DDD:60:VAL:O	2.00	0.60
1:DDD:122:PRO:HD2	1:AAA:187:MET:HE1	1.81	0.60
1:BBB:93:GLY:HA2	1:BBB:218:VAL:O	2.02	0.60
1:CCC:176:ARG:NH2	5:CCC:305:HOH:O	2.28	0.60
1:AAA:137:MET:HE1	1:AAA:242:VAL:HG23	1.82	0.60
1:BBB:130:ASN:HD21	1:BBB:132:GLU:HB3	1.68	0.59
1:DDD:141:CYS:HB2	5:DDD:402:HOH:O	2.02	0.59
1:CCC:225:ILE:HG22	1:CCC:226:PRO:O	2.01	0.59
1:EEE:24:ASP:HB3	1:EEE:27:ARG:HG3	1.84	0.59
1:BBB:134:THR:O	1:BBB:138:VAL:HG23	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:130:ASN:HD21	1:CCC:132:GLU:HB3	1.67	0.58
1:EEE:76:GLU:O	1:EEE:80:GLN:HG3	2.03	0.58
1:EEE:155:SER:HB3	1:EEE:197:ALA:HB2	1.85	0.58
1:DDD:108:GLN:HE21	1:DDD:151:GLY:HA2	1.69	0.58
1:FFF:130:ASN:HD22	1:FFF:133:CYS:H	1.50	0.58
1:BBB:84:ASN:ND2	1:BBB:85:THR:OG1	2.36	0.58
1:DDD:64:THR:OG1	1:DDD:88[B]:ARG:NH1	2.37	0.58
1:DDD:103:ASP:HA	5:DDD:520:HOH:O	2.04	0.58
1:DDD:159:PHE:HE1	3:DDD:302:GOL:H2	1.69	0.57
1:AAA:130:ASN:HD22	1:AAA:133:CYS:H	1.51	0.57
1:AAA:108:GLN:HE21	1:AAA:151:GLY:HA2	1.68	0.57
1:BBB:208:TRP:CH2	5:BBB:439:HOH:O	2.52	0.57
1:DDD:122:PRO:HB2	1:DDD:124:GLU:CD	2.29	0.57
1:EEE:202:MET:O	1:EEE:206:GLN:HG2	2.05	0.56
4:FFF:301:URA:N1	2:FFF:303:SO4:O4	2.37	0.56
1:BBB:118:LEU:HD21	1:BBB:123:MET:HE2	1.87	0.56
1:DDD:104:VAL:HG22	1:DDD:146:VAL:HG11	1.86	0.56
1:CCC:75:VAL:HG13	1:CCC:86:PHE:CE1	2.41	0.56
1:BBB:54:ALA:HB1	1:BBB:247:LYS:HG2	1.88	0.56
1:BBB:208:TRP:HH2	5:BBB:439:HOH:O	1.88	0.56
1:AAA:108:GLN:NE2	5:AAA:405:HOH:O	2.21	0.56
1:AAA:4:PHE:HD2	1:AAA:5:HIS:CE1	2.24	0.56
1:DDD:41:LEU:HD11	1:DDD:51:LEU:HB2	1.88	0.55
1:AAA:178:ALA:HB1	5:AAA:536:HOH:O	2.06	0.55
1:AAA:129:ALA:O	5:AAA:403:HOH:O	2.18	0.55
1:BBB:83:VAL:HG12	1:BBB:86:PHE:CZ	2.41	0.55
1:FFF:8:LEU:HD21	1:FFF:49:SER:OG	2.05	0.55
1:FFF:19:ALA:HB2	1:FFF:60:VAL:CG1	2.36	0.55
1:FFF:193:GLU:HB2	2:FFF:303:SO4:O2	2.07	0.55
1:EEE:84:ASN:C	1:EEE:84:ASN:HD22	2.14	0.55
1:FFF:143:ASP:OD2	1:FFF:248:LYS:NZ	2.22	0.55
1:AAA:84:ASN:ND2	1:AAA:85:THR:OG1	2.39	0.54
1:CCC:118:LEU:HD21	1:CCC:123:MET:HE2	1.89	0.54
1:DDD:130:ASN:HD21	1:DDD:132:GLU:HB3	1.73	0.54
1:DDD:130:ASN:HD22	1:DDD:133:CYS:N	2.05	0.54
1:FFF:16:ALA:HB2	1:FFF:58:PRO:HB2	1.90	0.54
1:FFF:122:PRO:HB2	1:FFF:124:GLU:CD	2.33	0.54
1:AAA:92:THR:HA	3:AAA:302:GOL:O2	2.08	0.53
1:DDD:101:VAL:O	1:DDD:231:MET:CE	2.57	0.53
1:CCC:27:ARG:HG3	5:CCC:406:HOH:O	2.08	0.53
1:DDD:181:MET:O	1:DDD:185:GLN:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:84:ASN:C	1:BBB:84:ASN:HD22	2.17	0.53
1:DDD:159:PHE:CE1	3:DDD:302:GOL:H2	2.45	0.52
1:AAA:84:ASN:C	1:AAA:84:ASN:HD22	2.17	0.52
1:DDD:73:ILE:HD11	1:CCC:159:PHE:HB2	1.91	0.52
1:FFF:16:ALA:O	5:FFF:401:HOH:O	2.18	0.52
1:FFF:19:ALA:HB2	1:FFF:60:VAL:HG13	1.92	0.52
1:DDD:88[B]:ARG:HG2	1:DDD:212:CYS:SG	2.49	0.52
1:EEE:12:MET:HB3	1:EEE:41:LEU:HD22	1.92	0.52
1:AAA:47:TYR:O	5:AAA:404:HOH:O	2.19	0.51
1:EEE:164:GLU:O	1:EEE:164:GLU:HG2	2.09	0.51
1:AAA:118:LEU:HD21	1:AAA:123:MET:HE2	1.92	0.51
1:DDD:124:GLU:OE2	5:DDD:406:HOH:O	2.18	0.51
1:AAA:183:GLU:O	1:AAA:187:MET:HG3	2.11	0.51
1:CCC:158:THR:C	1:CCC:194:MET:HE3	2.36	0.51
1:DDD:163:GLN:OE1	3:DDD:302:GOL:O2	2.21	0.50
1:CCC:237:SER:O	1:CCC:241:ILE:HG13	2.11	0.50
1:AAA:161:PRO:HG3	1:BBB:120:PHE:CE1	2.46	0.50
1:FFF:88[B]:ARG:HG2	1:FFF:212:CYS:SG	2.51	0.50
1:CCC:23:GLY:HA3	5:CCC:318:HOH:O	2.10	0.50
1:CCC:24:ASP:C	1:CCC:24:ASP:OD1	2.52	0.50
1:AAA:3:VAL:HG13	1:AAA:81:LEU:HD21	1.93	0.50
1:FFF:10:LYS:NZ	5:FFF:412:HOH:O	2.45	0.50
1:FFF:83:VAL:HG12	1:FFF:86:PHE:CZ	2.46	0.49
1:FFF:47:TYR:CE1	1:FFF:74:ALA:HB2	2.47	0.49
1:DDD:112:ARG:HD2	1:DDD:127:ALA:HB2	1.94	0.48
1:DDD:225:ILE:HG23	1:DDD:226:PRO:HD2	1.95	0.48
1:FFF:160:TYR:CB	1:FFF:161:PRO:CD	2.91	0.48
1:FFF:25:PRO:HA	1:FFF:48[B]:THR:HG22	1.95	0.48
1:FFF:72:SER:HA	1:FFF:202:MET:SD	2.54	0.48
1:FFF:160:TYR:HB2	1:FFF:161:PRO:CD	2.44	0.48
1:FFF:84:ASN:C	1:FFF:84:ASN:HD22	2.21	0.48
1:AAA:108:GLN:NE2	1:AAA:151:GLY:HA2	2.29	0.48
1:BBB:29:LYS:HB2	1:BBB:50:TYR:CZ	2.49	0.48
1:BBB:64:THR:HG1	1:BBB:88:ARG:HH12	1.60	0.48
1:DDD:104:VAL:HG21	1:DDD:146:VAL:HG11	1.96	0.48
1:DDD:46:GLU:HB3	1:CCC:46:GLU:HB3	1.95	0.48
1:CCC:18:LEU:C	1:CCC:18:LEU:HD23	2.39	0.47
1:FFF:122:PRO:HD2	1:CCC:187[A]:MET:HE1	1.96	0.47
1:DDD:30:ARG:NH1	5:DDD:417:HOH:O	2.46	0.47
1:CCC:67:GLY:HA2	1:CCC:194:MET:O	2.13	0.47
1:FFF:195:GLU:OE1	2:FFF:303:SO4:S	2.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:146:VAL:HG23	1:CCC:236:VAL:HG21	1.97	0.47
1:BBB:202:MET:O	1:BBB:206:GLN:HG2	2.15	0.47
1:FFF:19:ALA:CB	1:FFF:60:VAL:HG13	2.45	0.47
1:DDD:124:GLU:N	5:DDD:406:HOH:O	2.48	0.46
1:CCC:75:VAL:HG13	1:CCC:86:PHE:CD1	2.49	0.46
1:BBB:8:LEU:CD2	1:BBB:12:MET:HE2	2.45	0.46
1:BBB:124:GLU:H	1:BBB:124:GLU:CD	2.22	0.46
1:FFF:67:GLY:HA2	1:FFF:194:MET:O	2.16	0.46
1:BBB:14:ASP:OD2	1:BBB:53:TYR:OH	2.25	0.46
1:BBB:176:ARG:HG2	1:BBB:177:PHE:CD2	2.51	0.46
1:AAA:18:LEU:HD23	1:AAA:18:LEU:C	2.40	0.46
1:AAA:13:LEU:HD22	1:AAA:81:LEU:HB3	1.98	0.46
1:EEE:154:ALA:O	1:EEE:192:TYR:HA	2.16	0.46
1:CCC:137:MET:HE1	1:CCC:242:VAL:HG23	1.97	0.46
1:AAA:236:VAL:O	1:AAA:240:SER:HB3	2.15	0.46
1:DDD:84:ASN:C	1:DDD:84:ASN:ND2	2.74	0.45
1:DDD:193:GLU:HA	3:DDD:302:GOL:H12	1.98	0.45
1:CCC:83:VAL:HG12	1:CCC:86:PHE:CZ	2.51	0.45
1:CCC:84:ASN:ND2	1:CCC:85:THR:OG1	2.49	0.45
1:DDD:29:LYS:HE3	1:DDD:33:GLU:OE2	2.17	0.45
1:FFF:195:GLU:OE2	2:FFF:303:SO4:O3	2.35	0.45
1:EEE:32:ALA:HB2	1:EEE:61:ILE:HD13	1.97	0.45
1:DDD:27:ARG:O	1:DDD:31:ILE:HG13	2.17	0.45
1:DDD:31:ILE:HA	1:DDD:34:LEU:HD12	1.99	0.45
1:EEE:8:LEU:HD23	1:EEE:12:MET:HE1	1.98	0.45
1:DDD:206:GLN:NE2	1:CCC:170:THR:OG1	2.49	0.45
1:CCC:247:LYS:O	1:CCC:248:LYS:C	2.60	0.45
1:BBB:16:ALA:HB2	1:BBB:58:PRO:HB2	1.99	0.45
1:FFF:237:SER:O	1:FFF:241:ILE:HG13	2.17	0.45
1:AAA:76:GLU:O	1:AAA:80:GLN:HG3	2.17	0.45
1:AAA:158:THR:C	1:AAA:194[A]:MET:HE3	2.42	0.45
1:AAA:160:TYR:HB2	1:AAA:161:PRO:HD3	1.99	0.45
1:CCC:27:ARG:CD	1:CCC:31:ILE:HD11	2.47	0.45
1:CCC:143:ASP:OD2	1:CCC:248:LYS:NZ	2.44	0.45
1:EEE:163:GLN:HG2	1:EEE:192:TYR:CG	2.52	0.45
1:AAA:130:ASN:ND2	1:AAA:133:CYS:H	2.14	0.44
1:CCC:159:PHE:HD2	1:CCC:160:TYR:CE2	2.36	0.44
1:CCC:96:GLN:HB3	1:CCC:98:HIS:CE1	2.52	0.44
1:DDD:21:VAL:HA	1:DDD:62:CYS:O	2.18	0.44
1:DDD:138:VAL:HG21	1:AAA:131:PHE:CE2	2.52	0.44
1:FFF:88[A]:ARG:NH2	5:FFF:419:HOH:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:237:SER:O	1:EEE:241:ILE:HG13	2.17	0.44
1:AAA:66:ILE:HG23	1:AAA:194[B]:MET:HG2	1.99	0.44
1:AAA:72:SER:HA	1:AAA:202:MET:SD	2.57	0.44
1:AAA:182:LYS:HA	1:AAA:185:GLN:OE1	2.18	0.44
1:EEE:88:ARG:NH2	5:EEE:413:HOH:O	2.44	0.44
1:EEE:132:GLU:OE1	1:EEE:209:ARG:NH1	2.51	0.44
1:BBB:8:LEU:HD13	1:BBB:13:LEU:HD11	2.00	0.44
1:BBB:8:LEU:HD22	1:BBB:12:MET:HE2	2.00	0.44
1:FFF:167:ASP:O	1:FFF:167:ASP:OD2	2.35	0.44
1:BBB:45:ARG:NH1	5:BBB:409:HOH:O	2.43	0.44
1:DDD:19:ALA:HB2	1:DDD:60:VAL:HG13	1.98	0.43
1:FFF:44:HIS:HB3	5:FFF:416:HOH:O	2.16	0.43
1:FFF:76:GLU:O	1:FFF:80:GLN:HG3	2.18	0.43
1:EEE:19:ALA:HA	1:EEE:60:VAL:O	2.18	0.43
1:DDD:228:GLU:HG3	5:DDD:503:HOH:O	2.18	0.43
1:FFF:86:PHE:O	1:FFF:210:ALA:HA	2.17	0.43
1:FFF:22:PRO:O	1:FFF:63:SER:HA	2.18	0.43
1:AAA:92:THR:OG1	1:AAA:191:ASN:HB2	2.18	0.43
1:DDD:148:PRO:HD3	5:DDD:402:HOH:O	2.18	0.43
1:AAA:180:SER:O	1:AAA:183:GLU:HB2	2.17	0.43
1:CCC:3:VAL:CG1	1:CCC:81:LEU:HD21	2.48	0.43
1:BBB:102:GLY:HA2	1:BBB:234:THR:HG21	2.01	0.43
1:FFF:177:PHE:CE2	1:EEE:119:HIS:CD2	3.06	0.43
1:CCC:19:ALA:HB2	1:CCC:60:VAL:HG13	1.99	0.43
1:DDD:98:HIS:HB3	5:DDD:525:HOH:O	2.18	0.43
1:FFF:21:VAL:HA	1:FFF:62:CYS:O	2.18	0.43
1:AAA:176:ARG:HD3	1:AAA:177:PHE:CE2	2.54	0.43
1:CCC:46:GLU:HG3	1:CCC:65:GLY:HA3	2.01	0.42
1:FFF:155:SER:HB3	1:FFF:197:ALA:HB2	2.01	0.42
1:DDD:76:GLU:O	1:DDD:80:GLN:HG3	2.19	0.42
1:DDD:114:ASP:OD2	1:DDD:117:SER:HB3	2.19	0.42
1:FFF:34:LEU:CD1	1:FFF:239:VAL:HG12	2.49	0.42
1:DDD:194:MET:CG	3:DDD:302:GOL:O1	2.66	0.42
1:FFF:18:LEU:HD23	1:FFF:18:LEU:C	2.45	0.42
1:FFF:46:GLU:HB3	1:EEE:46:GLU:HB3	2.01	0.42
1:EEE:6:LEU:HD23	1:EEE:6:LEU:N	2.33	0.42
1:AAA:159:PHE:HB2	1:BBB:73:ILE:HD11	2.00	0.42
1:CCC:181:MET:O	1:CCC:185:GLN:HG3	2.20	0.42
1:CCC:88[A]:ARG:NH2	1:CCC:193:GLU:OE2	2.52	0.42
1:DDD:48:THR:O	1:DDD:62:CYS:HA	2.20	0.42
1:FFF:166:TYR:O	1:FFF:171:GLY:HA2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FFF:69:PRO:HA	1:EEE:157:ASP:O	2.20	0.41
1:BBB:234:THR:HG23	5:BBB:507:HOH:O	2.19	0.41
1:EEE:2:ASP:OD1	1:EEE:9:THR:HG22	2.20	0.41
1:EEE:122:PRO:HB2	1:EEE:124:GLU:CD	2.45	0.41
1:EEE:180:SER:O	1:EEE:183:GLU:HB2	2.20	0.41
1:CCC:130:ASN:ND2	1:CCC:133:CYS:H	2.13	0.41
1:BBB:61:ILE:N	1:BBB:61:ILE:HD12	2.35	0.41
1:BBB:10:LYS:HE3	5:BBB:497:HOH:O	2.20	0.41
1:BBB:130:ASN:ND2	1:BBB:132:GLU:HB3	2.34	0.41
1:FFF:160:TYR:OH	1:EEE:77:GLU:OE2	2.26	0.41
1:AAA:68:GLY:N	1:AAA:69:PRO:CD	2.83	0.41
1:BBB:112:ARG:HD2	1:BBB:127:ALA:HB2	2.02	0.41
1:DDD:104:VAL:CG2	1:DDD:146:VAL:CG1	2.97	0.41
1:AAA:187:MET:HE2	5:CCC:363:HOH:O	2.20	0.41
1:BBB:57:LYS:HD2	1:BBB:250:LEU:HB3	2.03	0.41
1:FFF:134[B]:THR:OG1	1:FFF:135:THR:N	2.54	0.41
1:AAA:8:LEU:CD2	1:AAA:12:MET:HE2	2.51	0.41
1:AAA:49:SER:HA	1:AAA:61:ILE:O	2.21	0.41
1:EEE:8:LEU:HD23	1:EEE:12:MET:CE	2.50	0.41
1:BBB:37:ASN:ND2	5:BBB:415:HOH:O	2.53	0.41
1:BBB:247:LYS:O	1:BBB:248:LYS:C	2.64	0.41
1:AAA:250:LEU:O	1:AAA:251:ALA:C	2.63	0.40
1:EEE:18:LEU:HD12	1:EEE:85:THR:HG21	2.01	0.40
1:FFF:118:LEU:HD21	1:FFF:123:MET:HE2	2.03	0.40
1:CCC:72:SER:HA	1:CCC:202:MET:SD	2.62	0.40
1:CCC:165:ARG:NH2	1:CCC:224:GLU:O	2.53	0.40
1:EEE:21:VAL:HA	1:EEE:62:CYS:O	2.22	0.40
1:EEE:175:ARG:O	1:EEE:176:ARG:C	2.63	0.40
1:BBB:195:GLU:OE1	5:BBB:405:HOH:O	2.21	0.40
5:DDD:487:HOH:O	1:AAA:126:PRO:HB3	2.22	0.40
1:FFF:78:LEU:O	1:FFF:81:LEU:N	2.51	0.40
1:FFF:130:ASN:HD21	1:FFF:132:GLU:HB3	1.86	0.40
1:AAA:71:THR:O	1:AAA:75:VAL:HG23	2.21	0.40
1:AAA:77:GLU:O	1:AAA:81:LEU:HG	2.21	0.40
1:AAA:236:VAL:N	5:AAA:427:HOH:O	2.55	0.40
1:DDD:218:VAL:HG22	1:DDD:219:ASN:N	2.37	0.40
1:AAA:202:MET:O	1:AAA:206:GLN:CG	2.63	0.40
1:BBB:64:THR:OG1	1:BBB:88:ARG:NH1	2.39	0.40
1:DDD:19:ALA:CB	1:DDD:60:VAL:HG13	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:228:GLU:OE1	1:BBB:185:GLN:HE21[2_646]	1.51	0.09

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	AAA	243/251 (97%)	235 (97%)	7 (3%)	1 (0%)	30	15
1	BBB	236/251 (94%)	226 (96%)	9 (4%)	1 (0%)	30	15
1	CCC	248/251 (99%)	236 (95%)	11 (4%)	1 (0%)	30	15
1	DDD	251/251 (100%)	242 (96%)	6 (2%)	3 (1%)	10	2
1	EEE	239/251 (95%)	226 (95%)	12 (5%)	1 (0%)	30	15
1	FFF	243/251 (97%)	234 (96%)	8 (3%)	1 (0%)	30	15
All	All	1460/1506 (97%)	1399 (96%)	53 (4%)	8 (0%)	21	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	160	TYR
1	DDD	235	GLU
1	FFF	160	TYR
1	AAA	160	TYR
1	CCC	160	TYR
1	EEE	160	TYR
1	BBB	160	TYR
1	DDD	233	LYS

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	AAA	191/197 (97%)	182 (95%)	9 (5%)	23	5
1	BBB	185/197 (94%)	176 (95%)	9 (5%)	22	5
1	CCC	195/197 (99%)	190 (97%)	5 (3%)	40	17
1	DDD	195/197 (99%)	188 (96%)	7 (4%)	31	9
1	EEE	187/197 (95%)	185 (99%)	2 (1%)	65	48
1	FFF	193/197 (98%)	187 (97%)	6 (3%)	35	12
All	All	1146/1182 (97%)	1108 (97%)	38 (3%)	36	11

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	13	LEU
1	DDD	39	THR
1	DDD	84	ASN
1	DDD	88[A]	ARG
1	DDD	88[B]	ARG
1	DDD	193	GLU
1	DDD	231	MET
1	FFF	84	ASN
1	FFF	88[A]	ARG
1	FFF	88[B]	ARG
1	FFF	193	GLU
1	FFF	237	SER
1	FFF	250	LEU
1	AAA	22	PRO
1	AAA	27	ARG
1	AAA	84	ASN
1	AAA	88[A]	ARG
1	AAA	88[B]	ARG
1	AAA	126	PRO
1	AAA	193	GLU
1	AAA	237	SER
1	AAA	240	SER
1	CCC	30	ARG
1	CCC	84	ASN
1	CCC	88[A]	ARG
1	CCC	88[B]	ARG
1	CCC	193	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	EEE	84	ASN
1	EEE	193	GLU
1	BBB	29	LYS
1	BBB	30	ARG
1	BBB	39	THR
1	BBB	57	LYS
1	BBB	84	ASN
1	BBB	88	ARG
1	BBB	91	SER
1	BBB	193	GLU
1	BBB	234	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

11 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
3	GOL	AAA	302	-	5,5,5	0.20	0	5,5,5	0.66	0
3	GOL	DDD	302	-	5,5,5	0.52	0	5,5,5	0.41	0
2	SO4	AAA	301	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	DDD	301	-	4,4,4	0.26	0	6,6,6	0.50	0
2	SO4	FFF	303	-	4,4,4	0.55	0	6,6,6	0.35	0
2	SO4	EEE	301	-	4,4,4	1.45	1 (25%)	6,6,6	1.21	0
2	SO4	BBB	302	-	4,4,4	0.34	0	6,6,6	0.12	0
4	URA	FFF	301	-	8,8,8	0.97	0	10,10,10	1.69	2 (20%)
2	SO4	BBB	301[A]	-	4,4,4	0.71	0	6,6,6	0.36	0
2	SO4	BBB	301[B]	-	4,4,4	0.50	0	6,6,6	0.45	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	GOL	AAA	302	-	-	4/4/4/4	-
3	GOL	DDD	302	-	-	1/4/4/4	-
4	URA	FFF	301	-	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EEE	301	SO4	O1-S	-2.14	1.32	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	FFF	301	URA	O2-C2-N1	3.09	125.97	122.79
4	FFF	301	URA	O4-C4-N3	-2.89	115.08	119.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	302	GOL	O1-C1-C2-C3
3	AAA	302	GOL	C1-C2-C3-O3
3	AAA	302	GOL	O1-C1-C2-O2
3	AAA	302	GOL	O2-C2-C3-O3
3	DDD	302	GOL	O1-C1-C2-O2

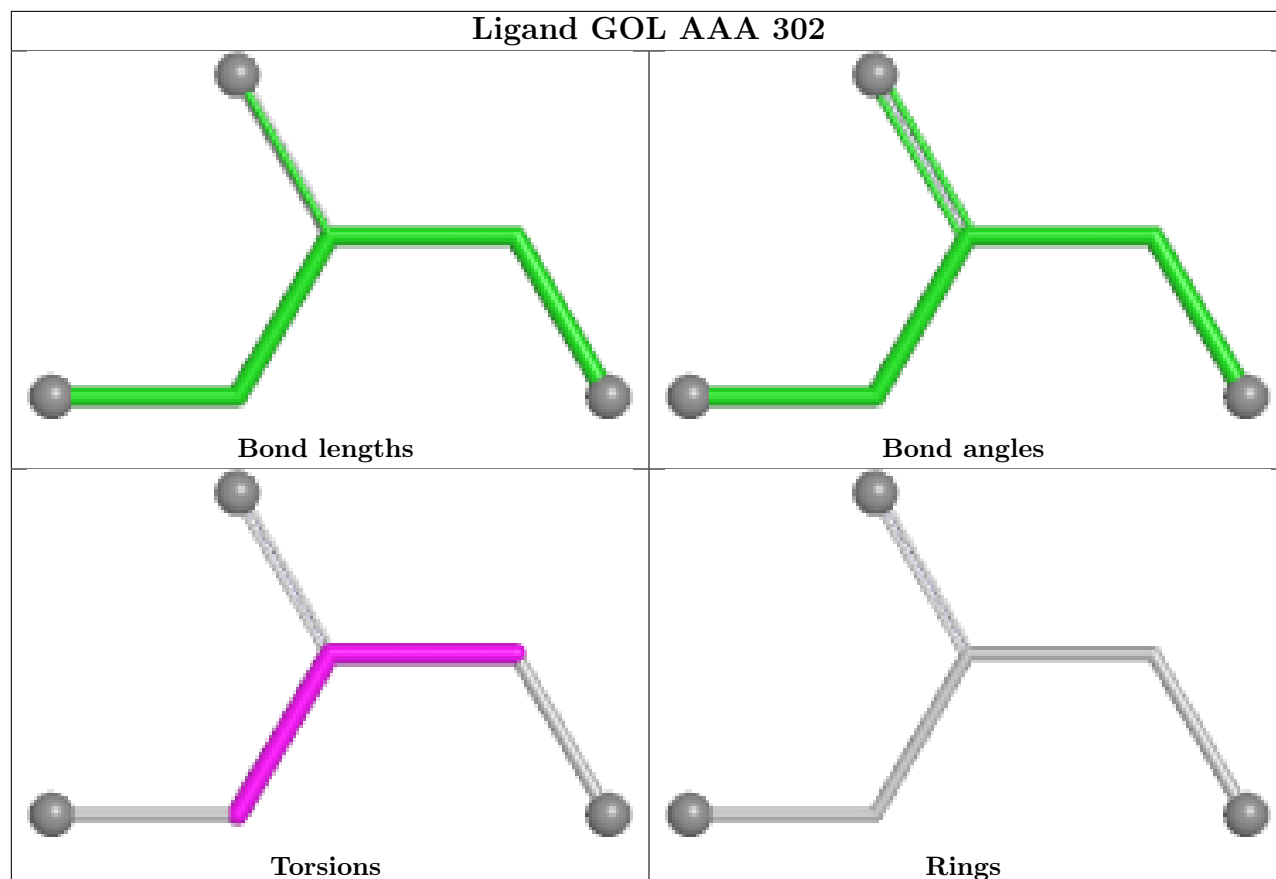
There are no ring outliers.

6 monomers are involved in 15 short contacts:

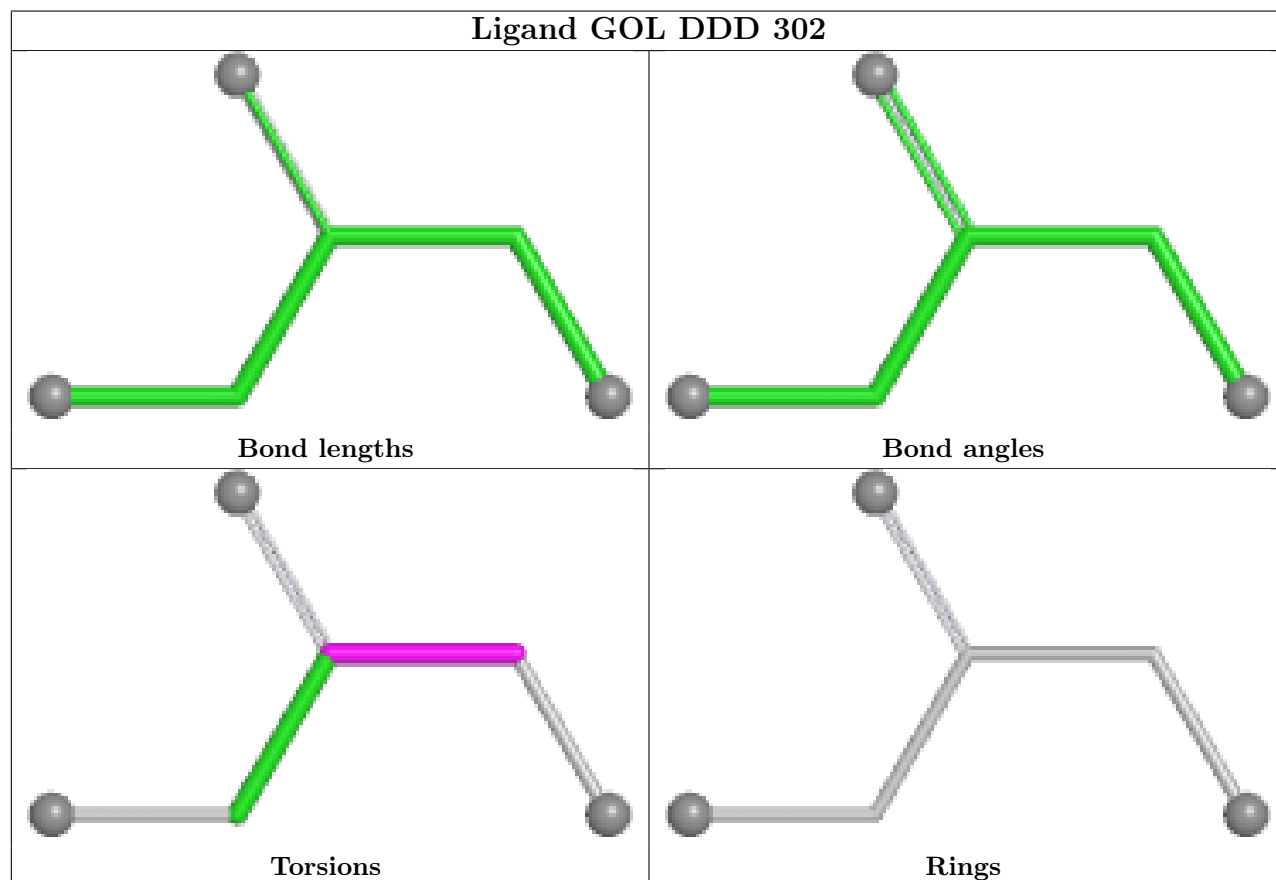
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	302	GOL	1	0
3	DDD	302	GOL	6	0
2	FFF	303	SO4	5	0
2	EEE	301	SO4	2	0
4	FFF	301	URA	1	0
2	BBB	301[A]	SO4	1	0

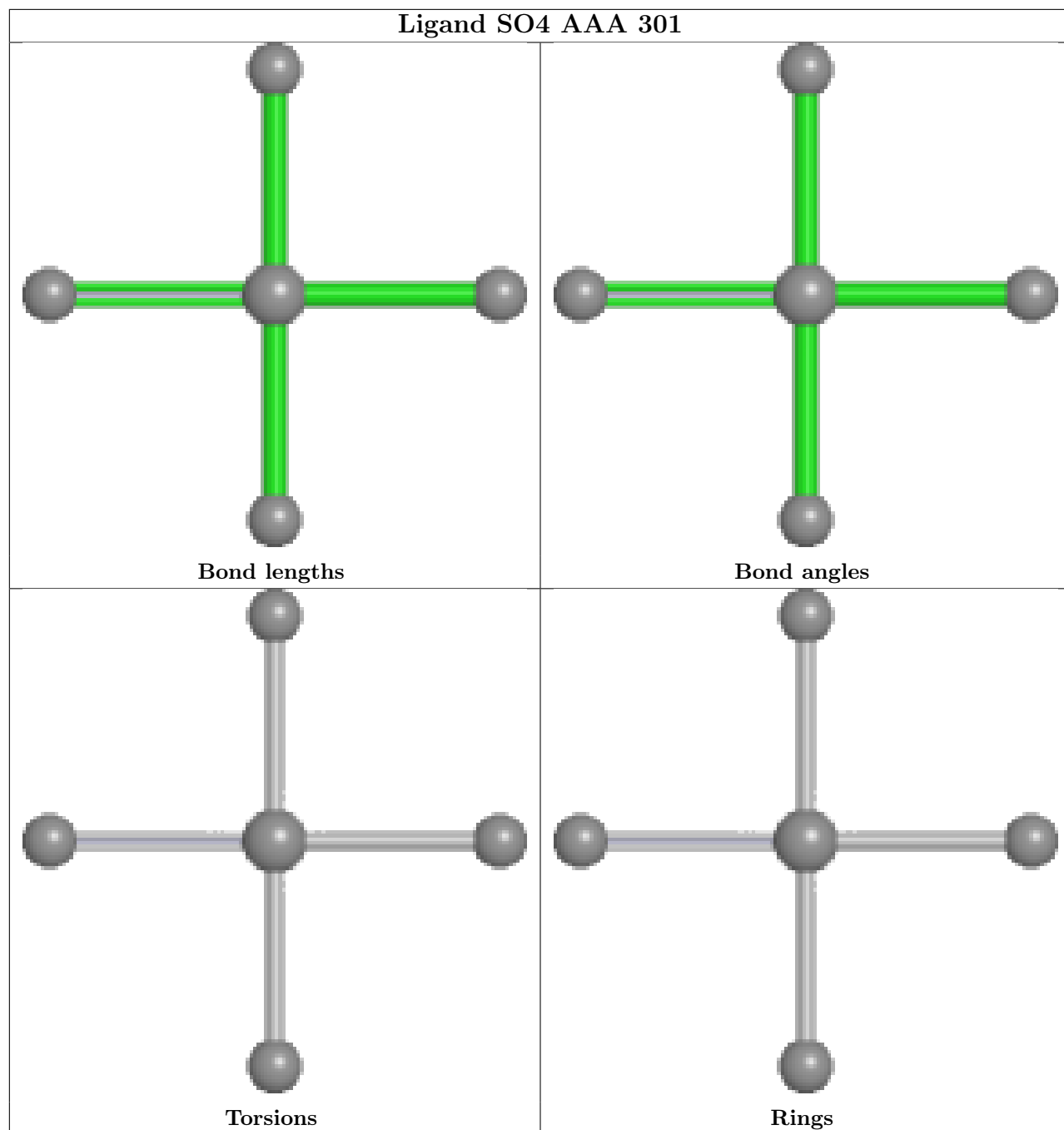
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

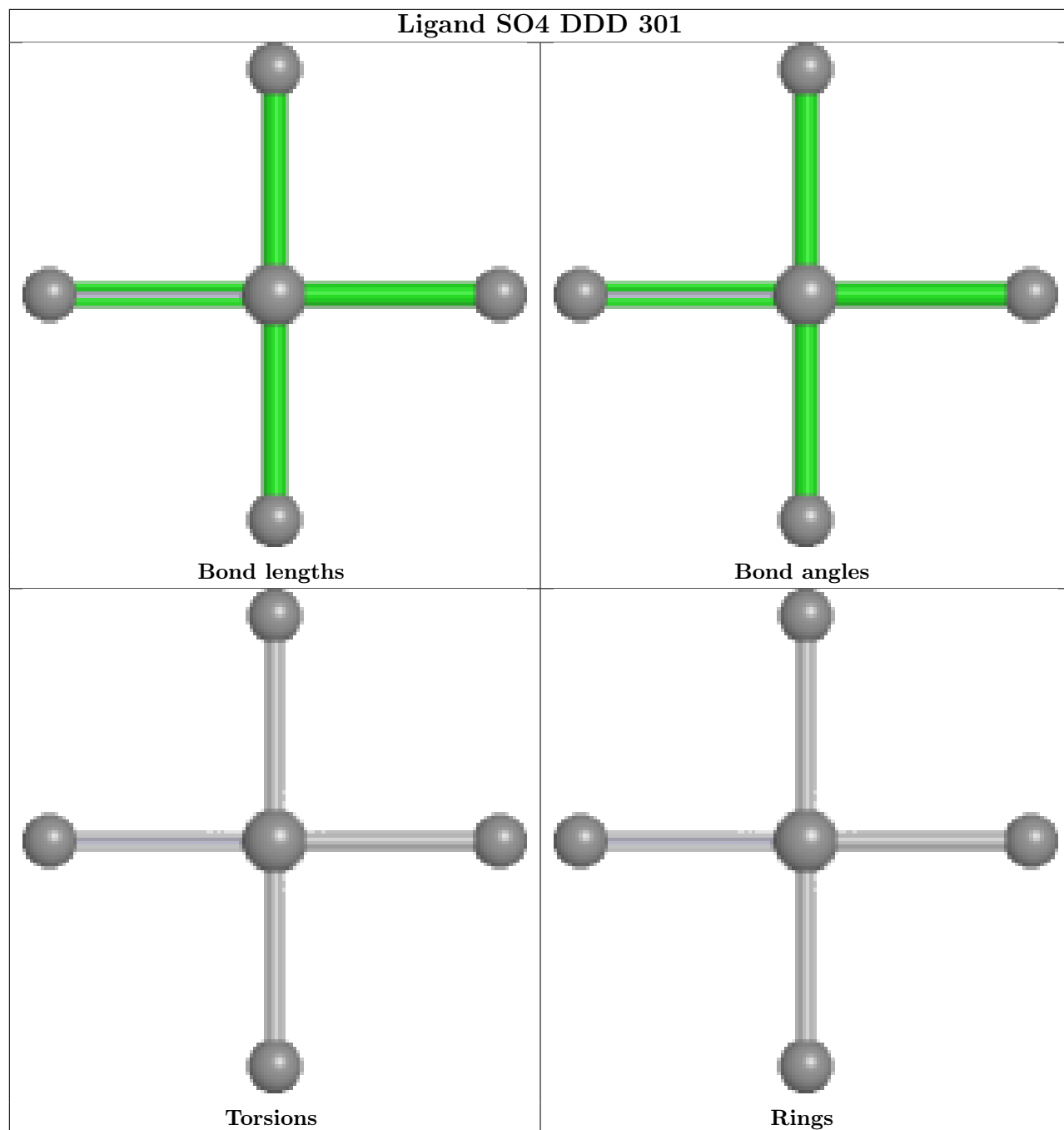
Ligand GOL AAA 302

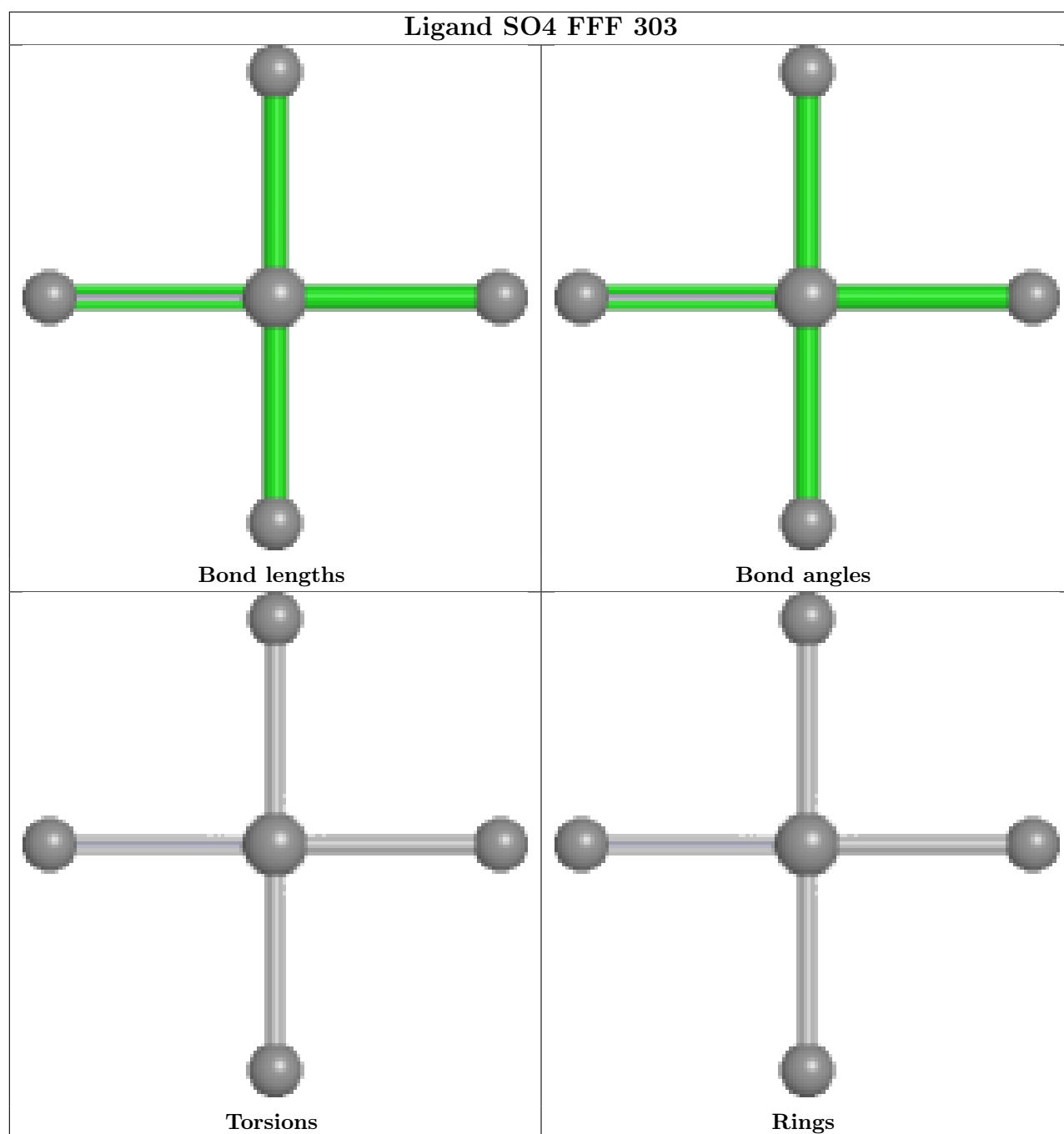


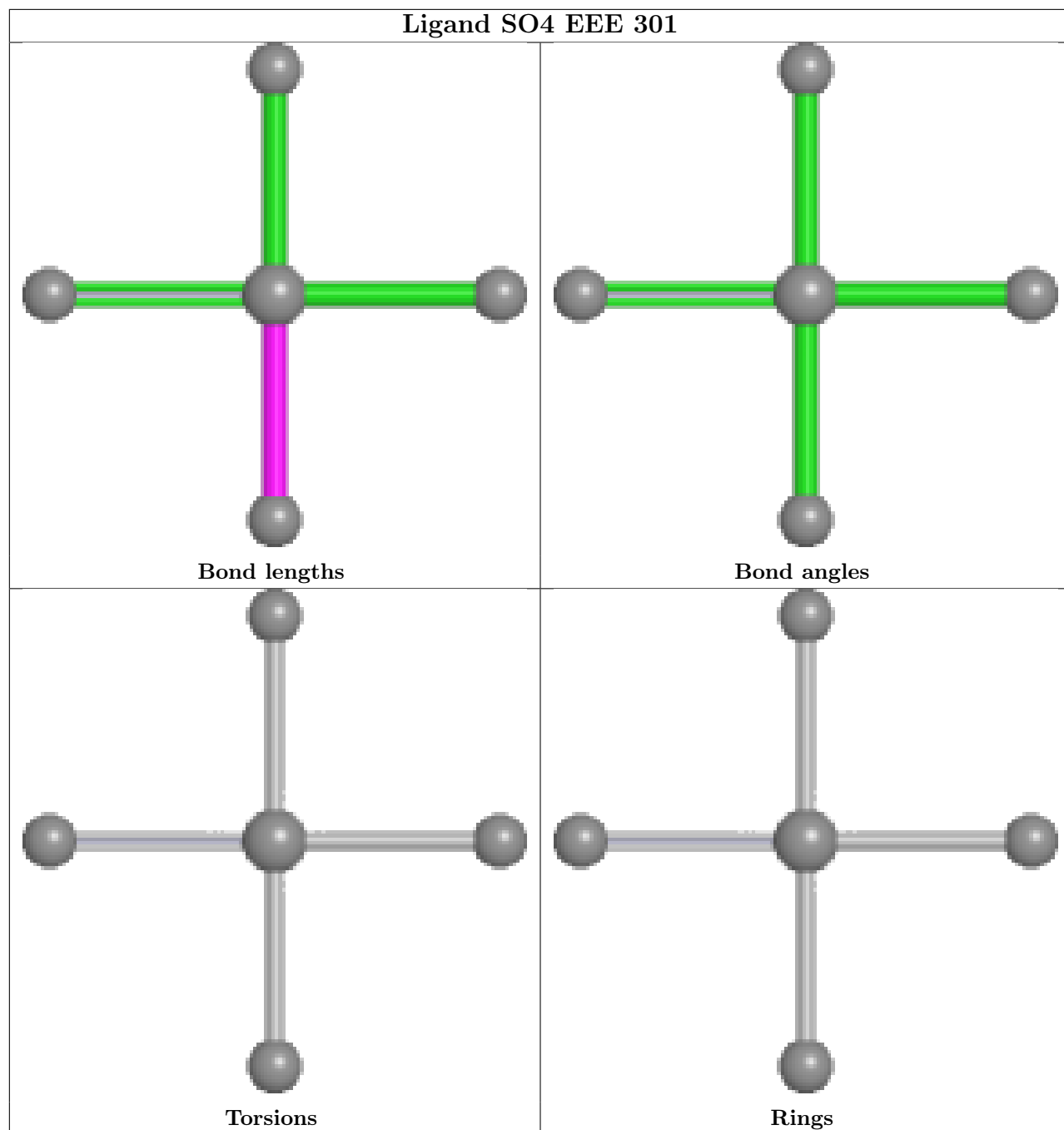
Ligand GOL DDD 302

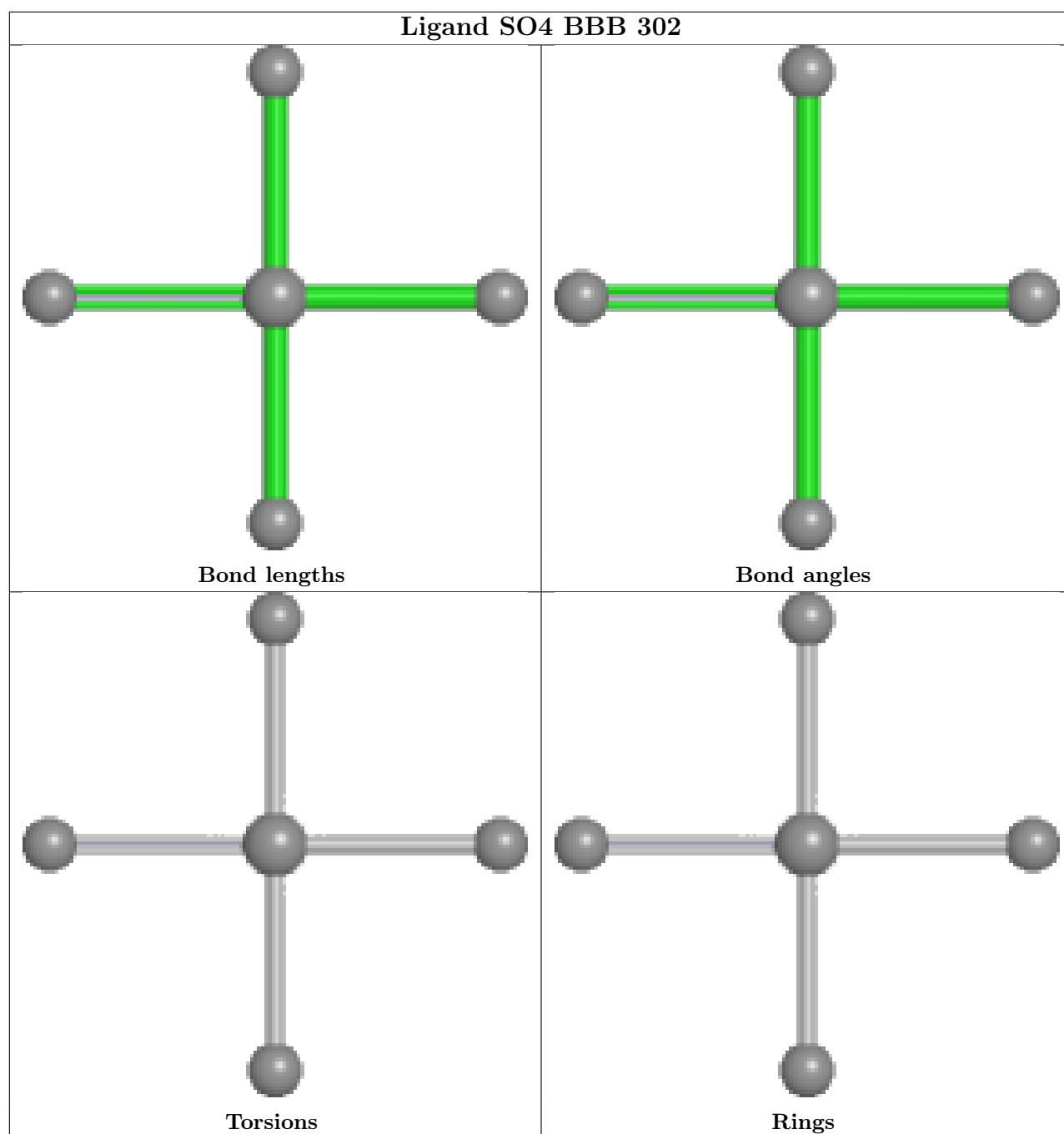


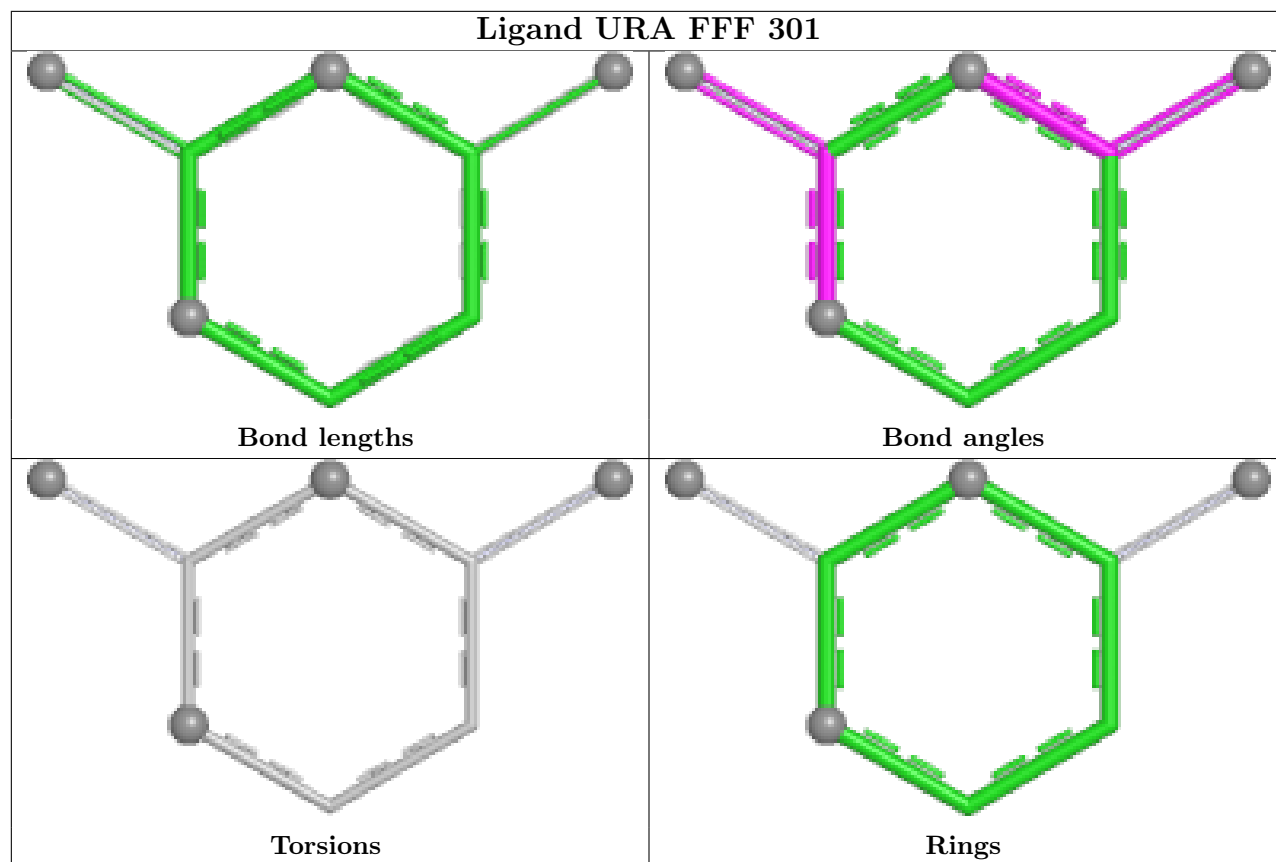


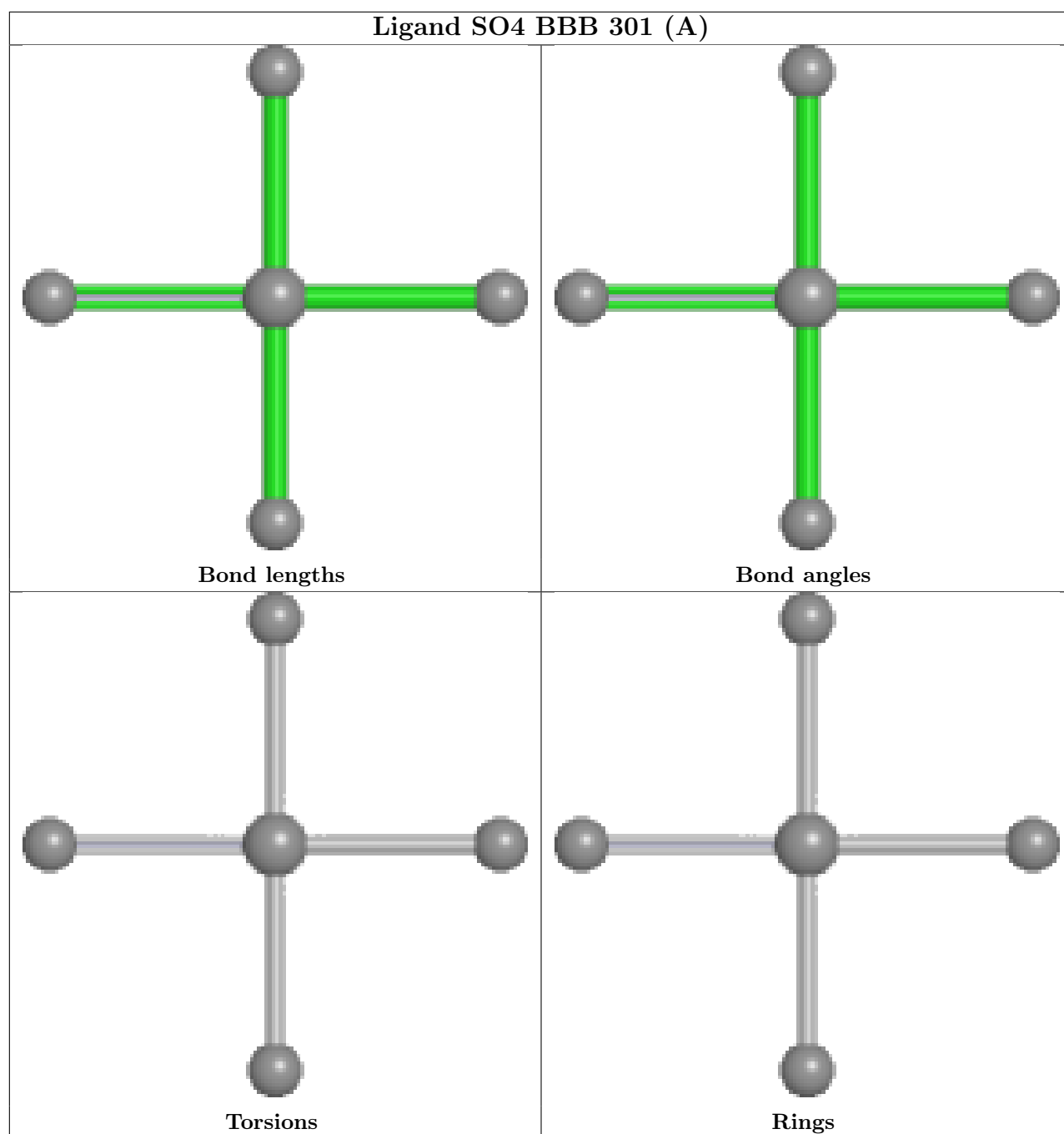


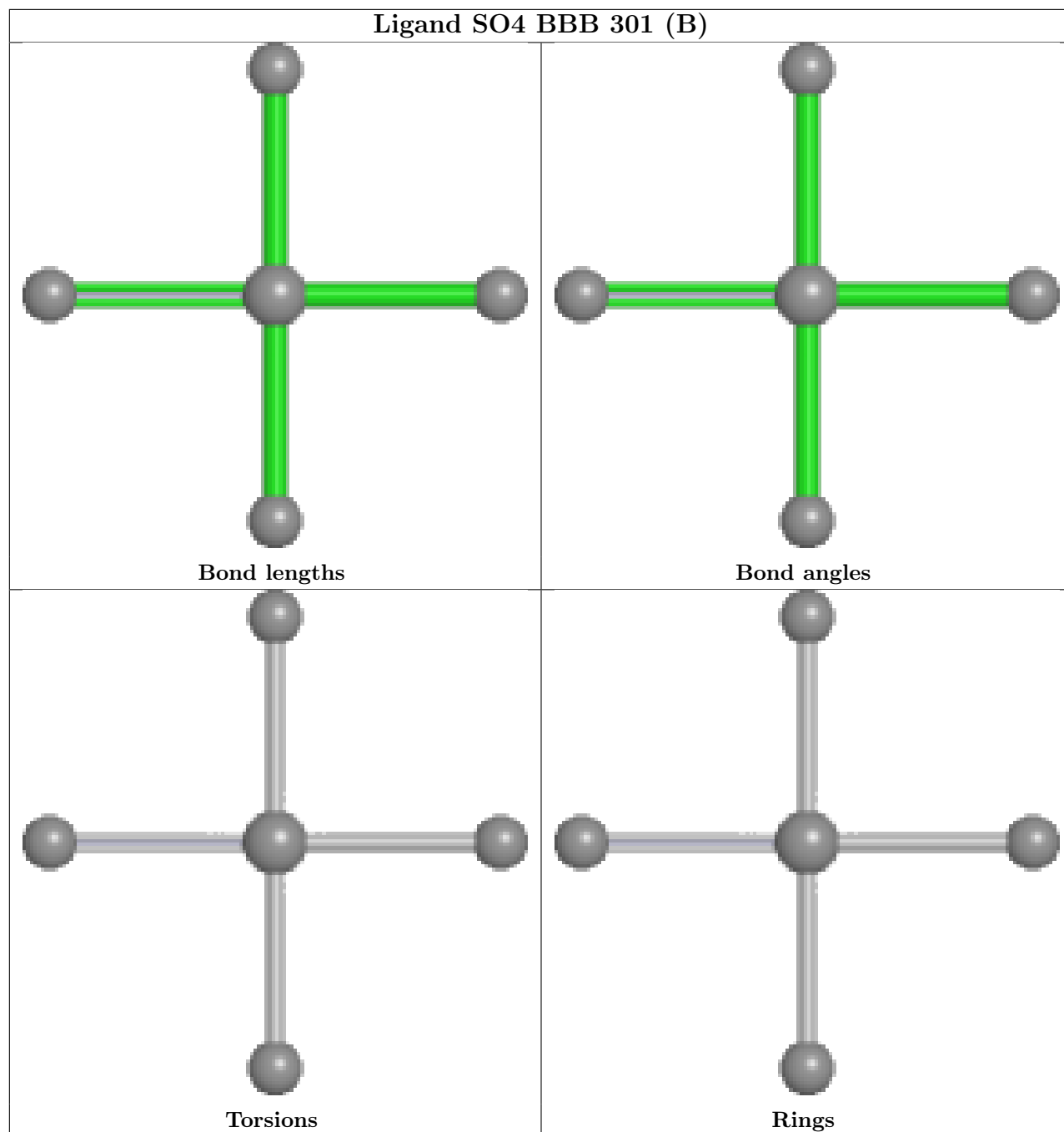












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	245/251 (97%)	-0.82	0 100 100	8, 17, 29, 51	2 (0%)
1	BBB	240/251 (95%)	-0.82	0 100 100	10, 17, 27, 38	0
1	CCC	250/251 (99%)	-0.88	0 100 100	8, 16, 26, 47	2 (0%)
1	DDD	251/251 (100%)	-0.85	0 100 100	9, 17, 28, 45	2 (0%)
1	EEE	242/251 (96%)	-0.86	0 100 100	10, 17, 27, 41	1 (0%)
1	FFF	244/251 (97%)	-0.83	0 100 100	7, 18, 31, 48	3 (1%)
All	All	1472/1506 (97%)	-0.84	0 100 100	7, 17, 28, 51	10 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	AAA	301	5/5	0.97	0.06	35,40,46,52	0

Continued on next page...

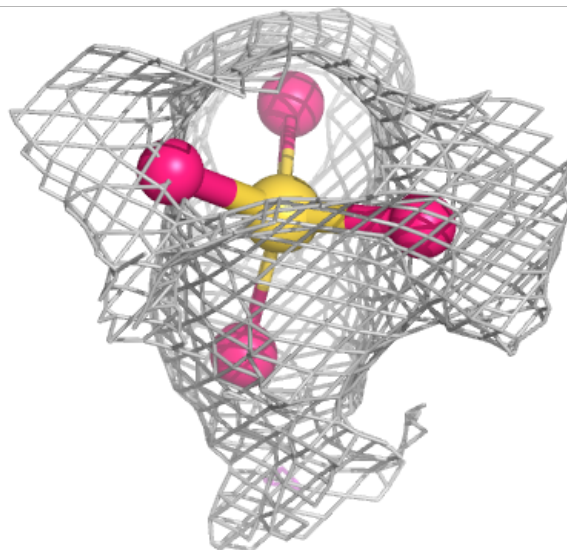
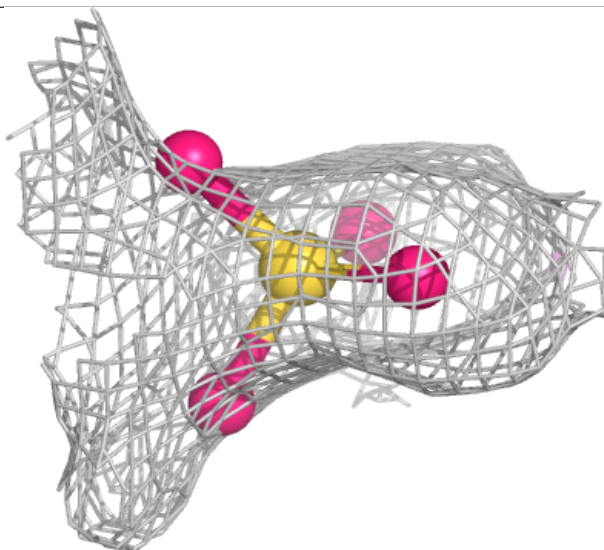
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	BBB	302	5/5	0.97	0.05	33,38,41,41	0
2	SO4	DDD	301	5/5	0.98	0.05	25,26,34,36	0
2	SO4	FFF	302[A]	5/5	0.98	0.07	21,22,23,30	5
3	GOL	AAA	302	6/6	0.98	0.05	19,23,29,29	2
4	URA	FFF	301	8/8	0.98	0.05	22,28,30,30	0
2	SO4	BBB	301[B]	5/5	0.99	0.04	8,9,10,11	5
2	SO4	FFF	303	5/5	0.99	0.06	15,16,19,20	5
3	GOL	DDD	302	6/6	0.99	0.05	15,19,24,27	2
2	SO4	EEE	301	5/5	0.99	0.05	11,14,18,20	0
2	SO4	BBB	301[A]	5/5	0.99	0.04	8,9,10,11	5

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.

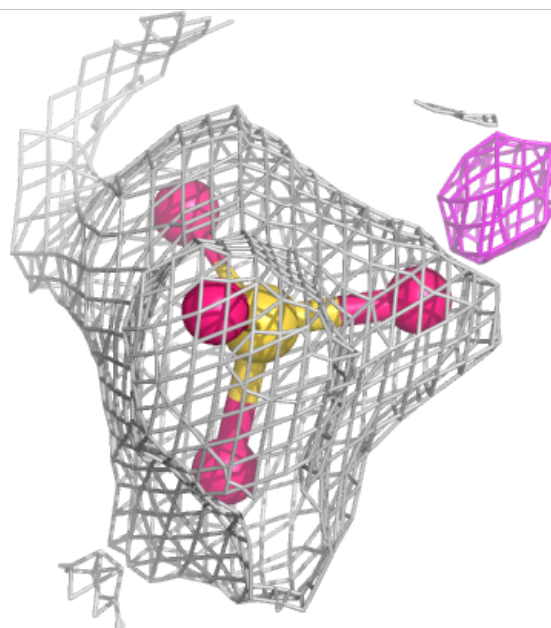
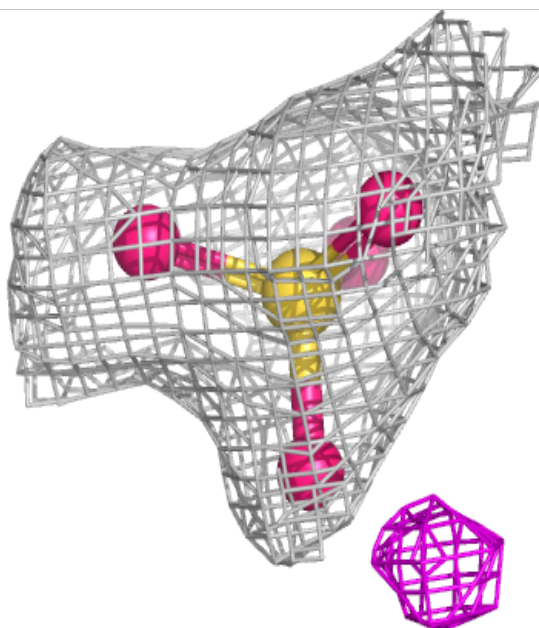
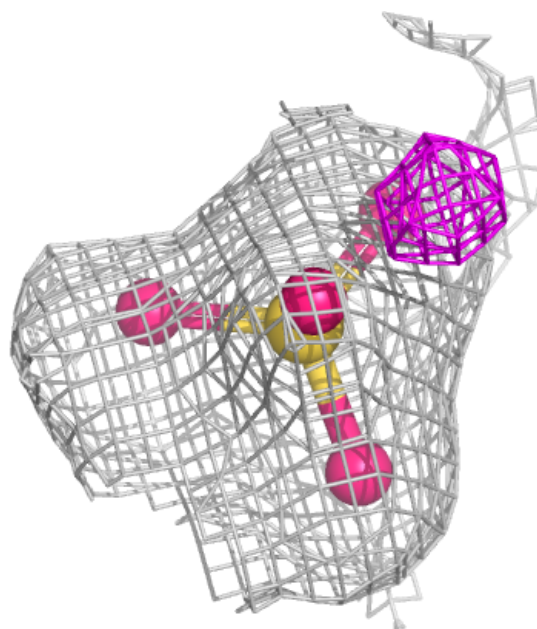
Electron density around SO4 AAA 301:

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



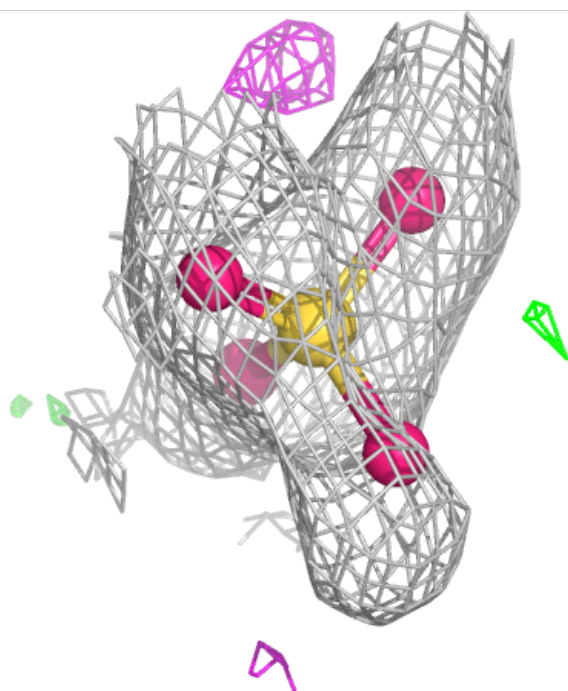
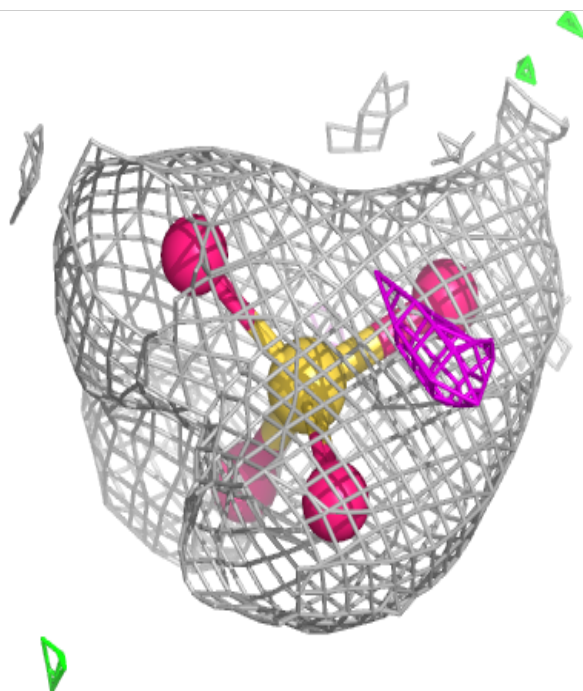
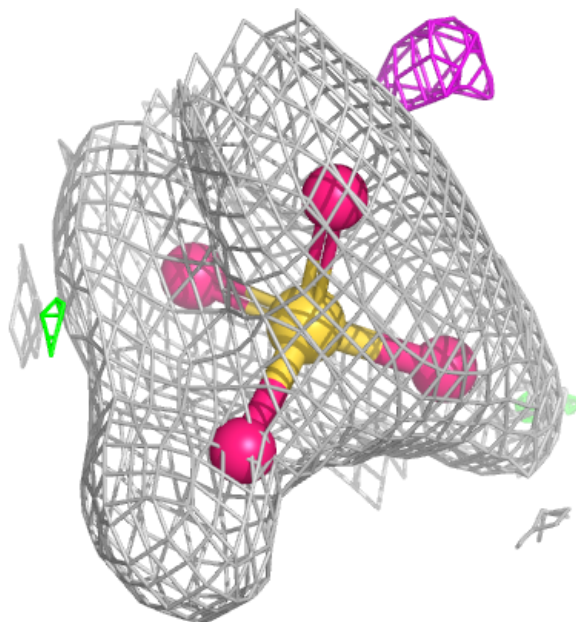
Electron density around SO4 BBB 302:

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



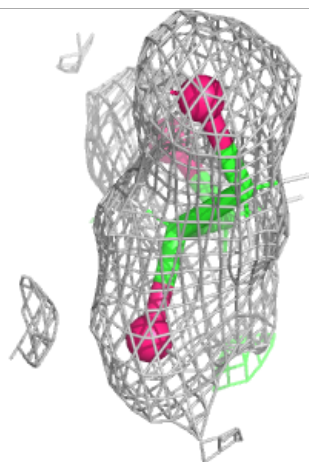
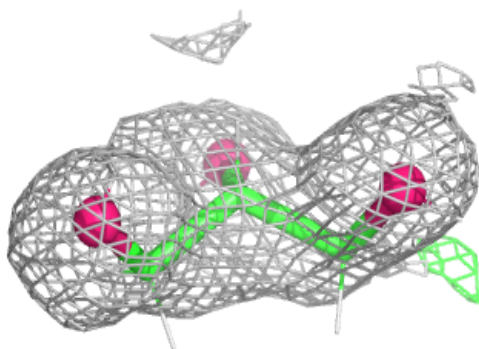
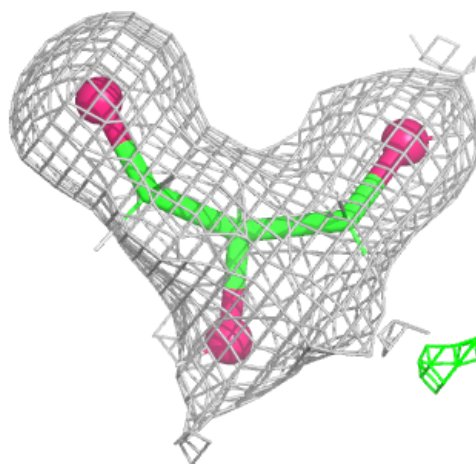
Electron density around SO4 DDD 301:

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



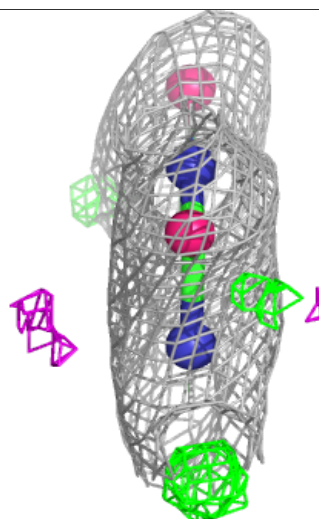
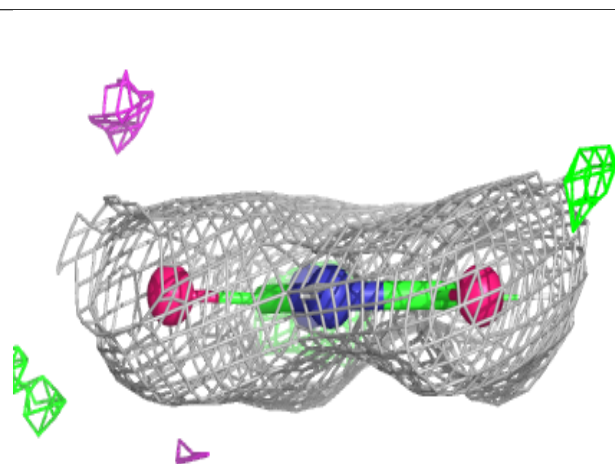
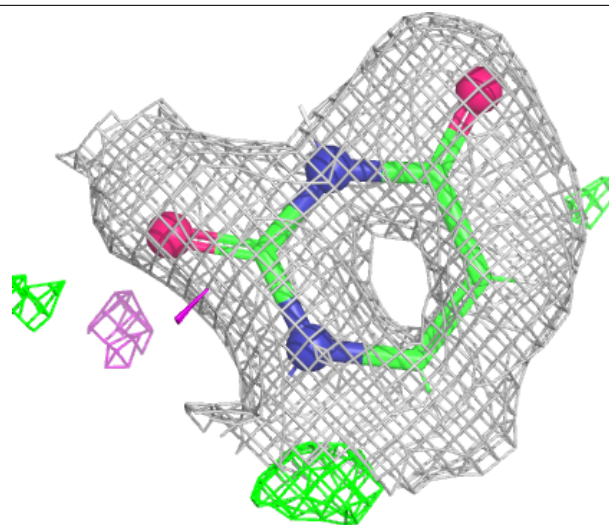
Electron density around GOL AAA 302:

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



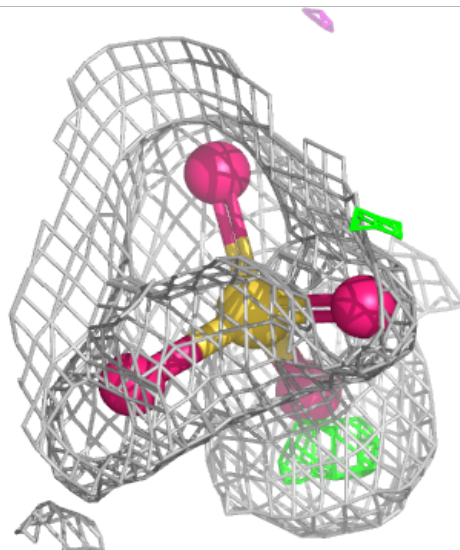
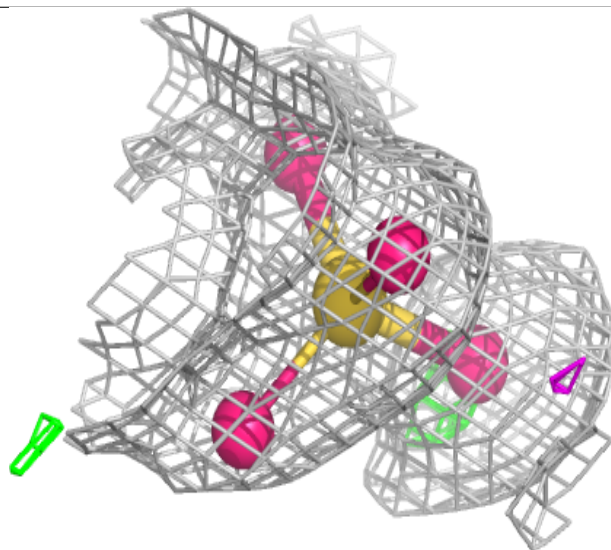
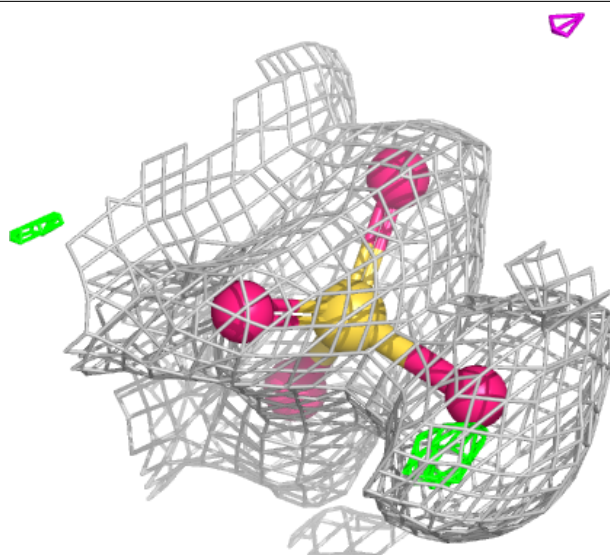
Electron density around URA FFF 301:

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



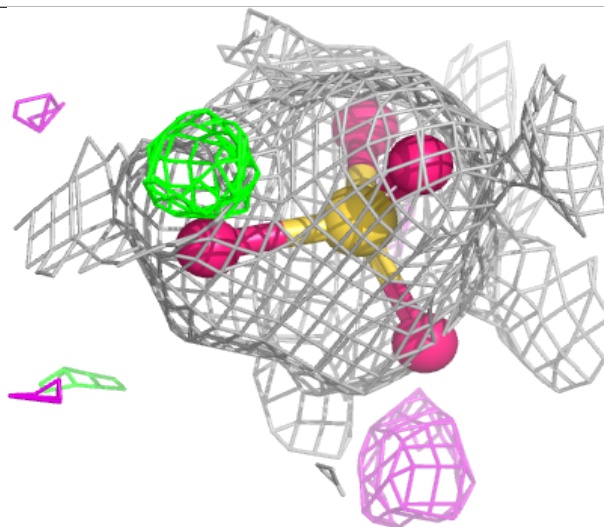
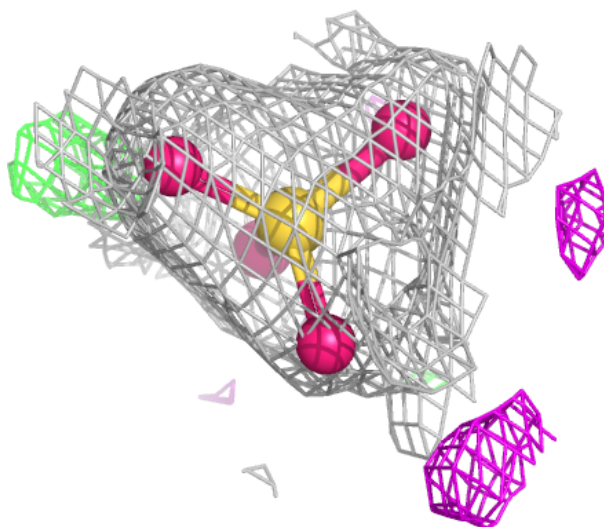
Electron density around SO4 BBB 301 (B):

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



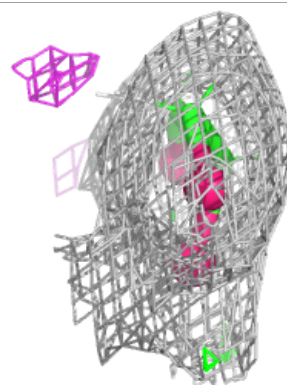
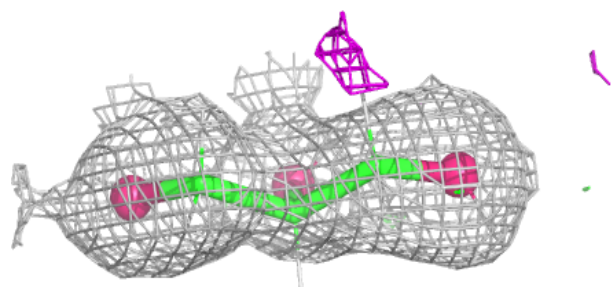
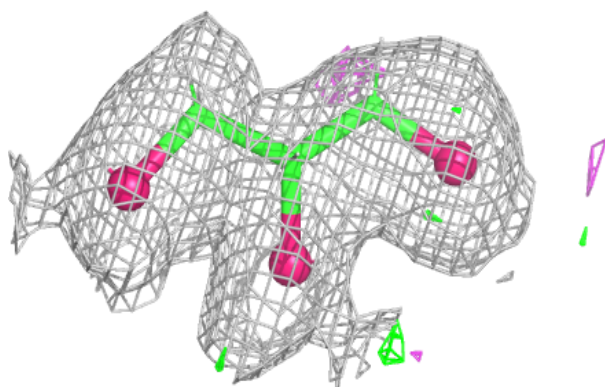
Electron density around SO4 FFF 303:

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



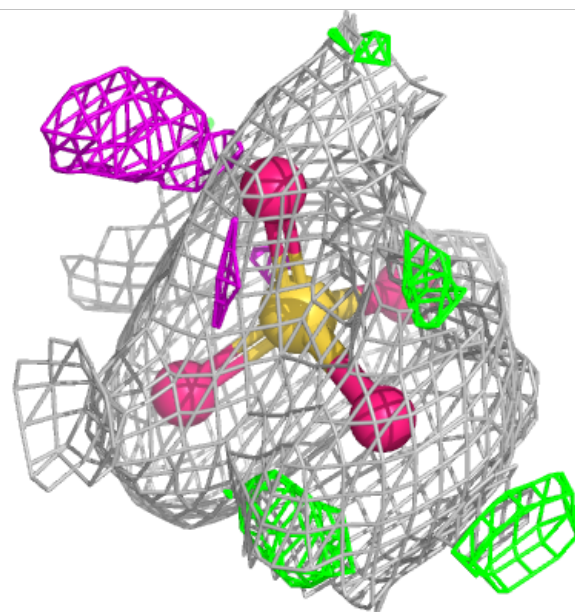
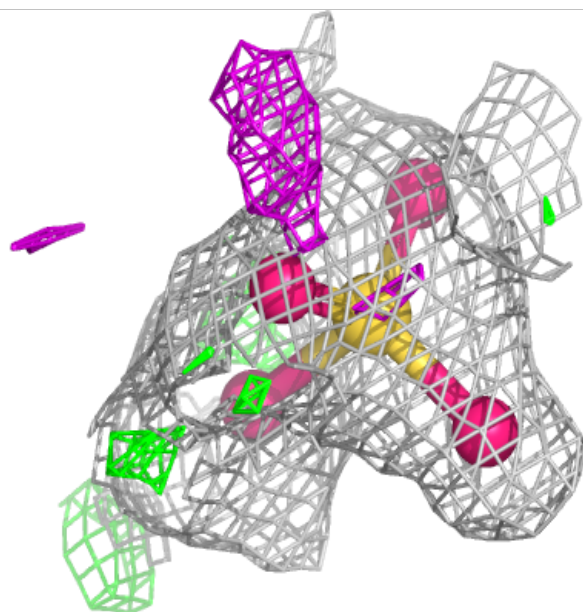
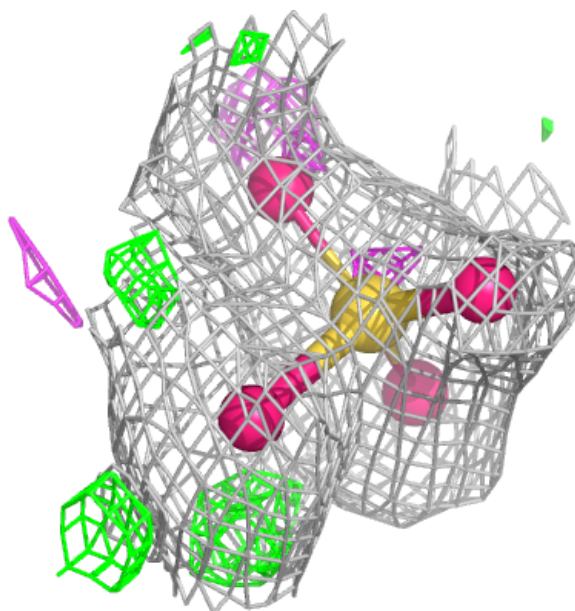
Electron density around GOL DDD 302:

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



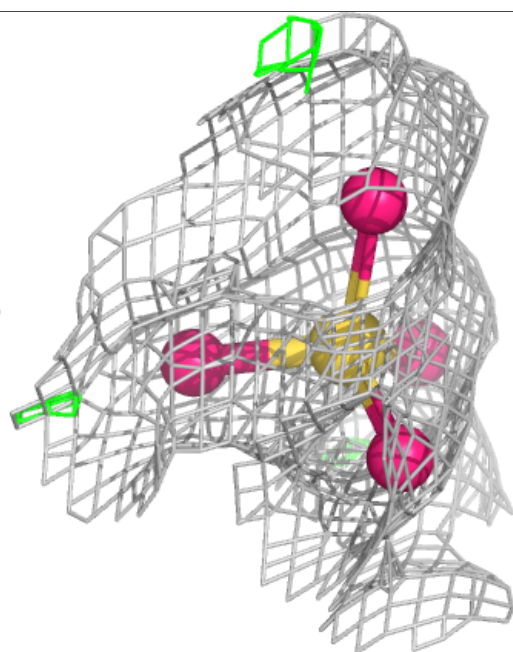
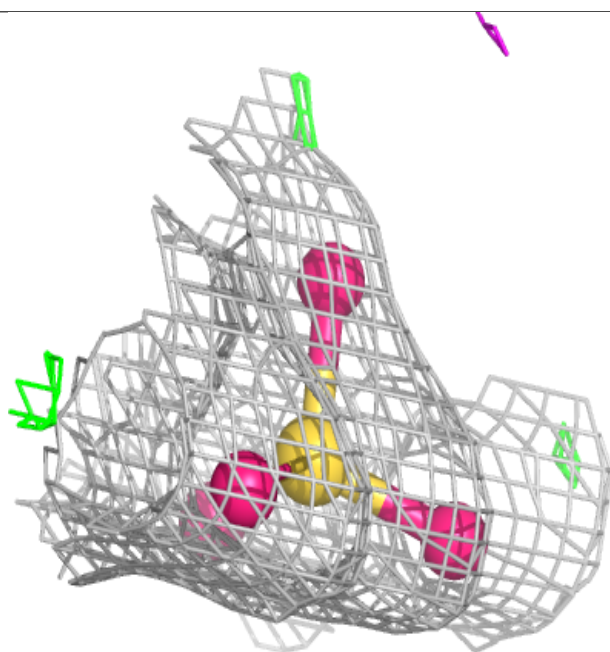
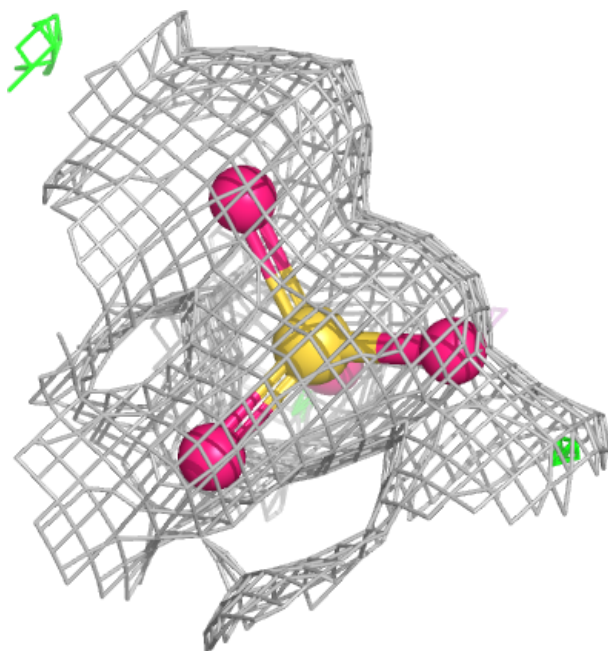
Electron density around SO4 EEE 301:

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



Electron density around SO4 BBB 301 (A):

$2mF_o - DF_c$ (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.