



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:08 AM UTC

PDB ID : 8BQG / pdb_00008bqg
Title : W-formate dehydrogenase from *Desulfovibrio vulgaris* - Soaking with Formate
1 min
Authors : Vilela-Alves, G.; Mota, C.; Oliveira, A.R.; Manuel, R.R.; Pereira, I.C.; Romao,
M.J.
Deposited on : 2022-11-21
Resolution : 1.95 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

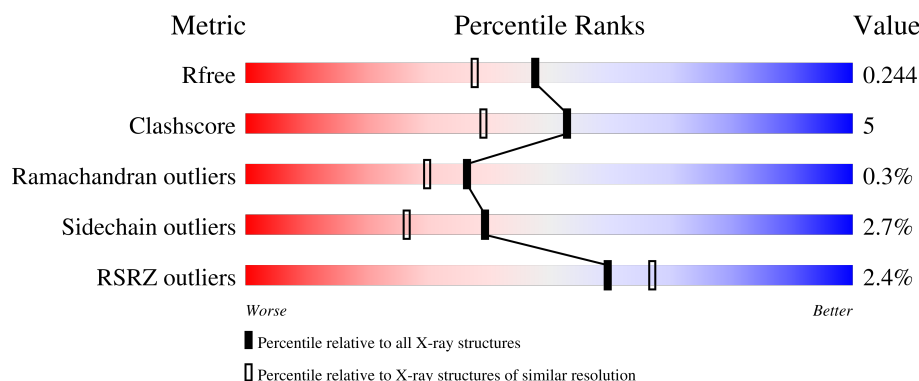
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

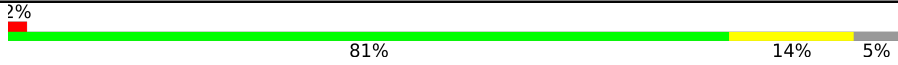
The reported resolution of this entry is 1.95 Å.

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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	1013	 2% 81% 14% 5%
2	B	236	 4% 78% 11% 9%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9509 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 Formate dehydrogenase, alpha subunit, selenocysteine-containing.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	963	Total	C	N	O	S	Se	0	0	0
			7533	4800	1313	1378	41	1			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q72EJ1
A	2	THR	-	expression tag	UNP Q72EJ1
A	3	VAL	-	expression tag	UNP Q72EJ1
A	4	THR	-	expression tag	UNP Q72EJ1
A	5	ARG	-	expression tag	UNP Q72EJ1
A	6	ARG	-	expression tag	UNP Q72EJ1
A	7	HIS	-	expression tag	UNP Q72EJ1
A	8	PHE	-	expression tag	UNP Q72EJ1
A	9	LEU	-	expression tag	UNP Q72EJ1
A	10	LYS	-	expression tag	UNP Q72EJ1
A	11	LEU	-	expression tag	UNP Q72EJ1
A	12	SER	-	expression tag	UNP Q72EJ1
A	13	ALA	-	expression tag	UNP Q72EJ1
A	14	GLY	-	expression tag	UNP Q72EJ1
A	15	ALA	-	expression tag	UNP Q72EJ1
A	16	ALA	-	expression tag	UNP Q72EJ1
A	17	VAL	-	expression tag	UNP Q72EJ1
A	18	ALA	-	expression tag	UNP Q72EJ1
A	19	GLY	-	expression tag	UNP Q72EJ1
A	20	ALA	-	expression tag	UNP Q72EJ1
A	21	PHE	-	expression tag	UNP Q72EJ1
A	22	THR	-	expression tag	UNP Q72EJ1
A	23	GLY	-	expression tag	UNP Q72EJ1
A	24	LEU	-	expression tag	UNP Q72EJ1
A	25	GLY	-	expression tag	UNP Q72EJ1
A	26	LEU	-	expression tag	UNP Q72EJ1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	expression tag	UNP Q72EJ1
A	28	LEU	-	expression tag	UNP Q72EJ1
A	29	ALA	-	expression tag	UNP Q72EJ1
A	30	PRO	-	expression tag	UNP Q72EJ1
A	31	THR	-	expression tag	UNP Q72EJ1
A	32	VAL	-	expression tag	UNP Q72EJ1
A	33	ALA	-	expression tag	UNP Q72EJ1
A	34	ARG	-	expression tag	UNP Q72EJ1
A	35	ALA	-	expression tag	UNP Q72EJ1
A	1006	TRP	-	expression tag	UNP Q72EJ1
A	1007	SER	-	expression tag	UNP Q72EJ1
A	1008	HIS	-	expression tag	UNP Q72EJ1
A	1009	PRO	-	expression tag	UNP Q72EJ1
A	1010	GLN	-	expression tag	UNP Q72EJ1
A	1011	PHE	-	expression tag	UNP Q72EJ1
A	1012	GLU	-	expression tag	UNP Q72EJ1
A	1013	LYS	-	expression tag	UNP Q72EJ1

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1664	1041	291	316	16			

There are 22 discrepancies between the modelled and reference sequences:

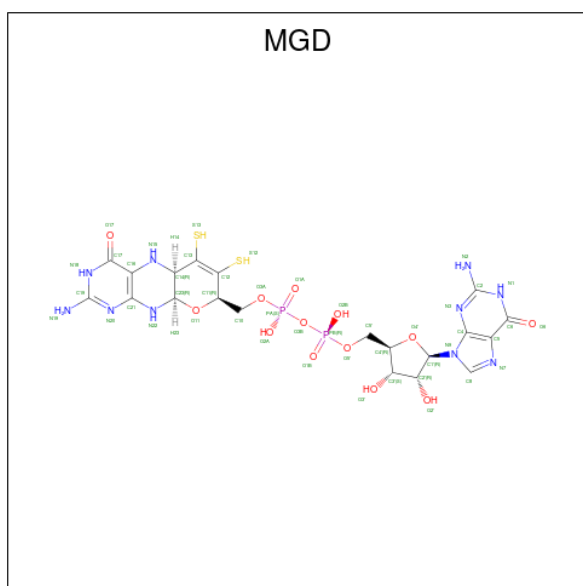
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q72EJ0
B	216	ASP	-	expression tag	UNP Q72EJ0
B	217	LEU	-	expression tag	UNP Q72EJ0
B	218	ALA	-	expression tag	UNP Q72EJ0
B	219	PRO	-	expression tag	UNP Q72EJ0
B	220	SER	-	expression tag	UNP Q72EJ0
B	221	MET	-	expression tag	UNP Q72EJ0
B	222	MET	-	expression tag	UNP Q72EJ0
B	223	THR	-	expression tag	UNP Q72EJ0
B	224	ARG	-	expression tag	UNP Q72EJ0
B	225	GLN	-	expression tag	UNP Q72EJ0
B	226	GLN	-	expression tag	UNP Q72EJ0
B	227	LEU	-	expression tag	UNP Q72EJ0
B	228	PHE	-	expression tag	UNP Q72EJ0
B	229	ALA	-	expression tag	UNP Q72EJ0

Continued on next page...

Continued from previous page...

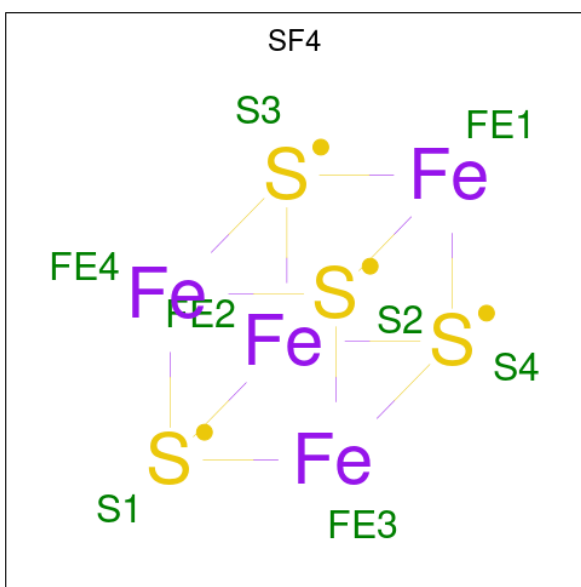
Chain	Residue	Modelled	Actual	Comment	Reference
B	230	ARG	-	expression tag	UNP Q72EJ0
B	231	LEU	-	expression tag	UNP Q72EJ0
B	232	PHE	-	expression tag	UNP Q72EJ0
B	233	ARG	-	expression tag	UNP Q72EJ0
B	234	PRO	-	expression tag	UNP Q72EJ0
B	235	ARG	-	expression tag	UNP Q72EJ0
B	236	ALA	-	expression tag	UNP Q72EJ0

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).



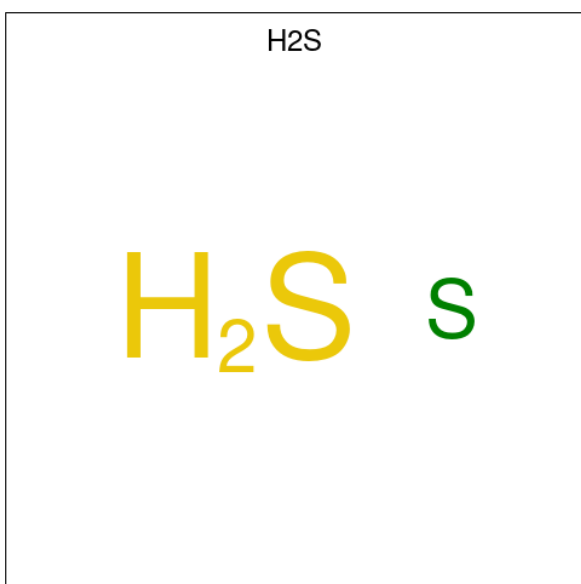
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).

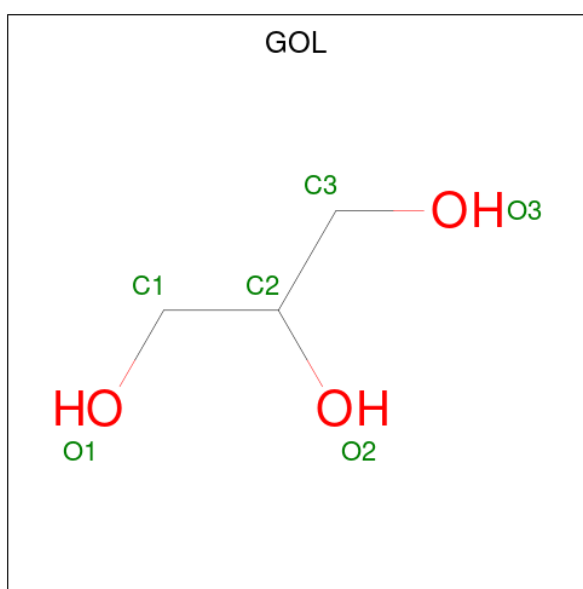


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 1 1	0	0

- Molecule 6 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total W 1 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		

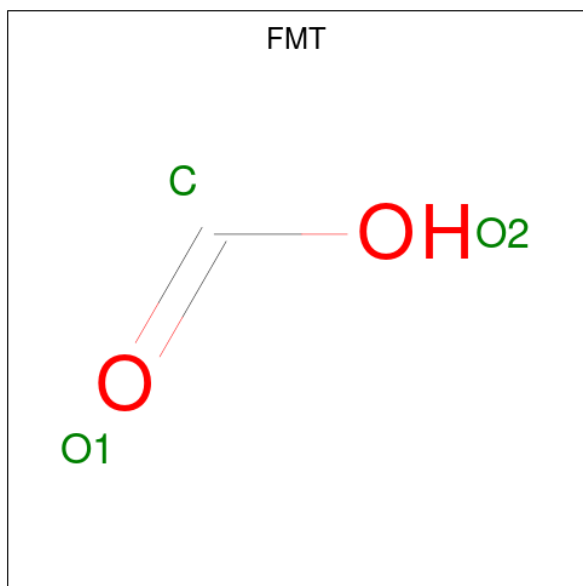
- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			3	1	2		

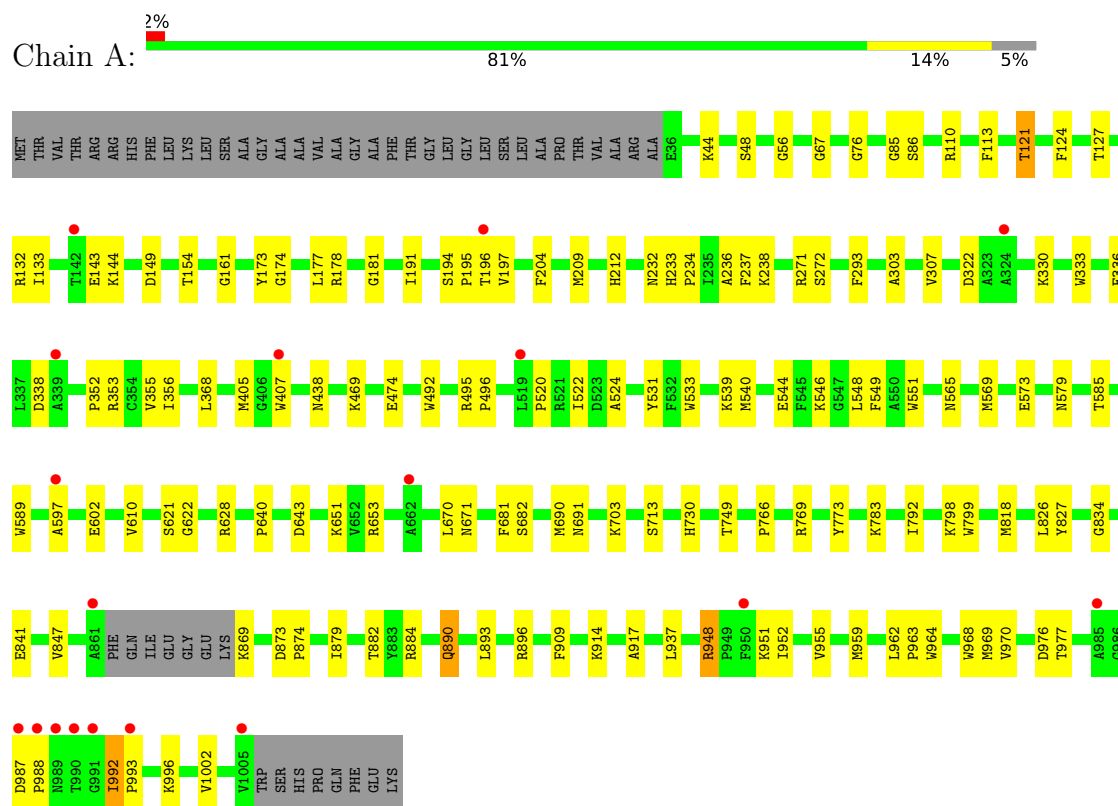
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	122	Total	O	0	0
			122	122		
11	B	26	Total	O	0	0
			26	26		

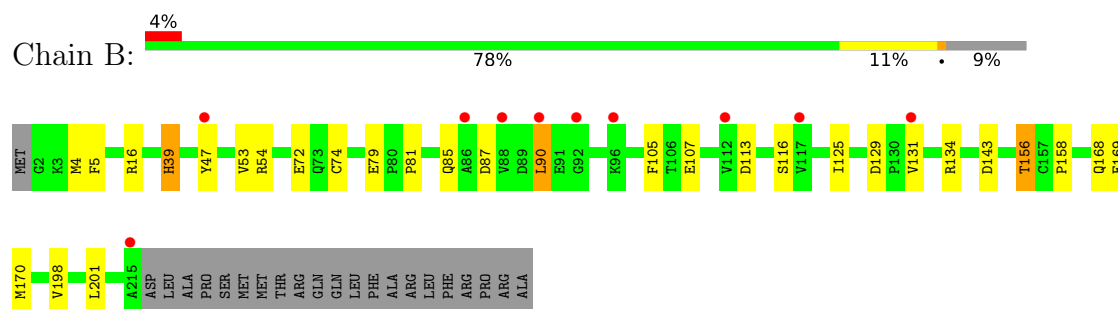
3 Residue-property plots [i](#)

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: Formate dehydrogenase, alpha subunit, selenocysteine-containing



- Molecule 2: Formate dehydrogenase, beta subunit, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.54Å 122.78Å 148.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.93 – 1.95 94.75 – 1.95	Depositor EDS
% Data completeness (in resolution range)	83.7 (94.93-1.95) 83.7 (94.75-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.243 0.198 , 0.244	Depositor DCC
R_{free} test set	3564 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9509	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PEG, GOL, W, EDO, FMT, MGD, SF4, SEC, H2S

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	1.07	4/7733 (0.1%)	1.39	13/10490 (0.1%)
2	B	1.06	0/1699	1.39	1/2302 (0.0%)
All	All	1.07	4/9432 (0.0%)	1.39	14/12792 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ALA	C-O	-6.23	1.16	1.24
1	A	352	PRO	C-O	-5.46	1.17	1.24
1	A	977	THR	C-O	5.08	1.29	1.23
1	A	682	SER	CA-CB	-5.07	1.47	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	610	VAL	CA-C-N	6.05	128.70	120.54
1	A	610	VAL	C-N-CA	6.05	128.70	120.54
1	A	890	GLN	CB-CA-C	-5.75	109.42	117.23
1	A	338	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	546	LYS	CA-C-N	5.50	125.39	121.65
1	A	546	LYS	C-N-CA	5.50	125.39	121.65
1	A	307	VAL	CA-C-N	5.30	125.13	120.10
1	A	307	VAL	C-N-CA	5.30	125.13	120.10
1	A	749	THR	CA-CB-OG1	-5.23	101.75	109.60
2	B	39	HIS	CA-CB-CG	-5.18	108.61	113.80
1	A	681	PHE	CA-C-O	-5.17	115.33	120.96
1	A	976	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	826	LEU	CA-C-N	5.01	129.06	122.30
1	A	826	LEU	C-N-CA	5.01	129.06	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7533	0	7366	76	0
2	B	1664	0	1633	18	0
3	A	94	0	44	4	0
4	A	8	0	0	1	0
4	B	24	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	18	0	24	1	0
8	A	7	0	10	0	0
9	A	4	0	6	0	0
9	B	4	0	6	1	0
10	A	3	0	1	0	0
11	A	122	0	0	1	0
11	B	26	0	0	0	0
All	All	9509	0	9090	92	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 (92) 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:579:ASN:OD1	3:A:1102:MGD:O2'	1.96	0.83
1:A:181:GLY:HA2	1:A:520:PRO:HG3	1.62	0.82
1:A:44:LYS:HE3	1:A:67:GLY:HA3	1.66	0.76
1:A:569:MET:HE1	1:A:585:THR:HG23	1.71	0.73
1:A:113:PHE:HD1	1:A:597:ALA:O	1.73	0.71
2:B:113:ASP:OD2	2:B:116:SER:OG	2.10	0.67
1:A:690:MET:HE2	1:A:730:HIS:CE1	2.33	0.64
1:A:336:GLU:OE1	1:A:353:ARG:NH2	2.30	0.63
1:A:405:MET:HE1	1:A:884:ARG:NH1	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:MET:HE1	1:A:884:ARG:HH12	1.63	0.62
2:B:79:GLU:O	2:B:81:PRO:HD3	1.99	0.62
1:A:209:MET:HG3	1:A:438:ASN:HA	1.81	0.62
1:A:948:ARG:CG	1:A:948:ARG:HH11	2.16	0.58
1:A:113:PHE:CD1	1:A:597:ALA:O	2.55	0.57
1:A:127:THR:HG22	1:A:651:LYS:HD3	1.87	0.57
1:A:132:ARG:NH2	1:A:602:GLU:OE2	2.37	0.57
1:A:209:MET:HE2	1:A:622:GLY:HA2	1.88	0.56
1:A:792:ILE:HD12	1:A:799:TRP:CE3	2.41	0.56
1:A:173:TYR:CE2	1:A:177:LEU:HD11	2.42	0.55
1:A:191:ILE:HD11	1:A:533:TRP:CE2	2.42	0.55
1:A:893:LEU:C	1:A:893:LEU:HD23	2.33	0.54
2:B:105:PHE:HB2	9:B:304:EDO:H12	1.91	0.53
1:A:405:MET:CE	1:A:884:ARG:NH1	2.72	0.53
1:A:173:TYR:CZ	1:A:177:LEU:HD11	2.44	0.53
1:A:144:LYS:HA	1:A:149:ASP:O	2.09	0.52
1:A:884:ARG:HH22	3:A:1102:MGD:H15	1.56	0.52
1:A:540:MET:HE1	1:A:548:LEU:HD22	1.91	0.52
1:A:539:LYS:NZ	1:A:544:GLU:OE1	2.44	0.51
1:A:952:ILE:O	1:A:955:VAL:HG12	2.11	0.50
1:A:209:MET:HE3	1:A:212:HIS:HA	1.93	0.50
2:B:201:LEU:C	2:B:201:LEU:HD23	2.37	0.50
1:A:565:ASN:O	1:A:569:MET:HG3	2.12	0.50
1:A:194:SER:N	1:A:195:PRO:CD	2.75	0.50
1:A:896:ARG:HD2	1:A:970:VAL:O	2.12	0.49
2:B:85:GLN:HE21	2:B:116:SER:HB3	1.78	0.49
1:A:948:ARG:HH11	1:A:948:ARG:HG3	1.79	0.48
1:A:968:TRP:CH2	1:A:969:MET:HE3	2.48	0.48
1:A:890:GLN:HA	1:A:964:TRP:CH2	2.49	0.47
2:B:47:TYR:CE1	2:B:129:ASP:HB2	2.48	0.47
1:A:56:GLY:HA2	11:A:1237:HOH:O	2.15	0.47
1:A:204:PHE:HB3	1:A:773:TYR:CZ	2.50	0.47
1:A:469:LYS:HG2	1:A:524:ALA:CB	2.45	0.47
7:A:1109:GOL:H31	2:B:39:HIS:CE1	2.50	0.46
1:A:174:GLY:O	1:A:178:ARG:HG3	2.16	0.46
1:A:882:THR:HA	1:A:962:LEU:O	2.15	0.46
1:A:937:LEU:C	1:A:937:LEU:HD12	2.40	0.46
1:A:330:LYS:HG2	1:A:333:TRP:CZ3	2.50	0.46
1:A:191:ILE:HG21	3:A:1102:MGD:H14	1.97	0.45
1:A:44:LYS:HE3	1:A:67:GLY:CA	2.41	0.45
1:A:48:SER:HA	1:A:628:ARG:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HA	1:A:651:LYS:HD3	1.99	0.45
1:A:879:ILE:O	1:A:959:MET:HA	2.16	0.45
1:A:303:ALA:HB1	1:A:356:ILE:HB	1.99	0.45
1:A:234:PRO:HD2	4:A:1103:SF4:S3	2.57	0.44
1:A:495:ARG:N	1:A:496:PRO:CD	2.80	0.44
2:B:90:LEU:C	2:B:90:LEU:HD23	2.41	0.44
1:A:407:TRP:CD1	1:A:996:LYS:HB2	2.53	0.44
2:B:85:GLN:NE2	2:B:116:SER:HB3	2.32	0.44
1:A:127:THR:CG2	1:A:651:LYS:HD3	2.48	0.44
1:A:209:MET:HE2	1:A:621:SER:C	2.42	0.44
1:A:987:ASP:O	1:A:988:PRO:C	2.60	0.44
1:A:522:ILE:HB	1:A:531:TYR:CE2	2.52	0.44
1:A:873:ASP:HA	1:A:874:PRO:HD3	1.89	0.44
2:B:74:CYS:HB2	2:B:125:ILE:HG21	2.00	0.44
2:B:107:GLU:HG3	2:B:134:ARG:NH1	2.32	0.44
1:A:653:ARG:NH2	1:A:670:LEU:O	2.43	0.44
1:A:133:ILE:HD11	1:A:549:PHE:HZ	1.83	0.43
1:A:992:ILE:HG23	1:A:993:PRO:HD2	2.01	0.43
1:A:238:LYS:HB2	2:B:158:PRO:O	2.19	0.43
1:A:322:ASP:OD1	1:A:322:ASP:C	2.62	0.43
1:A:233:HIS:N	1:A:234:PRO:HD3	2.34	0.43
2:B:5:PHE:CD1	2:B:198:VAL:HG22	2.54	0.43
2:B:107:GLU:H	2:B:107:GLU:CD	2.27	0.43
1:A:841:GLU:HG2	1:A:847:VAL:HG11	2.01	0.42
1:A:232:ASN:HA	3:A:1101:MGD:N20	2.34	0.42
1:A:86:SER:HB2	2:B:156:THR:O	2.19	0.42
1:A:110:ARG:HG3	1:A:589:TRP:CZ2	2.54	0.42
1:A:293:PHE:C	1:A:293:PHE:CD1	2.97	0.42
1:A:161:GLY:HA3	1:A:551:TRP:O	2.20	0.42
1:A:76:GLY:HA3	1:A:85:GLY:O	2.20	0.41
1:A:914:LYS:O	1:A:917:ALA:HB3	2.20	0.41
1:A:333:TRP:CH2	1:A:834:GLY:HA2	2.54	0.41
2:B:16:ARG:HG2	2:B:53:VAL:CG2	2.50	0.41
2:B:54:ARG:NH2	2:B:72:GLU:OE1	2.47	0.41
1:A:355:VAL:HG13	1:A:827:TYR:HB2	2.03	0.41
1:A:492:TRP:CD1	1:A:818:MET:HE3	2.56	0.41
1:A:766:PRO:HG2	1:A:769:ARG:HD2	2.02	0.41
2:B:4:MET:O	2:B:170:MET:HG3	2.19	0.41
1:A:110:ARG:HG3	1:A:589:TRP:CE2	2.56	0.40
1:A:121:THR:HG23	1:A:124:PHE:H	1.86	0.40
1:A:909:PHE:CE1	1:A:963:PRO:HD3	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:PRO:HG2	1:A:643:ASP:OD2	2.22	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	958/1013 (95%)	922 (96%)	36 (4%)	0	100	100
2	B	212/236 (90%)	198 (93%)	11 (5%)	3 (1%)	9	2
All	All	1170/1249 (94%)	1120 (96%)	47 (4%)	3 (0%)	36	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	90	LEU
2	B	131	VAL
2	B	87	ASP

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	782/819 (96%)	760 (97%)	22 (3%)	38	25
2	B	185/204 (91%)	181 (98%)	4 (2%)	45	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	967/1023 (94%)	941 (97%)	26 (3%)	39	26

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	THR
1	A	143	GLU
1	A	154	THR
1	A	196	THR
1	A	197	VAL
1	A	237	PHE
1	A	271	ARG
1	A	272	SER
1	A	368	LEU
1	A	474	GLU
1	A	573	GLU
1	A	671	ASN
1	A	691	ASN
1	A	703	LYS
1	A	713	SER
1	A	783	LYS
1	A	798	LYS
1	A	869	LYS
1	A	948	ARG
1	A	951	LYS
1	A	992	ILE
1	A	1002	VAL
2	B	143	ASP
2	B	156	THR
2	B	168	GLN
2	B	169	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	325	ASN
1	A	595	ASN
1	A	671	ASN
1	A	679	ASN
2	B	85	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	212	HIS

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 ⓘ

Of 15 ligands modelled in this entry, 1 is modelled with single atom and 1 is monoatomic - leaving 13 for Mogul analysis.

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	$\# Z > 2$
4	SF4	A	1103	1	0,12,12	-	-	-		
7	GOL	A	1107	-	5,5,5	0.15	0	5,5,5	0.33	0
10	FMT	A	1111	-	2,2,2	0.29	0	1,1,1	0.16	0
4	SF4	B	301	2	0,12,12	-	-	-		
8	PEG	A	1108	-	6,6,6	0.20	0	5,5,5	0.17	0
9	EDO	B	304	-	3,3,3	0.48	0	2,2,2	0.47	0
3	MGD	A	1101	6	47,52,52	0.80	1 (2%)	58,81,81	1.21	5 (8%)
3	MGD	A	1102	6	47,52,52	0.80	2 (4%)	58,81,81	1.06	5 (8%)
7	GOL	A	1106	-	5,5,5	0.19	0	5,5,5	0.52	0
4	SF4	B	302	2	0,12,12	-	-	-		
7	GOL	A	1109	-	5,5,5	0.13	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	1110	-	3,3,3	0.14	0	2,2,2	0.23	0
4	SF4	B	303	2	0,12,12	-	-	-		

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
4	SF4	A	1103	1	-	-	0/6/5/5
7	GOL	A	1107	-	-	2/4/4/4	-
8	PEG	A	1108	-	-	2/4/4/4	-
4	SF4	B	301	2	-	-	0/6/5/5
9	EDO	B	304	-	-	0/1/1/1	-
3	MGD	A	1101	6	-	3/22/66/66	0/6/6/6
7	GOL	A	1106	-	-	2/4/4/4	-
3	MGD	A	1102	6	-	4/22/66/66	0/6/6/6
4	SF4	B	302	2	-	-	0/6/5/5
7	GOL	A	1109	-	-	2/4/4/4	-
9	EDO	A	1110	-	-	0/1/1/1	-
4	SF4	B	303	2	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	MGD	PA-O3B	3.20	1.63	1.59
3	A	1101	MGD	C23-C14	-2.91	1.51	1.53
3	A	1102	MGD	C23-C14	2.20	1.55	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	O11-C23-C14	4.73	112.12	108.96
3	A	1101	MGD	C23-C14-N15	4.30	112.09	107.87
3	A	1102	MGD	O11-C23-C14	3.22	111.11	108.96
3	A	1102	MGD	C23-C14-N15	2.81	110.63	107.87
3	A	1101	MGD	C19-N20-C21	2.49	117.76	113.36
3	A	1102	MGD	C19-N20-C21	2.33	117.47	113.36
3	A	1102	MGD	C17-C16-N15	2.28	122.49	116.27
3	A	1102	MGD	O11-C23-N22	-2.25	106.56	108.61
3	A	1101	MGD	C17-C16-N15	2.02	121.77	116.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	O2B-PB-O1B	2.01	121.81	112.44

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	C5'-O5'-PB-O1B
3	A	1102	MGD	C4'-C5'-O5'-PB
7	A	1106	GOL	O1-C1-C2-C3
7	A	1107	GOL	O1-C1-C2-C3
7	A	1109	GOL	O1-C1-C2-C3
3	A	1102	MGD	O4'-C4'-C5'-O5'
8	A	1108	PEG	O2-C3-C4-O4
3	A	1102	MGD	C3'-C4'-C5'-O5'
7	A	1107	GOL	O1-C1-C2-O2
7	A	1109	GOL	O1-C1-C2-O2
8	A	1108	PEG	O1-C1-C2-O2
7	A	1106	GOL	O1-C1-C2-O2
3	A	1101	MGD	PA-O3B-PB-O5'
3	A	1101	MGD	PA-O3B-PB-O1B
3	A	1101	MGD	PA-O3B-PB-O2B

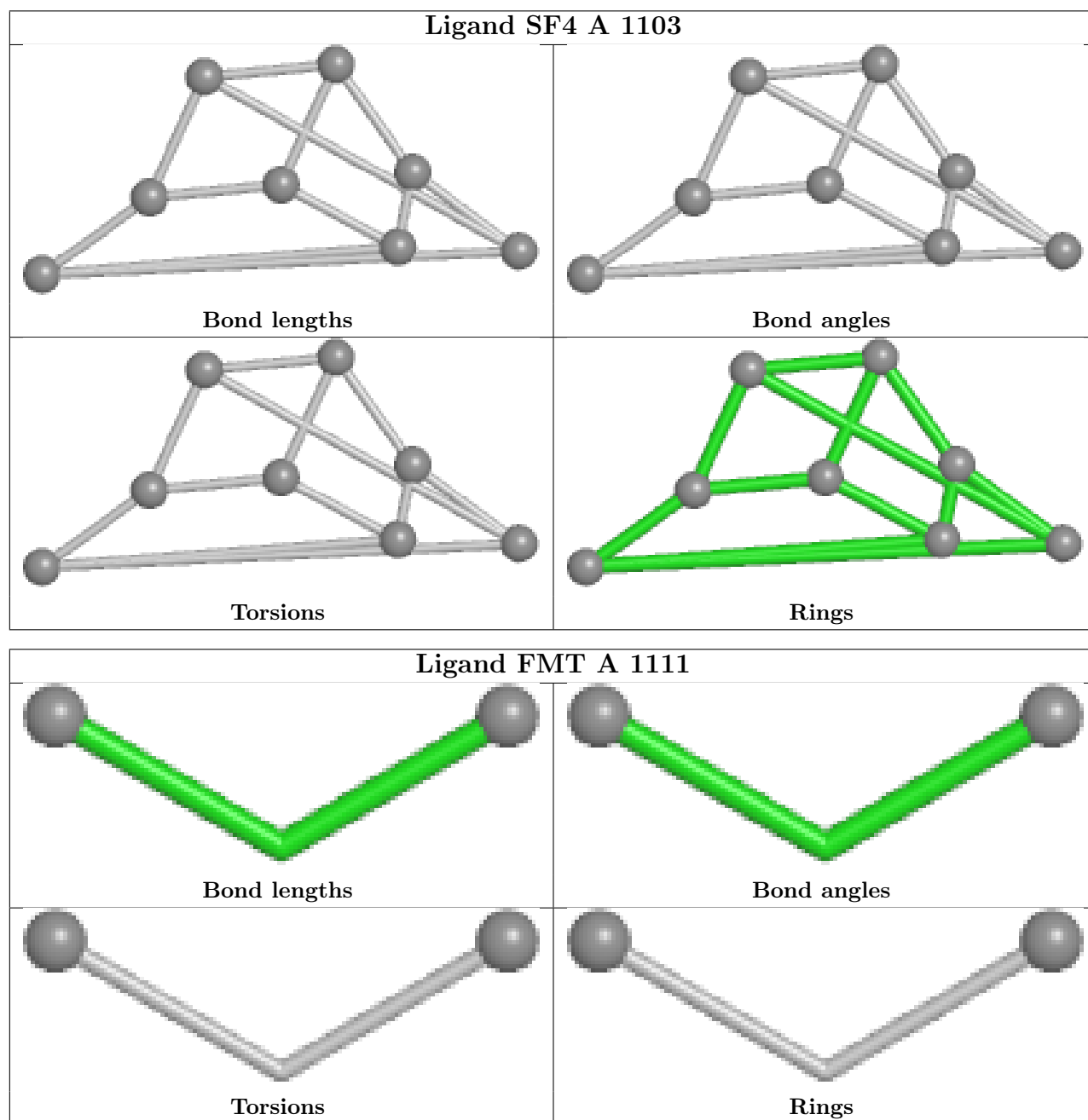
There are no ring outliers.

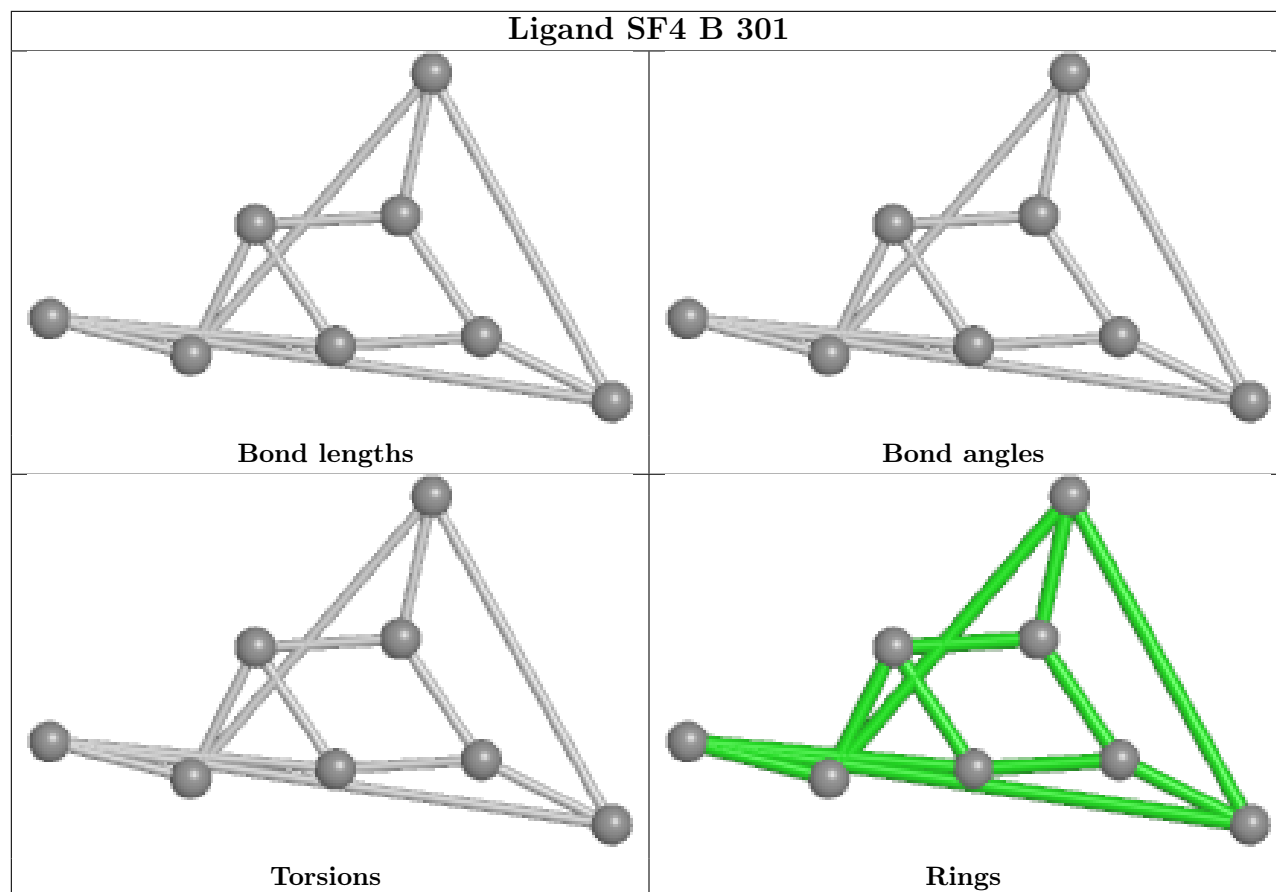
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103	SF4	1	0
9	B	304	EDO	1	0
3	A	1101	MGD	1	0
3	A	1102	MGD	3	0
7	A	1109	GOL	1	0

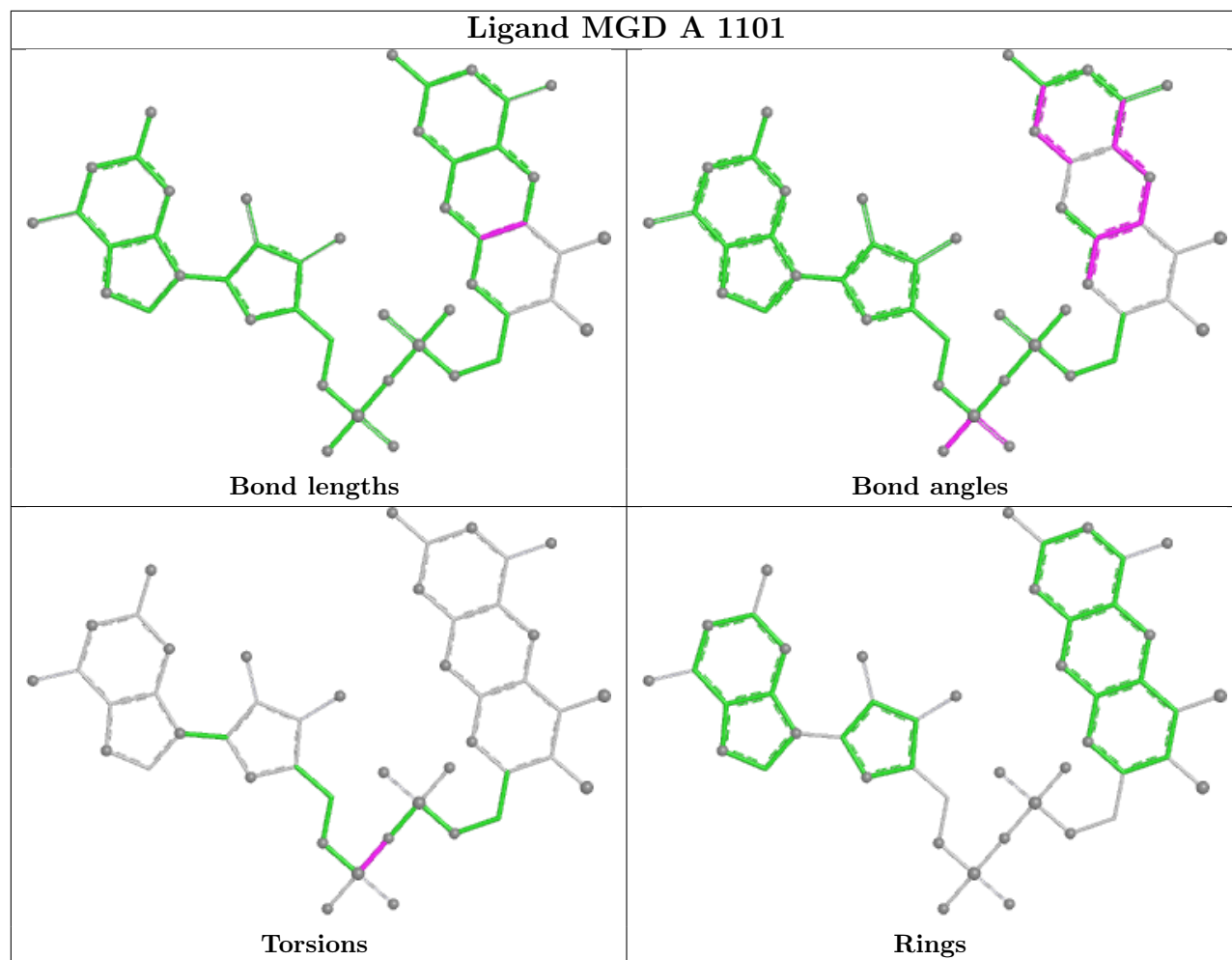
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

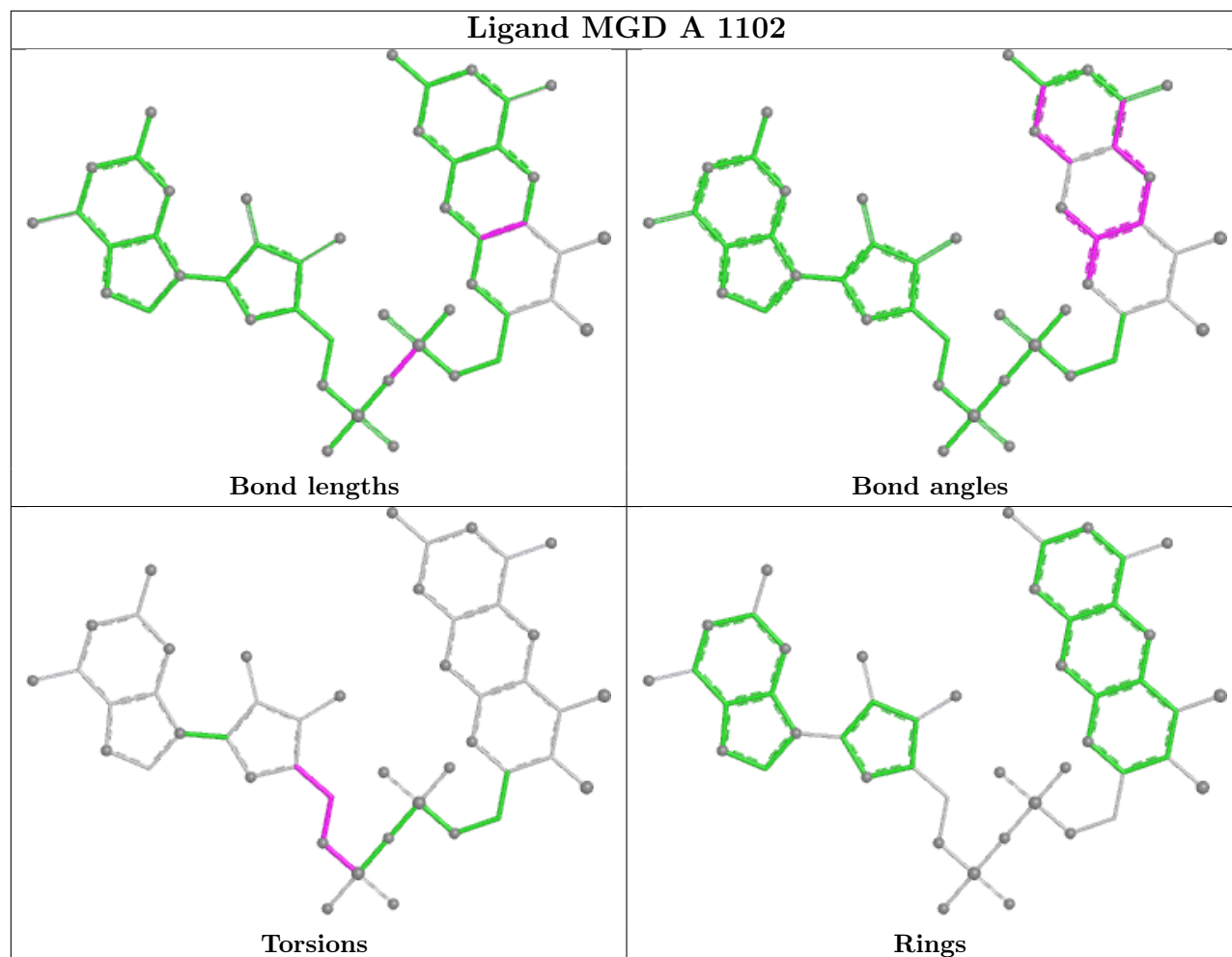




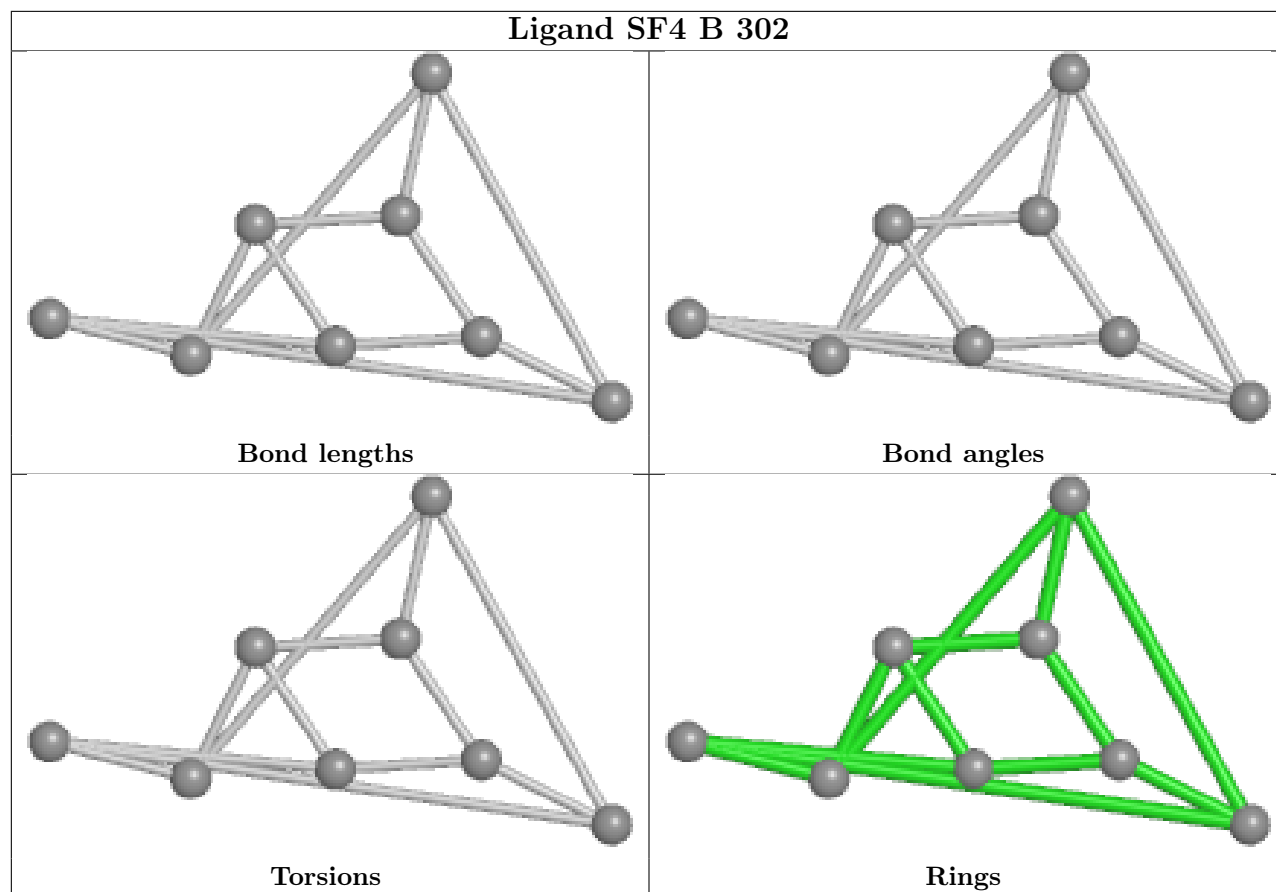
Ligand MGD A 1101



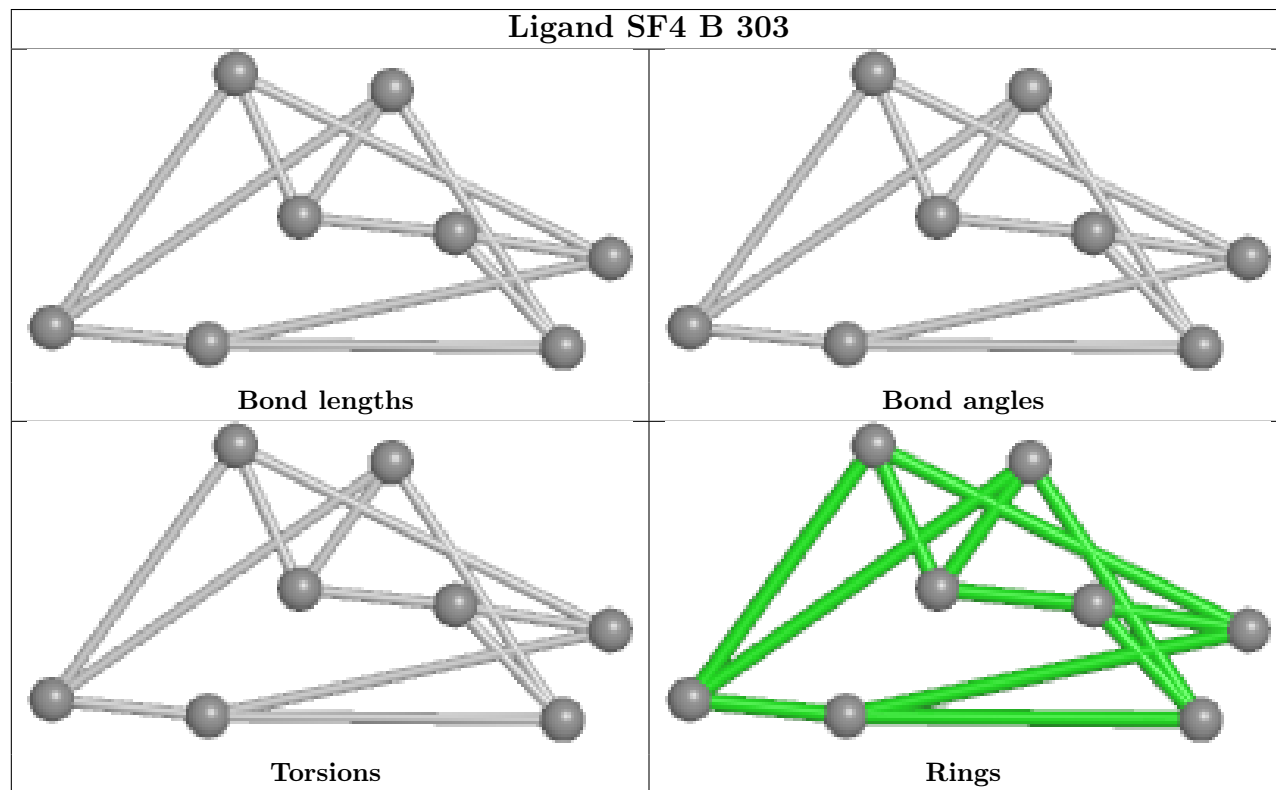
Ligand MGD A 1102



Ligand SF4 B 302



Ligand SF4 B 303



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	962/1013 (94%)	0.24	18 (1%) 66 72	23, 38, 61, 112	0
2	B	214/236 (90%)	0.53	10 (4%) 36 41	25, 44, 68, 76	0
All	All	1176/1249 (94%)	0.29	28 (2%) 59 67	23, 38, 62, 112	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	988	PRO	4.1
1	A	993	PRO	3.7
1	A	1005	VAL	3.6
1	A	985	ALA	3.6
1	A	989	ASN	3.3
2	B	88	VAL	3.0
2	B	215	ALA	2.9
2	B	117	VAL	2.7
2	B	90	LEU	2.6
1	A	196	THR	2.5
1	A	597	ALA	2.5
1	A	991	GLY	2.5
1	A	861	ALA	2.5
1	A	662	ALA	2.4
2	B	92	GLY	2.4
1	A	324	ALA	2.3
2	B	47	TYR	2.3
1	A	987	ASP	2.3
2	B	112	VAL	2.3
2	B	96	LYS	2.3
1	A	339	ALA	2.2
1	A	519	LEU	2.2
1	A	142	THR	2.2
1	A	407	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	990	THR	2.1
2	B	86	ALA	2.1
1	A	950	PHE	2.0
2	B	131	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

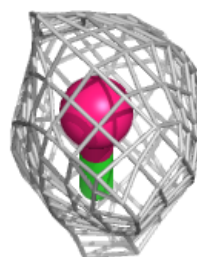
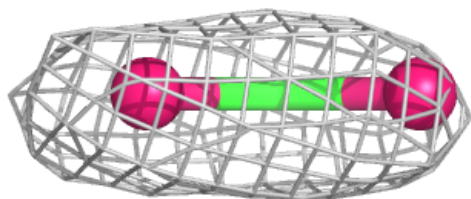
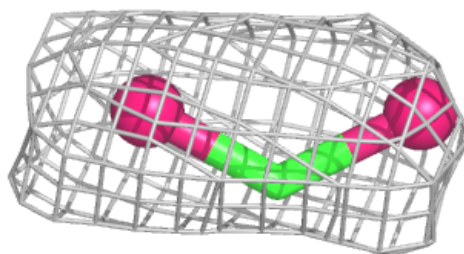
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	1106	6/6	0.89	0.11	47,49,51,56	0
8	PEG	A	1108	7/7	0.89	0.13	47,54,62,62	0
10	FMT	A	1111	3/3	0.89	0.21	57,57,65,67	0
7	GOL	A	1107	6/6	0.91	0.09	31,37,39,42	0
7	GOL	A	1109	6/6	0.91	0.11	36,40,46,47	0
9	EDO	A	1110	4/4	0.92	0.10	45,46,47,49	0
9	EDO	B	304	4/4	0.95	0.11	27,29,40,45	0
3	MGD	A	1102	47/47	0.98	0.05	27,32,39,49	0
4	SF4	B	302	8/8	0.98	0.04	39,41,43,43	0
3	MGD	A	1101	47/47	0.98	0.05	20,26,32,34	0
5	H2S	A	1104	1/1	0.99	0.07	36,36,36,36	0
4	SF4	B	301	8/8	0.99	0.02	27,28,28,29	0
4	SF4	A	1103	8/8	0.99	0.02	25,25,26,26	0
4	SF4	B	303	8/8	0.99	0.03	32,34,36,36	0
6	W	A	1105	1/1	1.00	0.01	28,28,28,28	0

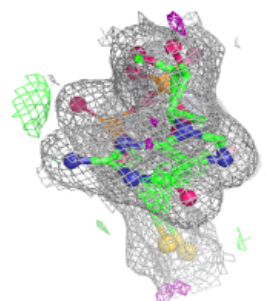
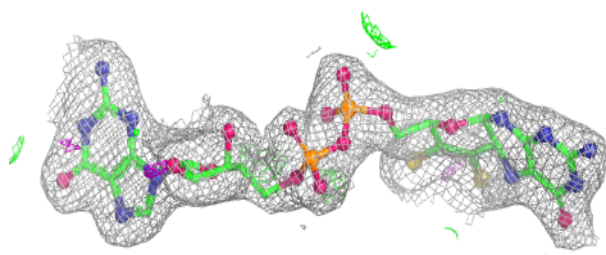
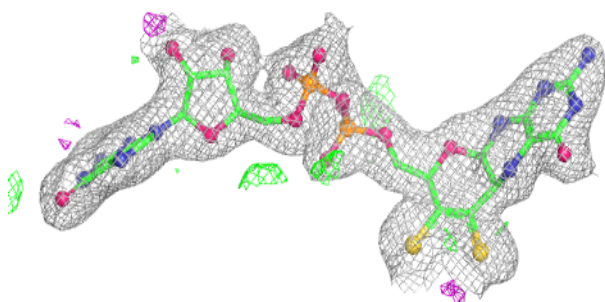
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMT A 1111:

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

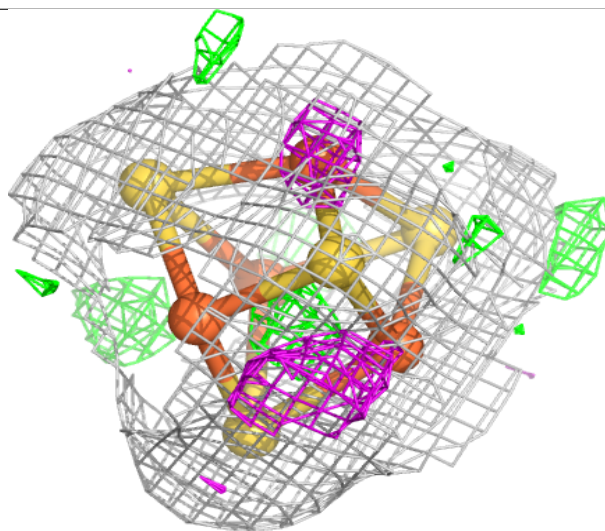
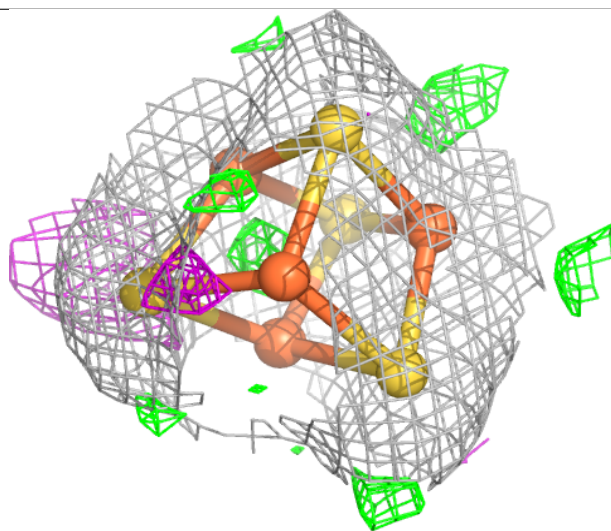
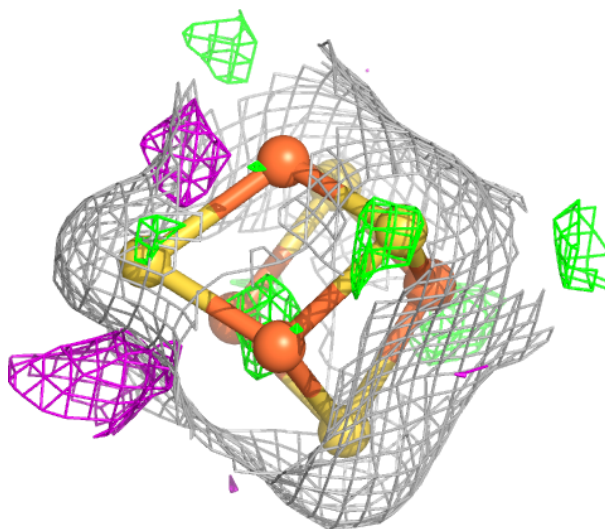
**Electron density around MGD A 1102:**

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



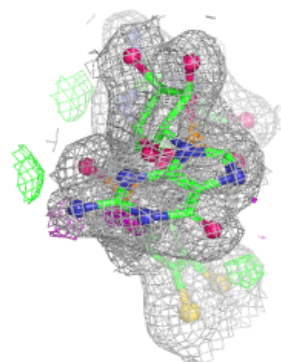
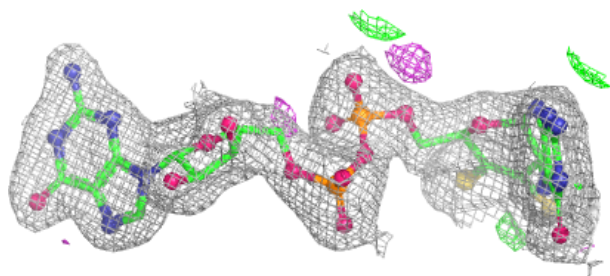
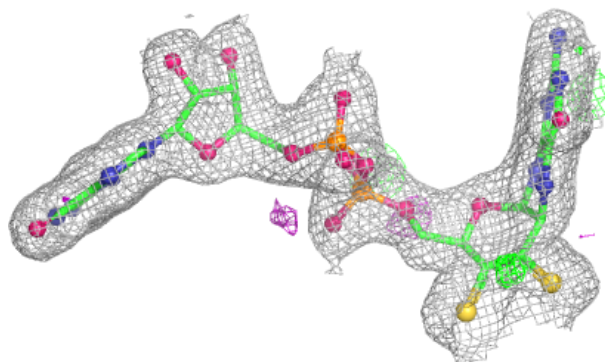
Electron density around SF4 B 302:

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



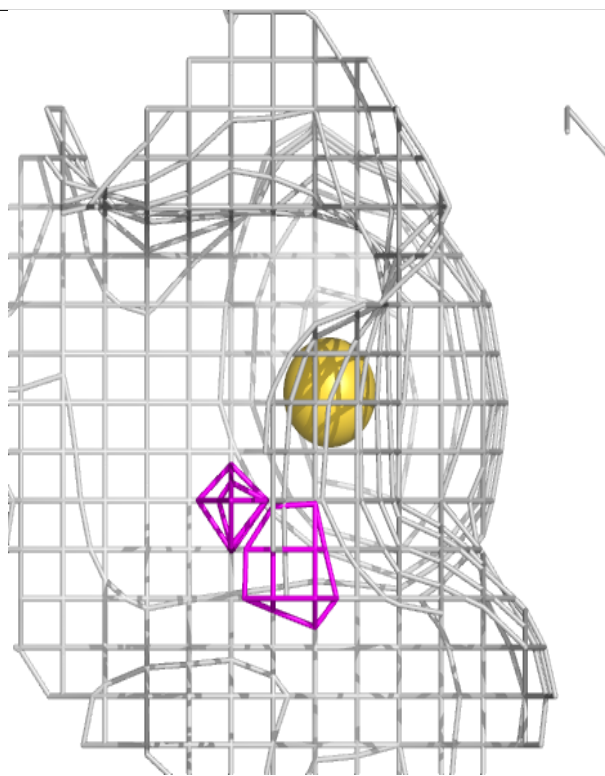
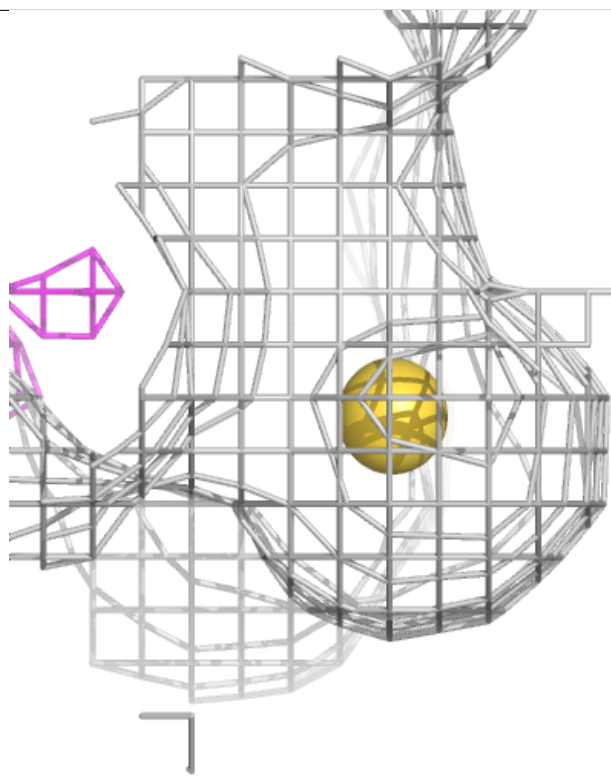
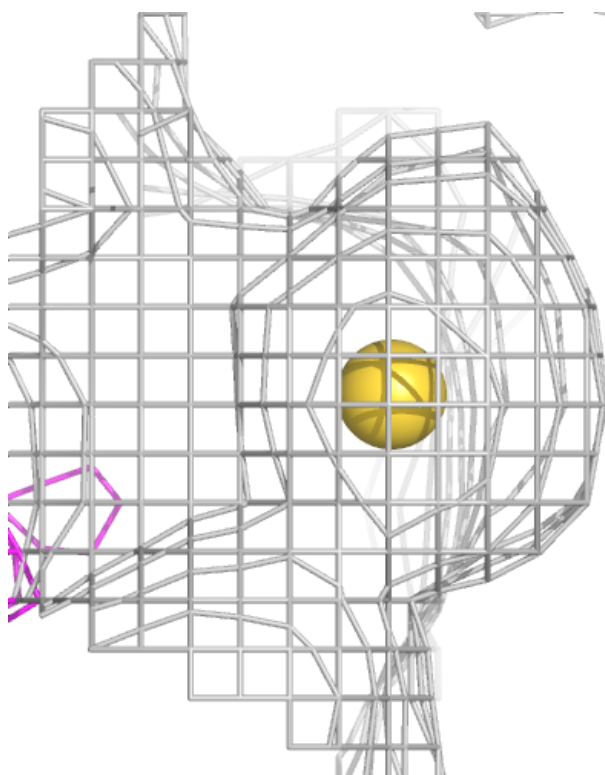
Electron density around MGD A 1101:

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



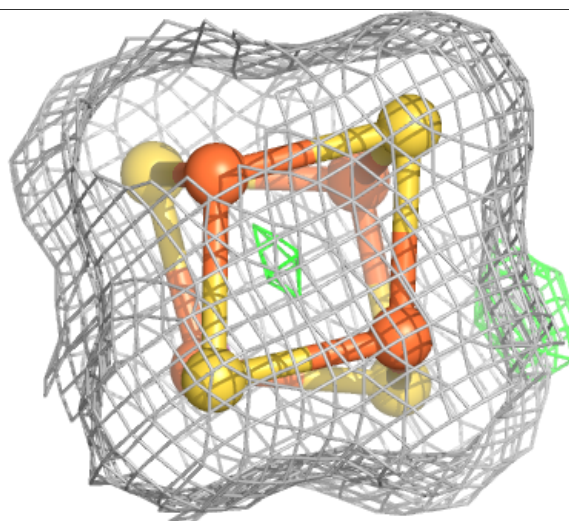
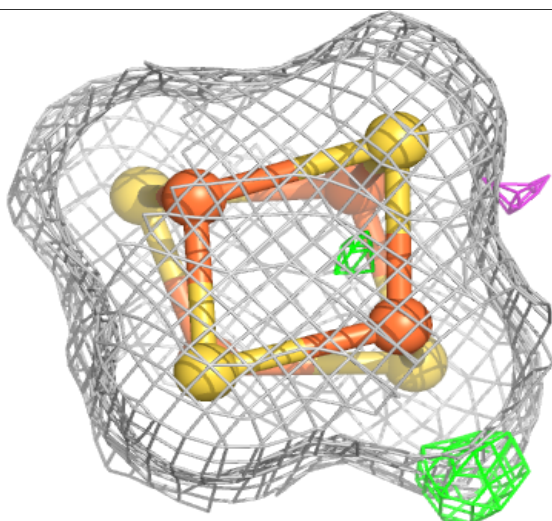
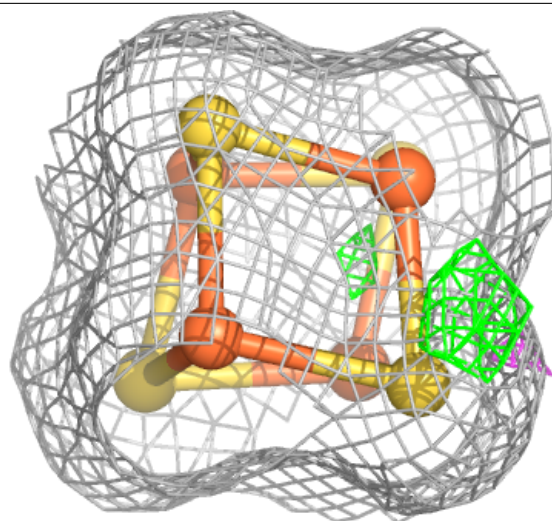
Electron density around H2S A 1104:

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



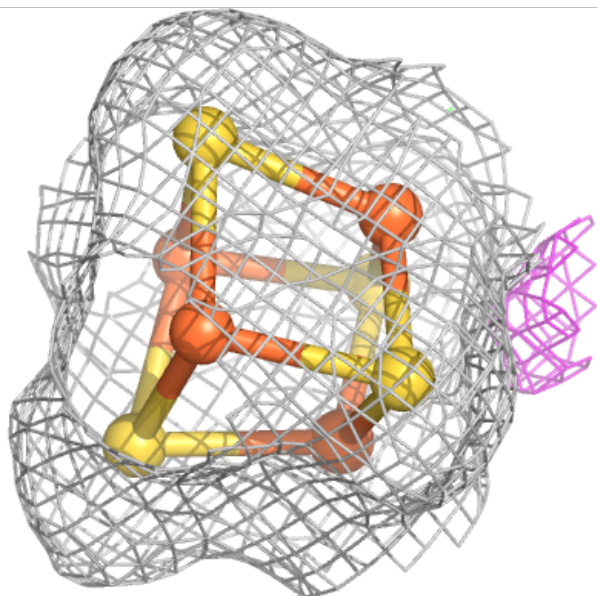
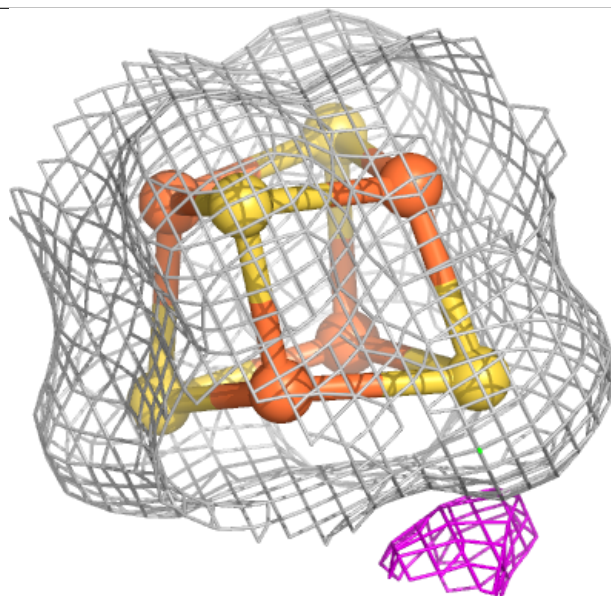
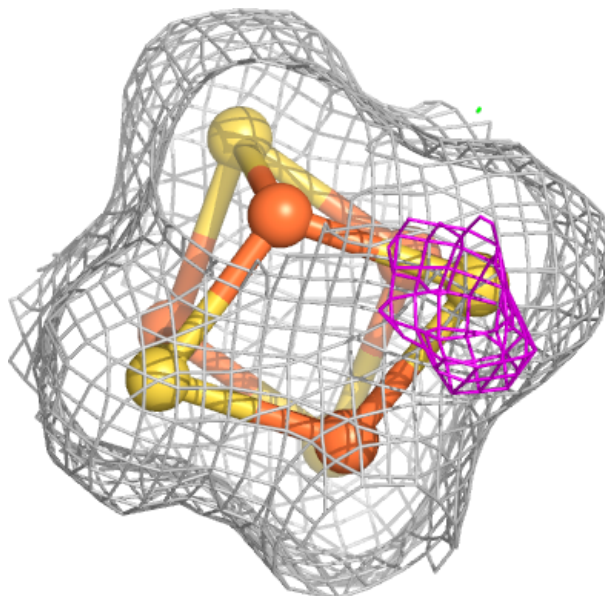
Electron density around SF4 B 301:

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



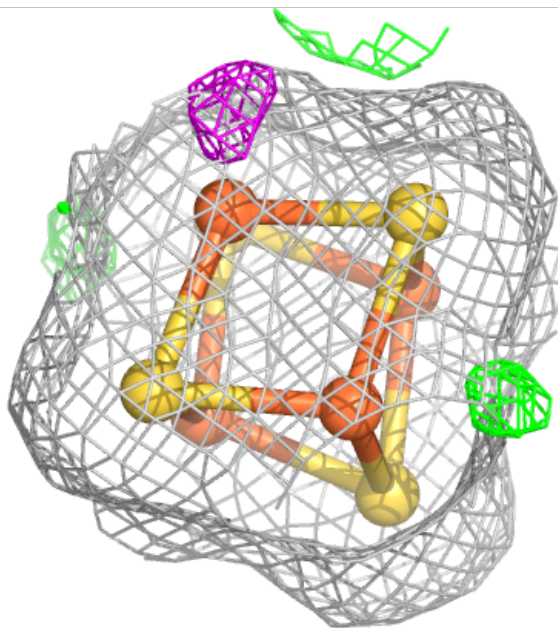
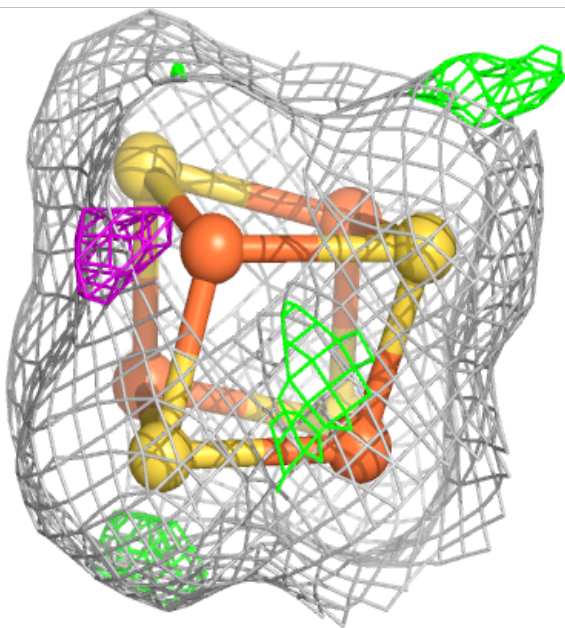
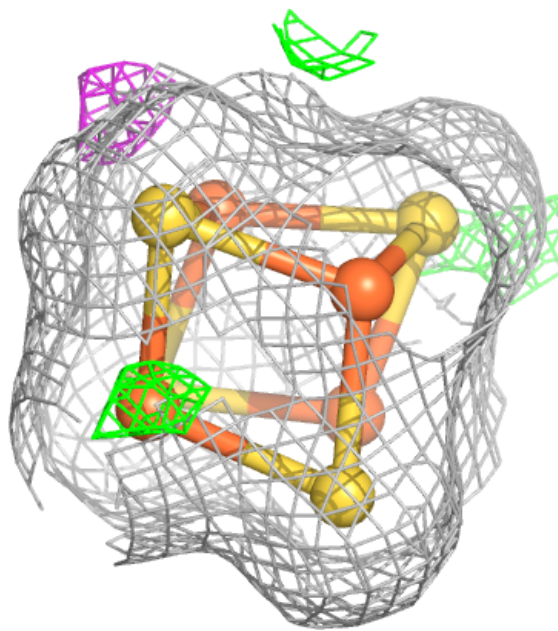
Electron density around SF4 A 1103:

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



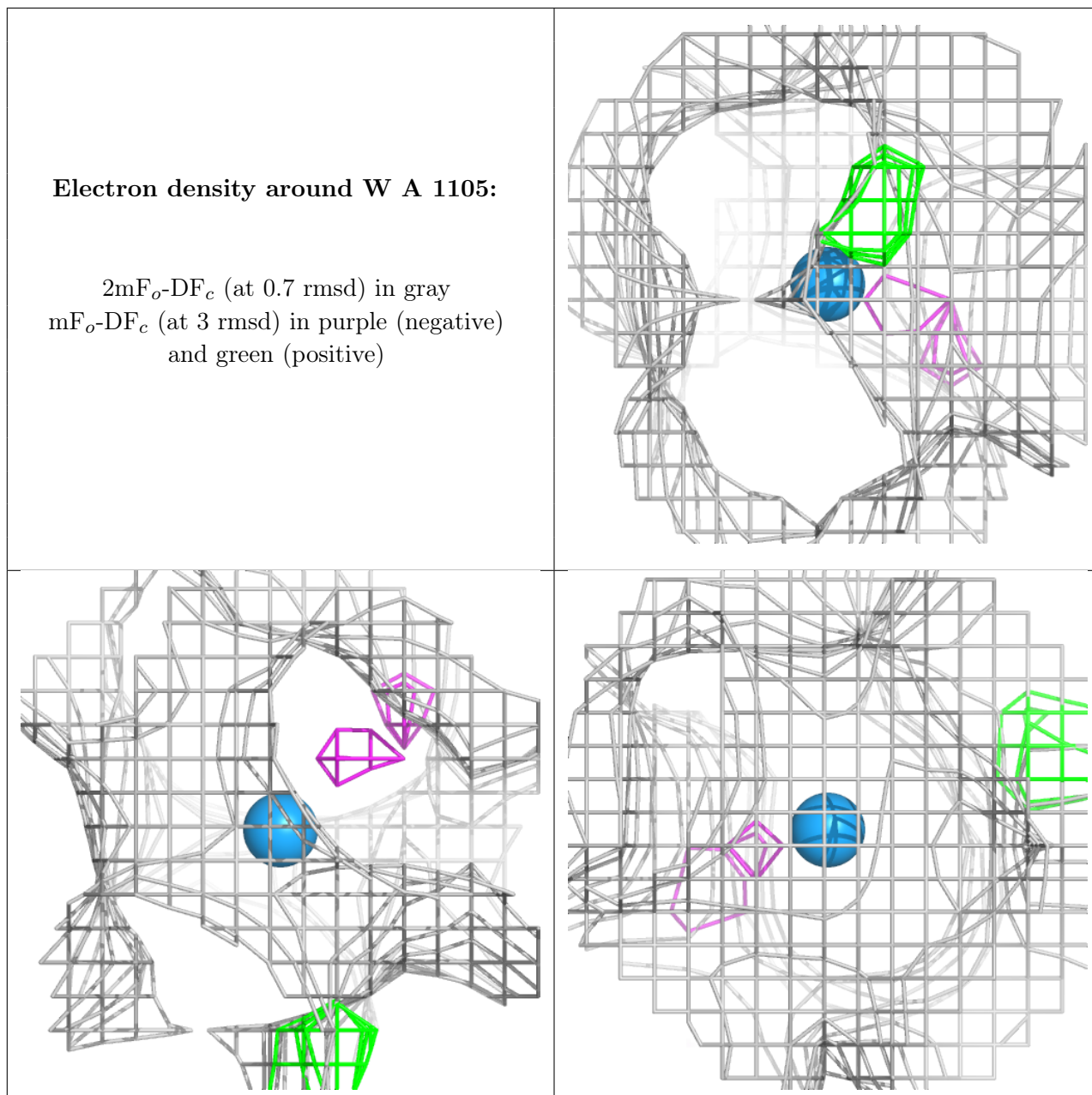
Electron density around SF4 B 303:

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



Electron density around W A 1105:

$2mF_o-DF_c$ (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.