



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 02:24 pm BST

PDB ID : 6ZRE / pdb_00006zre
Title : Deciphering the role of the channel constrictions in the opening mechanism of MexAB-OprM efflux pump from *Pseudomonas aeruginosa*
Authors : Ntsogo Enguene, Y.V.; Monlezun, L.; Ma, M.; Garnier, C.; Lascombe, M.B.; Salem, M.; Guenard, S.; Plesiat, P.; Llanes, C.; Phan, G.; Broutin, I.
Deposited on : 2020-07-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

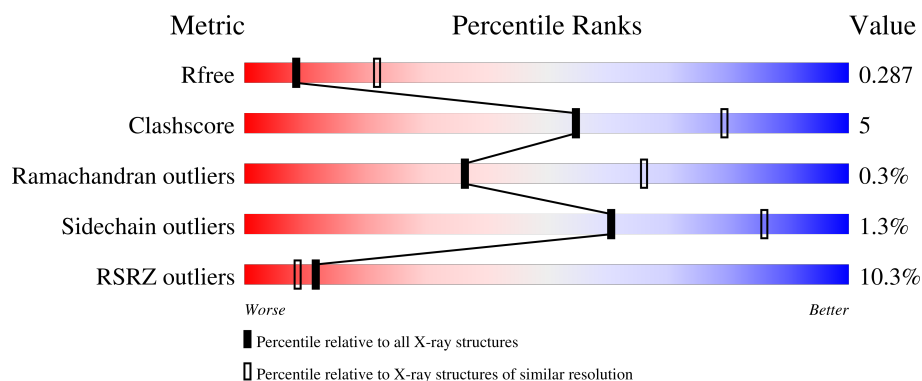
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	474	8% 85% 10% .
1	B	474	12% 84% 12% .

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
4	BOG	A	503	-	-	X	-
4	BOG	A	507	-	-	X	-
4	BOG	A	512	-	-	X	-
4	BOG	A	513	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7204 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.

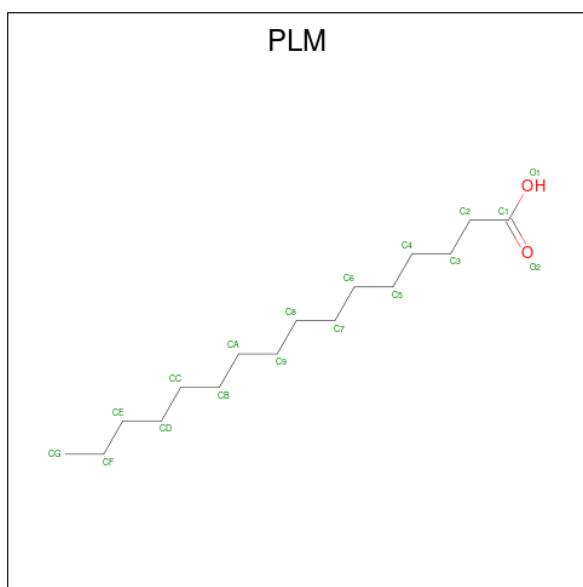
- Molecule 1 is a protein called Outer membrane protein OprM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	4	0	0
			3474	2178	615	678	3			
1	B	457	Total	C	N	O	S	4	0	0
			3490	2187	618	682	3			

There are 20 discrepancies between the modelled and reference sequences:

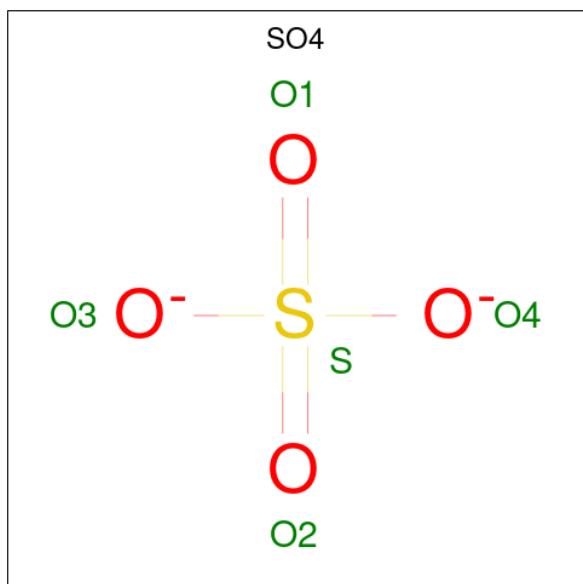
Chain	Residue	Modelled	Actual	Comment	Reference
A	403	LEU	ARG	engineered mutation	UNP Q51487
A	404	PHE	TYR	engineered mutation	UNP Q51487
A	416	ALA	ASP	engineered mutation	UNP Q51487
A	419	ALA	ARG	engineered mutation	UNP Q51487
A	469	HIS	-	expression tag	UNP Q51487
A	470	HIS	-	expression tag	UNP Q51487
A	471	HIS	-	expression tag	UNP Q51487
A	472	HIS	-	expression tag	UNP Q51487
A	473	HIS	-	expression tag	UNP Q51487
A	474	HIS	-	expression tag	UNP Q51487
B	403	LEU	ARG	engineered mutation	UNP Q51487
B	404	PHE	TYR	engineered mutation	UNP Q51487
B	416	ALA	ASP	engineered mutation	UNP Q51487
B	419	ALA	ARG	engineered mutation	UNP Q51487
B	469	HIS	-	expression tag	UNP Q51487
B	470	HIS	-	expression tag	UNP Q51487
B	471	HIS	-	expression tag	UNP Q51487
B	472	HIS	-	expression tag	UNP Q51487
B	473	HIS	-	expression tag	UNP Q51487
B	474	HIS	-	expression tag	UNP Q51487

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



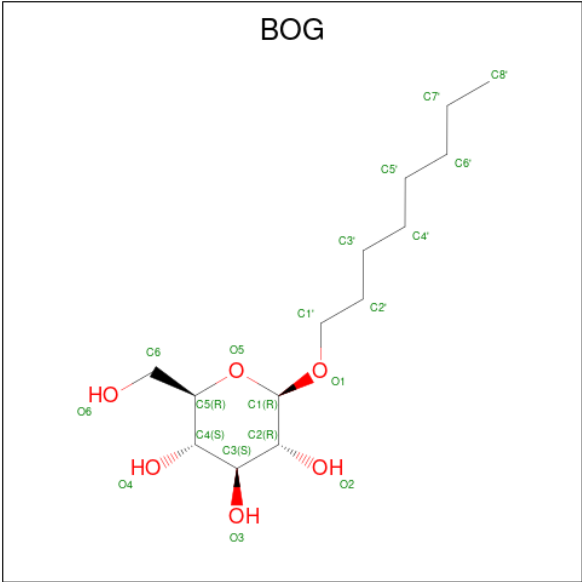
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆) (labeled as "Ligand of Interest" by depositor).

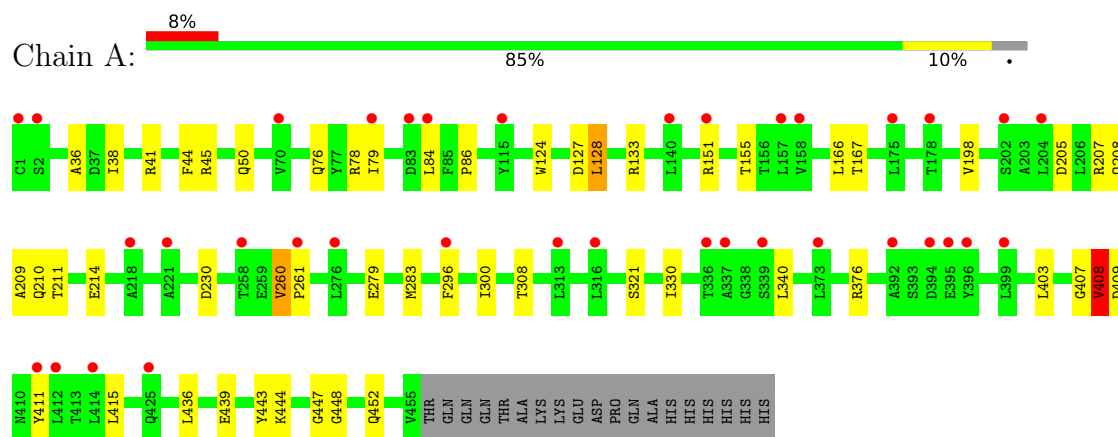


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		

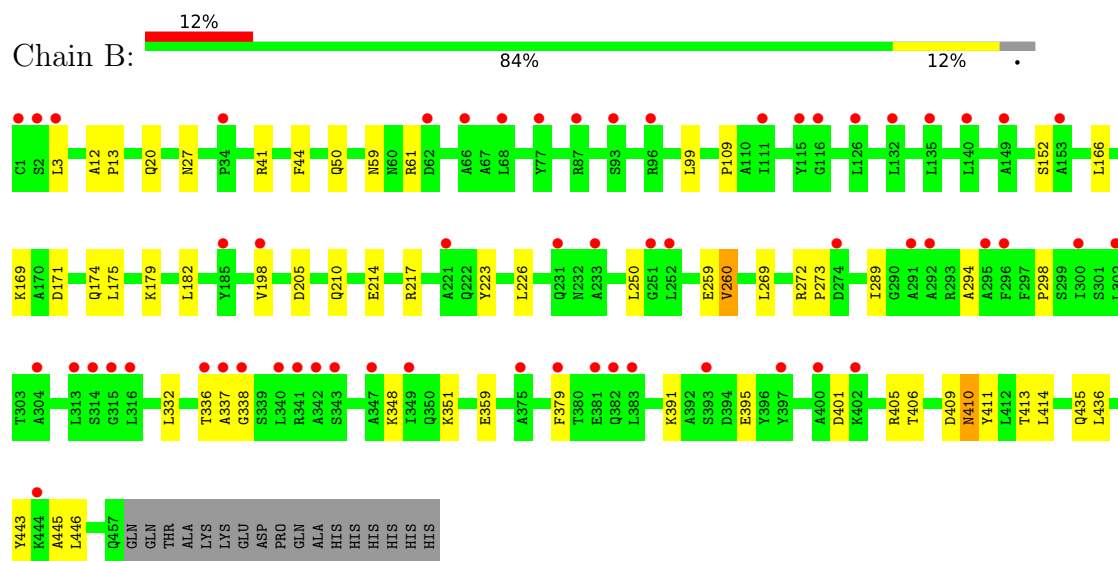
3 Residue-property plots [i](#)

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: Outer membrane protein OprM



• Molecule 1: Outer membrane protein OprM



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	86.80Å 86.80Å 1046.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.63 – 2.80 47.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.63-2.80) 99.7 (47.63-2.80)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.293 , 0.318 0.289 , 0.287	Depositor DCC
R_{free} test set	2160 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	97.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7204	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.77% 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, PLM, BOG

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	0.30	0/3530	0.45	0/4803
1	B	0.15	0/3546	0.28	0/4825
All	All	0.24	0/7076	0.37	0/9628

There are no bond length outliers.

There are no bond angle outliers.

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	3474	0	3456	33	0
1	B	3490	0	3472	32	0
2	A	17	0	31	2	0
3	A	5	0	0	1	0
4	A	218	0	301	7	144
All	All	7204	0	7260	70	144

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 (70) 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:208:GLN:HG3	1:A:415:LEU:HD12	1.64	0.79
1:A:41:ARG:NH2	1:A:452:GLN:OE1	2.16	0.79
1:B:409:ASP:O	1:B:410:ASN:ND2	2.25	0.70
1:A:209:ALA:HB2	1:A:411:TYR:HE2	1.57	0.68
1:B:401:ASP:OD2	1:B:405:ARG:NH1	2.27	0.68
1:B:152:SER:HB2	1:B:273:PRO:HB2	1.78	0.65
1:B:413:THR:O	1:B:414:LEU:HG	2.03	0.59
1:B:59:ASN:O	1:B:61:ARG:NH1	2.35	0.59
1:A:308:THR:HB	4:A:508:BOG:H1'1	1.84	0.58
4:A:507:BOG:H5'1	4:A:511:BOG:H5'1	1.85	0.58
1:A:376:ARG:NH2	1:A:439:GLU:OE2	2.30	0.58
1:A:209:ALA:HB2	1:A:411:TYR:CE2	2.38	0.57
1:B:166:LEU:HD13	1:B:436:LEU:HB3	1.86	0.57
1:B:336:THR:O	1:B:338:GLY:N	2.39	0.55
1:A:128:LEU:HD13	1:A:300:ILE:HD12	1.88	0.54
1:B:210:GLN:O	1:B:214:GLU:HG2	2.08	0.54
1:A:407:GLY:O	1:A:409:ASP:N	2.40	0.54
4:A:504:BOG:O6	4:A:510:BOG:O6	2.23	0.53
1:B:272:ARG:NH1	1:B:445:ALA:O	2.41	0.52
1:B:413:THR:HG22	1:B:414:LEU:H	1.74	0.52
1:B:289:ILE:HD11	1:B:348:LYS:HA	1.91	0.52
1:B:12:ALA:HB2	1:B:269:LEU:HD11	1.91	0.52
1:A:296:PHE:CZ	1:A:340:LEU:HB3	2.45	0.51
1:A:260:VAL:HG22	1:A:261:PRO:HD2	1.92	0.51
4:A:506:BOG:H3'1	4:A:506:BOG:H2	1.93	0.50
1:B:205:ASP:HB3	1:B:411:TYR:CD2	2.47	0.50
1:A:78:ARG:NH1	3:A:502:SO4:O2	2.44	0.50
1:A:210:GLN:O	1:A:214:GLU:HG2	2.12	0.49
1:A:45:ARG:NH2	1:B:406:THR:O	2.46	0.48
1:A:84:LEU:HD21	1:A:133:ARG:HG3	1.95	0.48
1:A:167:THR:HG22	1:A:230:ASP:OD2	2.14	0.48
1:B:169:LYS:NZ	1:B:250:LEU:O	2.43	0.48
1:A:41:ARG:O	1:A:50:GLN:NE2	2.47	0.48
1:A:86:PRO:HD3	1:A:124:TRP:CE2	2.48	0.47
1:A:205:ASP:HB3	1:A:411:TYR:CD2	2.50	0.47
1:A:36:ALA:HB2	1:A:447:GLY:HA3	1.97	0.47
1:B:41:ARG:O	1:B:50:GLN:NE2	2.47	0.47
1:B:20:GLN:HE22	1:B:27:ASN:H	1.62	0.47
4:A:507:BOG:C5'	4:A:511:BOG:H5'1	2.43	0.47
1:B:44:PHE:O	1:B:50:GLN:NE2	2.44	0.47
1:B:174:GLN:HB3	1:B:223:TYR:CE2	2.50	0.47
1:B:166:LEU:HD22	1:B:436:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:BOG:H2'1	4:A:503:BOG:H5'1	1.65	0.45
4:A:507:BOG:H7'1	4:A:507:BOG:H4'1	1.65	0.45
1:A:151:ARG:O	1:A:155:THR:HG23	2.17	0.45
1:A:38:ILE:O	1:A:443:TYR:OH	2.24	0.44
1:A:308:THR:HG1	1:A:321:SER:HG	1.62	0.44
1:A:444:LYS:HA	1:A:448:GLY:HA2	2.00	0.43
1:B:391:LYS:O	1:B:395:GLU:HG2	2.18	0.43
1:B:171:ASP:OD2	1:B:226:LEU:HB3	2.19	0.43
1:B:13:PRO:HG3	1:B:359:GLU:HB3	2.01	0.43
1:B:99:LEU:O	1:B:109:PRO:HA	2.18	0.43
1:A:86:PRO:HD3	1:A:124:TRP:CZ2	2.54	0.42
1:B:182:LEU:HD21	1:B:217:ARG:HH11	1.83	0.42
1:B:379:PHE:CD2	1:B:435:GLN:HA	2.55	0.42
1:A:166:LEU:HD13	1:A:436:LEU:HB3	2.02	0.42
1:A:207:ARG:O	1:A:211:THR:HG23	2.20	0.42
1:B:175:LEU:HG	1:B:179:LYS:HE3	2.02	0.42
1:A:279:GLU:O	1:A:283:MET:HG3	2.20	0.42
1:A:296:PHE:CZ	1:A:340:LEU:C	2.98	0.41
1:B:260:VAL:HG21	1:B:443:TYR:CD1	2.55	0.41
1:B:3:LEU:HD12	1:B:294:ALA:HA	2.02	0.41
1:B:298:PRO:HG3	1:B:332:LEU:HD13	2.02	0.41
1:A:403:LEU:O	1:A:408:VAL:HG13	2.21	0.41
1:B:272:ARG:HA	1:B:273:PRO:HD3	1.97	0.41
1:A:76:GLN:O	1:A:79:ILE:HG22	2.21	0.41
1:A:330:ILE:HD11	2:A:501:PLM:HC1	2.02	0.41
1:A:44:PHE:O	1:A:50:GLN:NE2	2.39	0.40
1:A:128:LEU:HD21	2:A:501:PLM:H51	2.03	0.40
1:B:289:ILE:HD12	1:B:351:LYS:HD2	2.03	0.40

All (144) 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)
4:A:507:BOG:C2	4:A:512:BOG:C2[2_665]	0.06	2.14
4:A:507:BOG:C6'	4:A:512:BOG:C6'[2_665]	0.10	2.10
4:A:503:BOG:O6	4:A:513:BOG:O6[5_665]	0.11	2.09
4:A:507:BOG:C3	4:A:512:BOG:C3[2_665]	0.26	1.94
4:A:503:BOG:C6	4:A:513:BOG:C6[5_665]	0.36	1.84
4:A:503:BOG:C5	4:A:513:BOG:C5[5_665]	0.37	1.83
4:A:503:BOG:C3'	4:A:513:BOG:C4'[5_665]	0.37	1.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:507:BOG:C1	4:A:512:BOG:C1[2_665]	0.38	1.82
4:A:503:BOG:O5	4:A:513:BOG:O5[5_665]	0.39	1.81
4:A:507:BOG:O2	4:A:512:BOG:O2[2_665]	0.39	1.81
4:A:507:BOG:C1'	4:A:512:BOG:C1'[2_665]	0.40	1.80
4:A:503:BOG:O4	4:A:513:BOG:O4[5_665]	0.41	1.79
4:A:503:BOG:C4	4:A:513:BOG:C4[5_665]	0.42	1.78
4:A:503:BOG:C3	4:A:513:BOG:C3[5_665]	0.44	1.76
4:A:503:BOG:C1	4:A:513:BOG:C1[5_665]	0.44	1.76
4:A:503:BOG:O2	4:A:513:BOG:O2[5_665]	0.46	1.74
4:A:503:BOG:C1'	4:A:513:BOG:C1'[5_665]	0.46	1.74
4:A:503:BOG:O3	4:A:513:BOG:O3[5_665]	0.46	1.74
4:A:503:BOG:C2	4:A:513:BOG:C2[5_665]	0.48	1.72
4:A:503:BOG:O1	4:A:513:BOG:O1[5_665]	0.52	1.68
4:A:507:BOG:O3	4:A:512:BOG:O3[2_665]	0.53	1.67
4:A:507:BOG:C4	4:A:512:BOG:C4[2_665]	0.53	1.67
4:A:503:BOG:C4'	4:A:513:BOG:C5'[5_665]	0.55	1.65
4:A:507:BOG:O5	4:A:512:BOG:O5[2_665]	0.59	1.61
4:A:507:BOG:C8'	4:A:512:BOG:C8'[2_665]	0.62	1.58
4:A:507:BOG:C5	4:A:512:BOG:C5[2_665]	0.63	1.57
4:A:507:BOG:O1	4:A:512:BOG:O1[2_665]	0.66	1.54
4:A:507:BOG:C6	4:A:512:BOG:O6[2_665]	0.69	1.51
4:A:507:BOG:O4	4:A:512:BOG:O4[2_665]	0.75	1.45
4:A:503:BOG:C2'	4:A:513:BOG:C2'[5_665]	0.77	1.43
4:A:503:BOG:C2'	4:A:513:BOG:C3'[5_665]	0.81	1.39
4:A:507:BOG:C3'	4:A:512:BOG:C3'[2_665]	0.82	1.38
4:A:507:BOG:O6	4:A:512:BOG:C6[2_665]	0.84	1.36
4:A:507:BOG:C4'	4:A:512:BOG:C4'[2_665]	0.88	1.32
4:A:507:BOG:O5	4:A:512:BOG:C5[2_665]	0.94	1.26
4:A:503:BOG:C1	4:A:513:BOG:O1[5_665]	0.97	1.23
4:A:503:BOG:O4	4:A:513:BOG:C4[5_665]	1.01	1.19
4:A:507:BOG:C5'	4:A:512:BOG:C5'[2_665]	1.01	1.19
4:A:503:BOG:C5'	4:A:513:BOG:C5'[5_665]	1.03	1.17
4:A:503:BOG:C3	4:A:513:BOG:C2[5_665]	1.04	1.16
4:A:507:BOG:C6	4:A:512:BOG:C6[2_665]	1.04	1.16
4:A:507:BOG:C2'	4:A:512:BOG:C2'[2_665]	1.05	1.15
4:A:507:BOG:C5	4:A:512:BOG:C4[2_665]	1.05	1.15
4:A:503:BOG:O1	4:A:513:BOG:C1'[5_665]	1.06	1.14
4:A:503:BOG:C5	4:A:513:BOG:O5[5_665]	1.10	1.10
4:A:507:BOG:C4'	4:A:512:BOG:C5'[2_665]	1.14	1.06
4:A:507:BOG:C1	4:A:512:BOG:O5[2_665]	1.14	1.06
4:A:507:BOG:C7'	4:A:512:BOG:C8'[2_665]	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:507:BOG:C7'	4:A:512:BOG:C7'[2_665]	1.18	1.02
4:A:507:BOG:C3'	4:A:512:BOG:C2'[2_665]	1.20	1.00
4:A:507:BOG:C2'	4:A:512:BOG:C3'[2_665]	1.20	1.00
4:A:507:BOG:O1	4:A:512:BOG:C1[2_665]	1.22	0.98
4:A:507:BOG:C5'	4:A:512:BOG:C4'[2_665]	1.24	0.96
4:A:503:BOG:C4'	4:A:513:BOG:C4'[5_665]	1.25	0.95
4:A:507:BOG:C4	4:A:512:BOG:O4[2_665]	1.25	0.95
4:A:503:BOG:C1'	4:A:513:BOG:C2'[5_665]	1.26	0.94
4:A:503:BOG:C3'	4:A:513:BOG:C3'[5_665]	1.26	0.94
4:A:503:BOG:C2	4:A:513:BOG:C1[5_665]	1.27	0.93
4:A:507:BOG:C4	4:A:512:BOG:C3[2_665]	1.27	0.93
4:A:507:BOG:C3'	4:A:512:BOG:C4'[2_665]	1.27	0.93
4:A:507:BOG:C1'	4:A:512:BOG:O1[2_665]	1.28	0.92
4:A:507:BOG:C3	4:A:512:BOG:O3[2_665]	1.28	0.92
4:A:507:BOG:O6	4:A:512:BOG:O6[2_665]	1.28	0.92
4:A:503:BOG:C2	4:A:513:BOG:O2[5_665]	1.29	0.91
4:A:503:BOG:O6	4:A:513:BOG:C6[5_665]	1.30	0.90
4:A:503:BOG:O3	4:A:513:BOG:C3[5_665]	1.30	0.90
4:A:503:BOG:C4'	4:A:513:BOG:C6'[5_665]	1.33	0.87
4:A:507:BOG:C4'	4:A:512:BOG:C3'[2_665]	1.34	0.86
4:A:503:BOG:C4	4:A:513:BOG:C3[5_665]	1.36	0.84
4:A:507:BOG:O2	4:A:512:BOG:C2[2_665]	1.37	0.83
4:A:503:BOG:C4	4:A:513:BOG:C5[5_665]	1.38	0.82
4:A:507:BOG:C8'	4:A:512:BOG:C7'[2_665]	1.38	0.82
4:A:503:BOG:O5	4:A:513:BOG:C1[5_665]	1.39	0.81
4:A:503:BOG:C6	4:A:513:BOG:C5[5_665]	1.40	0.80
4:A:507:BOG:O1	4:A:512:BOG:C1'[2_665]	1.41	0.79
4:A:507:BOG:C6'	4:A:512:BOG:C7'[2_665]	1.43	0.77
4:A:507:BOG:C2	4:A:512:BOG:C3[2_665]	1.44	0.76
4:A:507:BOG:C1'	4:A:512:BOG:C2'[2_665]	1.46	0.74
4:A:507:BOG:C3	4:A:512:BOG:C2[2_665]	1.46	0.74
4:A:507:BOG:C2	4:A:512:BOG:C1[2_665]	1.47	0.73
4:A:503:BOG:C6	4:A:513:BOG:O6[5_665]	1.48	0.72
4:A:507:BOG:C2	4:A:512:BOG:O2[2_665]	1.48	0.72
4:A:507:BOG:C5'	4:A:512:BOG:C6'[2_665]	1.49	0.71
4:A:507:BOG:C1	4:A:512:BOG:C2[2_665]	1.54	0.66
4:A:507:BOG:C6'	4:A:512:BOG:C5'[2_665]	1.55	0.65
4:A:507:BOG:C2'	4:A:512:BOG:C1'[2_665]	1.55	0.65
4:A:507:BOG:C7'	4:A:512:BOG:C6'[2_665]	1.58	0.62
4:A:507:BOG:C1	4:A:512:BOG:O1[2_665]	1.60	0.60
4:A:507:BOG:C5	4:A:512:BOG:C6[2_665]	1.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:BOG:C5	4:A:513:BOG:C6[5_665]	1.64	0.56
4:A:507:BOG:O3	4:A:512:BOG:C3[2_665]	1.65	0.55
4:A:503:BOG:C1	4:A:513:BOG:O5[5_665]	1.67	0.53
4:A:503:BOG:O2	4:A:513:BOG:C2[5_665]	1.67	0.53
4:A:503:BOG:C3	4:A:513:BOG:O3[5_665]	1.70	0.50
4:A:503:BOG:C3	4:A:513:BOG:C4[5_665]	1.70	0.50
4:A:503:BOG:C2'	4:A:513:BOG:C4'[5_665]	1.71	0.49
4:A:507:BOG:C3	4:A:512:BOG:C4[2_665]	1.72	0.48
4:A:503:BOG:C5	4:A:513:BOG:C4[5_665]	1.73	0.47
4:A:507:BOG:C6	4:A:512:BOG:C5[2_665]	1.74	0.46
4:A:507:BOG:O1	4:A:512:BOG:O5[2_665]	1.74	0.46
4:A:503:BOG:O1	4:A:513:BOG:C1[5_665]	1.76	0.44
4:A:507:BOG:C5	4:A:512:BOG:O4[2_665]	1.78	0.42
4:A:507:BOG:O4	4:A:512:BOG:C4[2_665]	1.79	0.41
4:A:507:BOG:C7'	4:A:512:BOG:C5'[2_665]	1.79	0.41
4:A:503:BOG:C1'	4:A:513:BOG:O1[5_665]	1.80	0.40
4:A:503:BOG:C1	4:A:513:BOG:C2[5_665]	1.80	0.40
4:A:503:BOG:O1	4:A:513:BOG:C2'[5_665]	1.81	0.39
4:A:503:BOG:C4	4:A:513:BOG:O4[5_665]	1.82	0.38
4:A:503:BOG:O5	4:A:513:BOG:C5[5_665]	1.82	0.38
4:A:503:BOG:C3'	4:A:513:BOG:C5'[5_665]	1.83	0.37
4:A:503:BOG:C1	4:A:513:BOG:C1'[5_665]	1.84	0.36
4:A:503:BOG:C2	4:A:513:BOG:O1[5_665]	1.84	0.36
4:A:507:BOG:C2'	4:A:512:BOG:O1[2_665]	1.84	0.36
4:A:507:BOG:O5	4:A:512:BOG:C1[2_665]	1.86	0.34
4:A:507:BOG:O5	4:A:512:BOG:C6[2_665]	1.87	0.33
4:A:503:BOG:C2	4:A:513:BOG:C3[5_665]	1.90	0.30
4:A:507:BOG:C4	4:A:512:BOG:O3[2_665]	1.93	0.27
4:A:503:BOG:C2'	4:A:513:BOG:C1'[5_665]	1.94	0.26
4:A:503:BOG:O3	4:A:513:BOG:C2[5_665]	1.94	0.26
4:A:503:BOG:O4	4:A:513:BOG:C3[5_665]	1.95	0.25
4:A:503:BOG:O5	4:A:513:BOG:O1[5_665]	1.98	0.22
4:A:503:BOG:C6'	4:A:513:BOG:C5'[5_665]	1.99	0.21
4:A:507:BOG:O5	4:A:512:BOG:C4[2_665]	1.99	0.21
4:A:503:BOG:C3	4:A:513:BOG:C1[5_665]	2.00	0.20
4:A:503:BOG:C3	4:A:513:BOG:O2[5_665]	2.00	0.20
4:A:507:BOG:C5	4:A:512:BOG:O5[2_665]	2.01	0.19
4:A:507:BOG:C4	4:A:512:BOG:C5[2_665]	2.01	0.19
4:A:503:BOG:C1'	4:A:513:BOG:C3'[5_665]	2.02	0.18
4:A:507:BOG:C6	4:A:512:BOG:C4[2_665]	2.03	0.17
4:A:503:BOG:C4	4:A:513:BOG:C2[5_665]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:507:BOG:C5	4:A:512:BOG:O6[2_665]	2.05	0.15
4:A:503:BOG:O4	4:A:513:BOG:C5[5_665]	2.08	0.12
4:A:507:BOG:C1'	4:A:512:BOG:C1[2_665]	2.08	0.12
4:A:507:BOG:C1	4:A:512:BOG:C5[2_665]	2.09	0.11
4:A:503:BOG:C4	4:A:513:BOG:O5[5_665]	2.10	0.10
4:A:503:BOG:C6	4:A:513:BOG:O5[5_665]	2.10	0.10
4:A:503:BOG:C5	4:A:513:BOG:C1[5_665]	2.11	0.09
4:A:507:BOG:C6	4:A:512:BOG:O4[2_665]	2.13	0.07
4:A:507:BOG:O2	4:A:512:BOG:C1[2_665]	2.14	0.06
4:A:503:BOG:C4'	4:A:513:BOG:C3'[5_665]	2.16	0.04
4:A:507:BOG:C3	4:A:512:BOG:O2[2_665]	2.16	0.04
4:A:507:BOG:C5	4:A:512:BOG:C3[2_665]	2.18	0.02
4:A:503:BOG:C5'	4:A:513:BOG:C4'[5_665]	2.19	0.01
4:A:507:BOG:O6	4:A:512:BOG:C5[2_665]	2.19	0.01

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	453/474 (96%)	441 (97%)	10 (2%)	2 (0%)	30	60
1	B	455/474 (96%)	439 (96%)	15 (3%)	1 (0%)	43	72
All	All	908/948 (96%)	880 (97%)	25 (3%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	VAL
1	B	337	ALA
1	A	127	ASP

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	356/373 (95%)	352 (99%)	4 (1%)	65	87
1	B	358/373 (96%)	353 (99%)	5 (1%)	59	85
All	All	714/746 (96%)	705 (99%)	9 (1%)	61	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	198	VAL
1	A	260	VAL
1	A	408	VAL
1	B	198	VAL
1	B	259	GLU
1	B	260	VAL
1	B	410	ASN
1	B	446	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	59	ASN
1	A	148	GLN
1	A	254	GLN
1	B	59	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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$
4	BOG	A	508	-	18,18,20	1.25	2 (11%)	23,23,25	0.84	0
4	BOG	A	512	-	20,20,20	1.28	3 (15%)	25,25,25	0.88	0
2	PLM	A	501	1	16,16,17	0.88	0	15,15,17	0.53	0
4	BOG	A	506	-	20,20,20	1.15	1 (5%)	25,25,25	1.68	7 (28%)
4	BOG	A	513	-	20,20,20	1.33	3 (15%)	25,25,25	1.17	1 (4%)
4	BOG	A	511	-	20,20,20	1.10	1 (5%)	25,25,25	0.92	0
4	BOG	A	505	-	20,20,20	1.20	2 (10%)	25,25,25	1.20	3 (12%)
4	BOG	A	509	-	20,20,20	1.14	1 (5%)	25,25,25	0.92	1 (4%)
4	BOG	A	504	-	20,20,20	1.21	2 (10%)	25,25,25	1.04	2 (8%)
4	BOG	A	507	-	20,20,20	1.38	3 (15%)	25,25,25	1.04	1 (4%)
4	BOG	A	510	-	20,20,20	1.17	1 (5%)	25,25,25	1.41	4 (16%)
3	SO4	A	502	-	4,4,4	0.14	0	6,6,6	0.22	0
4	BOG	A	503	-	20,20,20	1.20	3 (15%)	25,25,25	0.99	1 (4%)

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	BOG	A	508	-	-	4/9/29/31	0/1/1/1
4	BOG	A	512	-	-	5/11/31/31	0/1/1/1
2	PLM	A	501	1	-	7/13/14/15	-
4	BOG	A	506	-	-	6/11/31/31	0/1/1/1
4	BOG	A	513	-	-	8/11/31/31	0/1/1/1
4	BOG	A	511	-	-	4/11/31/31	0/1/1/1
4	BOG	A	505	-	-	6/11/31/31	0/1/1/1
4	BOG	A	509	-	-	7/11/31/31	0/1/1/1
4	BOG	A	504	-	-	9/11/31/31	0/1/1/1
4	BOG	A	507	-	-	6/11/31/31	0/1/1/1
4	BOG	A	510	-	-	9/11/31/31	0/1/1/1
4	BOG	A	503	-	-	5/11/31/31	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	513	BOG	O1-C1	-4.01	1.33	1.40
4	A	507	BOG	O1-C1	-3.80	1.33	1.40
4	A	510	BOG	O5-C1	3.71	1.51	1.41
4	A	508	BOG	O5-C1	3.65	1.51	1.41
4	A	506	BOG	O5-C1	3.61	1.51	1.41
4	A	504	BOG	O5-C1	3.58	1.51	1.41
4	A	509	BOG	O5-C1	3.55	1.50	1.41
4	A	505	BOG	O5-C1	3.43	1.50	1.41
4	A	511	BOG	O5-C1	3.42	1.50	1.41
4	A	512	BOG	O1-C1	-3.37	1.34	1.40
4	A	503	BOG	O1-C1	-2.94	1.35	1.40
4	A	507	BOG	O5-C1	2.80	1.49	1.41
4	A	512	BOG	O5-C1	2.75	1.48	1.41
4	A	503	BOG	O5-C1	2.49	1.48	1.41
4	A	507	BOG	C3-C2	-2.45	1.46	1.52
4	A	505	BOG	O1-C1	-2.42	1.36	1.40
4	A	513	BOG	C3-C2	-2.33	1.46	1.52
4	A	512	BOG	C3-C2	-2.33	1.46	1.52
4	A	513	BOG	O5-C1	2.30	1.47	1.41
4	A	508	BOG	O1-C1	-2.24	1.36	1.40
4	A	503	BOG	C3-C2	-2.18	1.46	1.52
4	A	504	BOG	O1-C1	-2.17	1.36	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	506	BOG	O3-C3-C2	-4.02	101.05	110.35
4	A	510	BOG	C1-C2-C3	3.41	117.09	110.00
4	A	505	BOG	O5-C5-C4	3.37	115.82	109.69
4	A	510	BOG	O5-C1-C2	3.11	116.93	110.35
4	A	506	BOG	C1-C2-C3	2.84	115.91	110.00
4	A	506	BOG	C4-C3-C2	2.80	115.70	110.82
4	A	510	BOG	O3-C3-C4	-2.65	104.22	110.35
4	A	506	BOG	O3-C3-C4	2.60	116.36	110.35
4	A	505	BOG	C3-C4-C5	2.60	114.88	110.24
4	A	504	BOG	O5-C5-C4	2.48	114.20	109.69
4	A	506	BOG	O5-C1-C2	2.37	115.36	110.35
4	A	504	BOG	C6-C5-C4	-2.26	107.71	113.00
4	A	505	BOG	C6-C5-C4	-2.24	107.77	113.00
4	A	503	BOG	C6-C5-C4	-2.18	107.89	113.00
4	A	510	BOG	O4-C4-C5	2.16	114.66	109.30
4	A	513	BOG	C1-O5-C5	-2.13	109.50	113.69
4	A	507	BOG	C6-C5-C4	-2.05	108.21	113.00
4	A	506	BOG	O4-C4-C3	-2.02	105.67	110.35
4	A	509	BOG	C1-C2-C3	2.00	114.16	110.00
4	A	506	BOG	O2-C2-C3	-2.00	105.72	110.35

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	BOG	C2'-C1'-O1-C1
4	A	506	BOG	C2-C1-O1-C1'
4	A	506	BOG	C2'-C1'-O1-C1
4	A	507	BOG	C2'-C1'-O1-C1
4	A	509	BOG	C2-C1-O1-C1'
4	A	509	BOG	C2'-C1'-O1-C1
4	A	511	BOG	C2'-C1'-O1-C1
4	A	512	BOG	C2'-C1'-O1-C1
4	A	505	BOG	O5-C5-C6-O6
4	A	504	BOG	O5-C5-C6-O6
4	A	509	BOG	O5-C5-C6-O6
4	A	506	BOG	C2'-C3'-C4'-C5'
4	A	503	BOG	C4-C5-C6-O6
4	A	504	BOG	C4-C5-C6-O6
4	A	505	BOG	C4-C5-C6-O6
4	A	506	BOG	O1-C1'-C2'-C3'
4	A	506	BOG	O5-C1-O1-C1'
4	A	509	BOG	O5-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
4	A	503	BOG	O5-C5-C6-O6
4	A	509	BOG	C4-C5-C6-O6
4	A	503	BOG	C2'-C3'-C4'-C5'
4	A	513	BOG	O1-C1'-C2'-C3'
4	A	513	BOG	C3'-C4'-C5'-C6'
4	A	509	BOG	C3'-C4'-C5'-C6'
4	A	513	BOG	C4-C5-C6-O6
4	A	510	BOG	C2-C1-O1-C1'
4	A	507	BOG	C3'-C4'-C5'-C6'
4	A	504	BOG	C2'-C3'-C4'-C5'
4	A	513	BOG	C2'-C3'-C4'-C5'
4	A	505	BOG	C3'-C4'-C5'-C6'
4	A	513	BOG	C4'-C5'-C6'-C7'
4	A	507	BOG	O5-C1-O1-C1'
4	A	512	BOG	C2'-C3'-C4'-C5'
2	A	501	PLM	CA-CB-CC-CD
4	A	508	BOG	O1-C1'-C2'-C3'
4	A	510	BOG	C4-C5-C6-O6
4	A	510	BOG	O5-C5-C6-O6
4	A	511	BOG	C3'-C4'-C5'-C6'
4	A	510	BOG	C1'-C2'-C3'-C4'
4	A	504	BOG	C2-C1-O1-C1'
4	A	507	BOG	C2-C1-O1-C1'
4	A	506	BOG	O5-C5-C6-O6
4	A	503	BOG	C3'-C4'-C5'-C6'
4	A	512	BOG	O5-C5-C6-O6
4	A	508	BOG	C1'-C2'-C3'-C4'
2	A	501	PLM	C7-C8-C9-CA
4	A	504	BOG	O1-C1'-C2'-C3'
4	A	512	BOG	C3'-C4'-C5'-C6'
4	A	509	BOG	C5'-C6'-C7'-C8'
4	A	510	BOG	C5'-C6'-C7'-C8'
4	A	511	BOG	C2'-C3'-C4'-C5'
4	A	512	BOG	C1'-C2'-C3'-C4'
4	A	513	BOG	O5-C5-C6-O6
4	A	508	BOG	C2'-C1'-O1-C1
4	A	510	BOG	C2'-C1'-O1-C1
4	A	508	BOG	C3'-C4'-C5'-C6'
4	A	507	BOG	C4'-C5'-C6'-C7'
2	A	501	PLM	C9-CA-CB-CC
4	A	513	BOG	C1'-C2'-C3'-C4'
4	A	510	BOG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
2	A	501	PLM	C8-C9-CA-CB
4	A	504	BOG	O5-C1-O1-C1'
2	A	501	PLM	CB-CC-CD-CE
4	A	504	BOG	C4'-C5'-C6'-C7'
4	A	504	BOG	C3'-C4'-C5'-C6'
4	A	507	BOG	O1-C1'-C2'-C3'
4	A	505	BOG	C5'-C6'-C7'-C8'
4	A	510	BOG	O1-C1'-C2'-C3'
2	A	501	PLM	C2-C3-C4-C5
4	A	510	BOG	O5-C1-O1-C1'
4	A	505	BOG	C1'-C2'-C3'-C4'
4	A	513	BOG	C2'-C1'-O1-C1
4	A	511	BOG	C4'-C5'-C6'-C7'
4	A	503	BOG	O5-C1-O1-C1'
2	A	501	PLM	C5-C6-C7-C8
4	A	505	BOG	O1-C1'-C2'-C3'

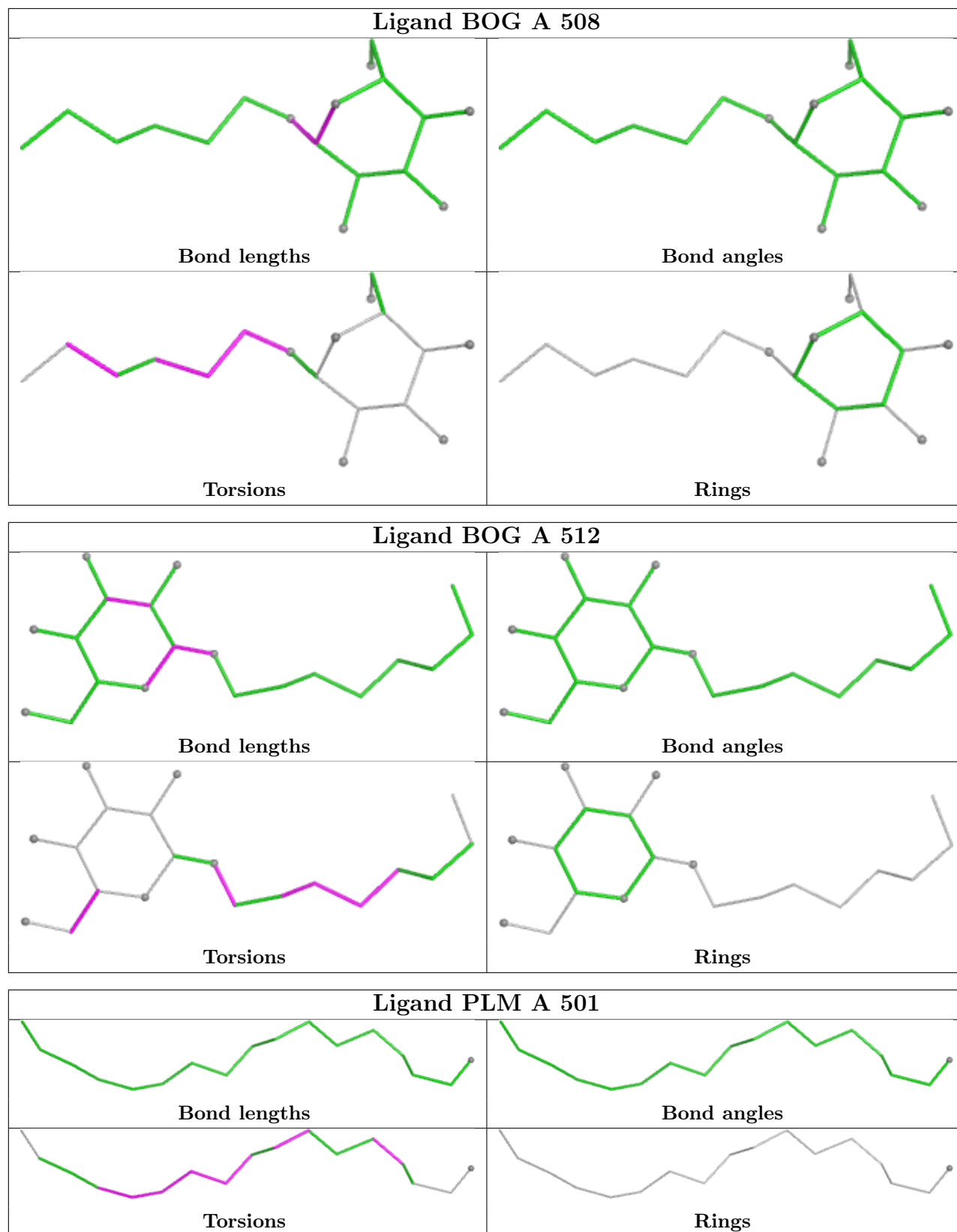
There are no ring outliers.

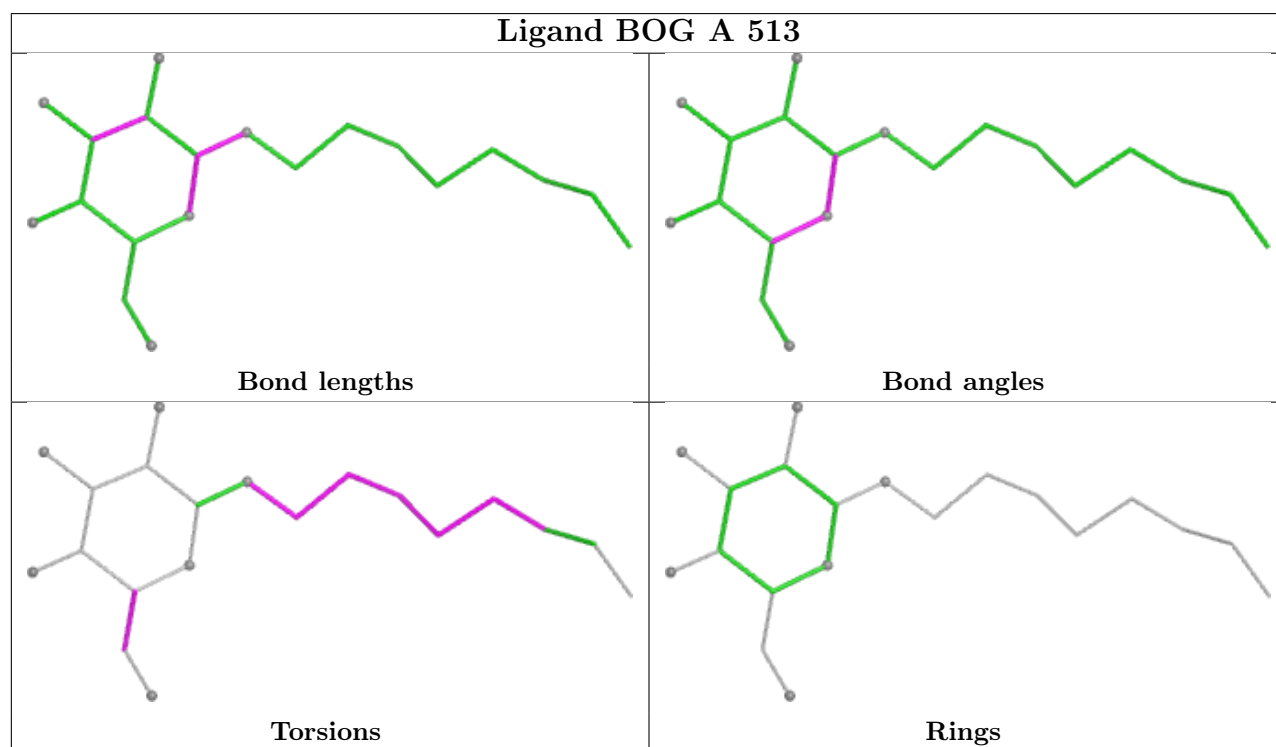
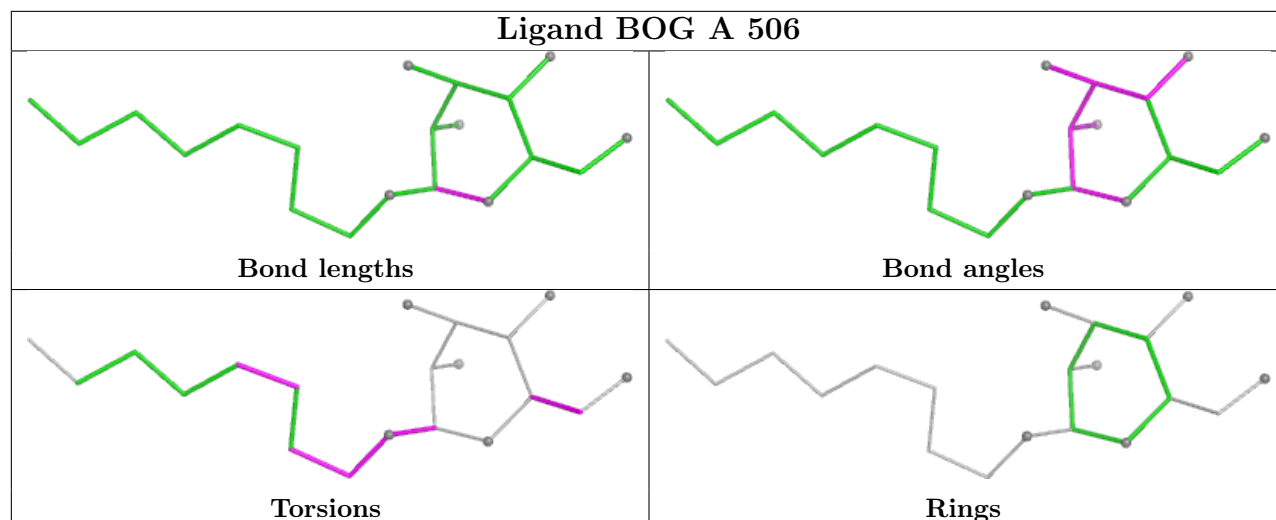
11 monomers are involved in 154 short contacts:

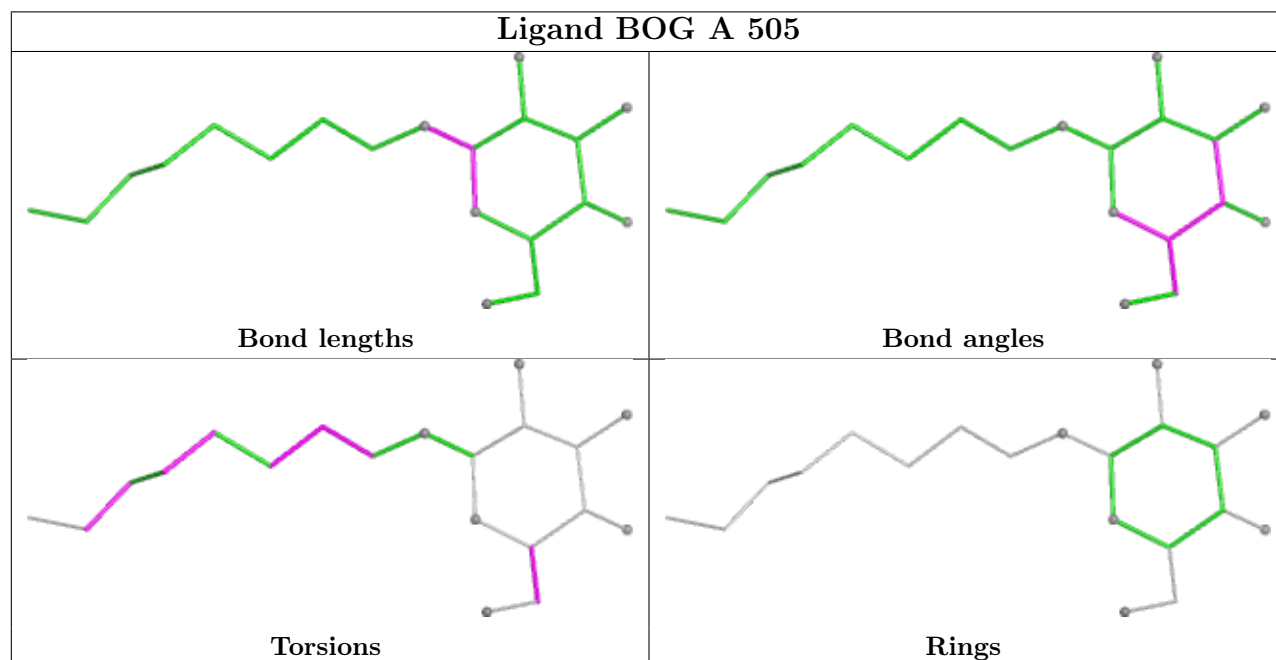
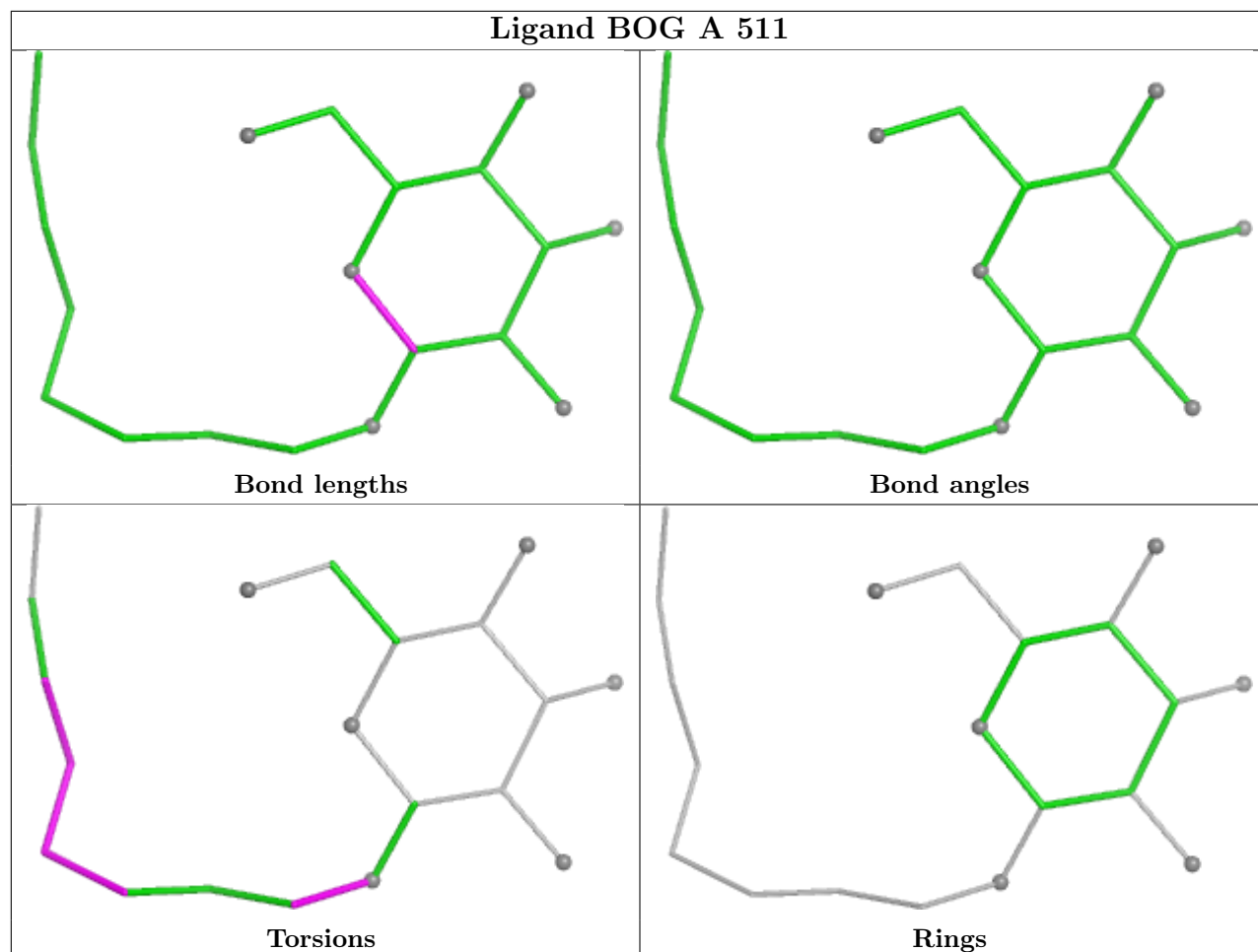
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	508	BOG	1	0
4	A	512	BOG	0	76
2	A	501	PLM	2	0
4	A	506	BOG	1	0
4	A	513	BOG	0	68
4	A	511	BOG	2	0
4	A	504	BOG	1	0
4	A	507	BOG	3	76
4	A	510	BOG	1	0
3	A	502	SO4	1	0
4	A	503	BOG	1	68

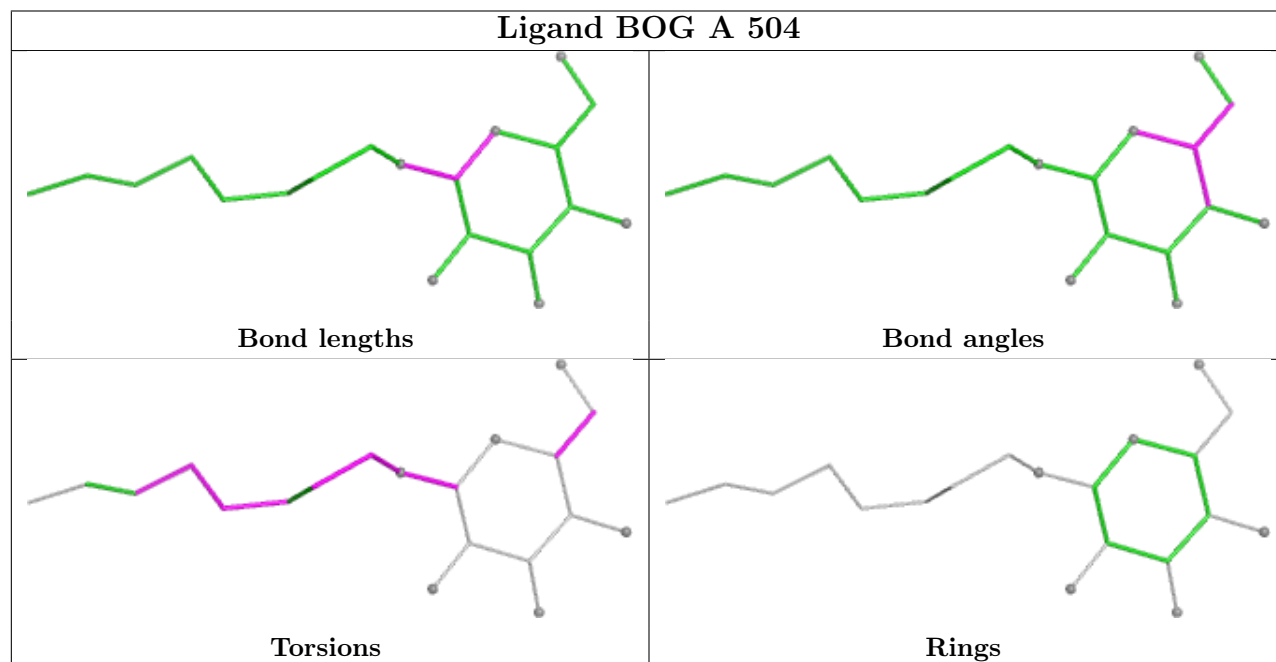
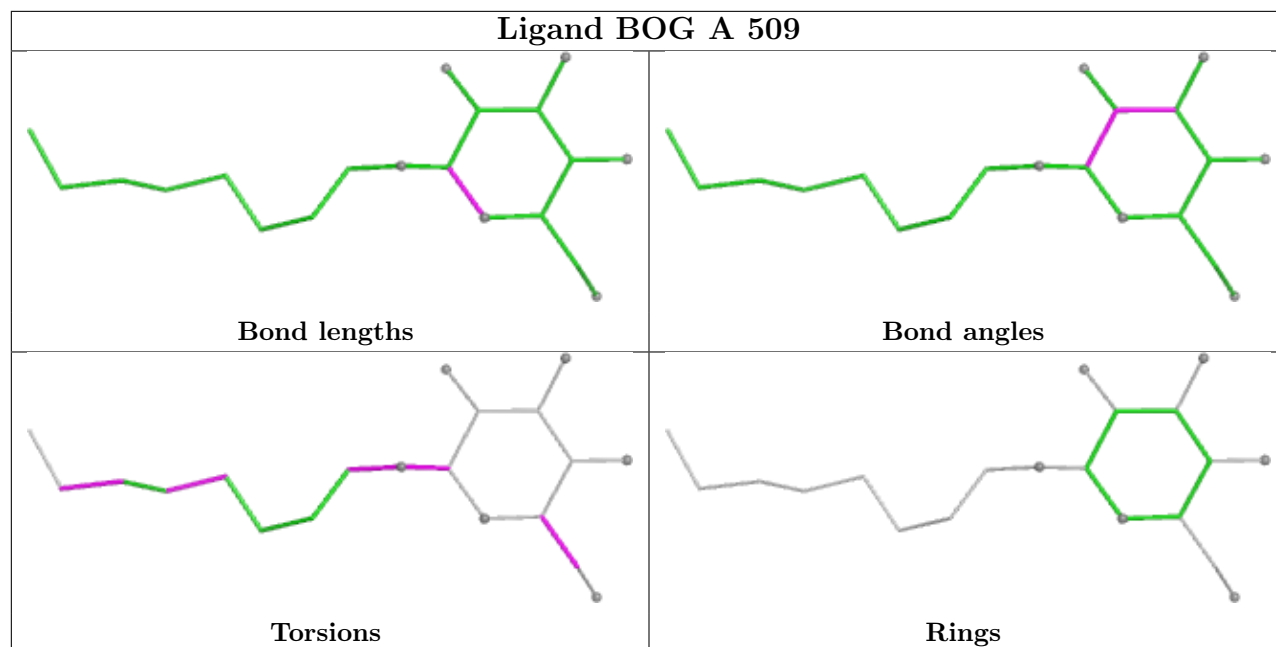
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

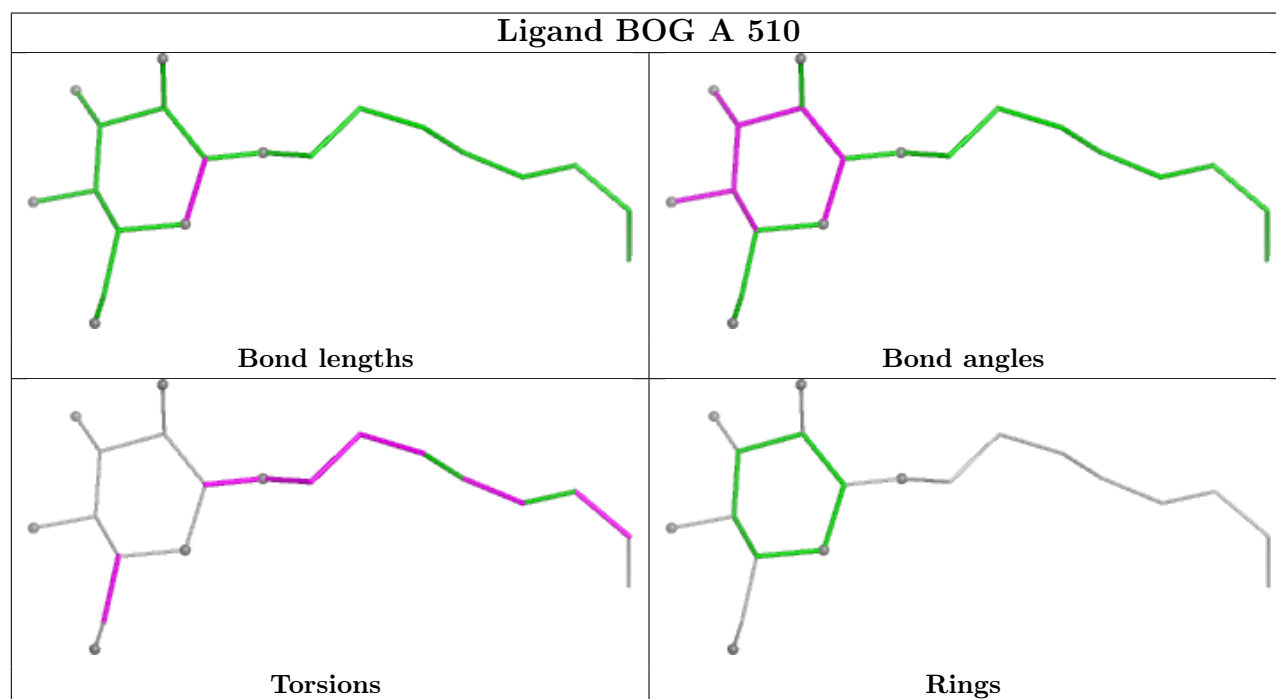
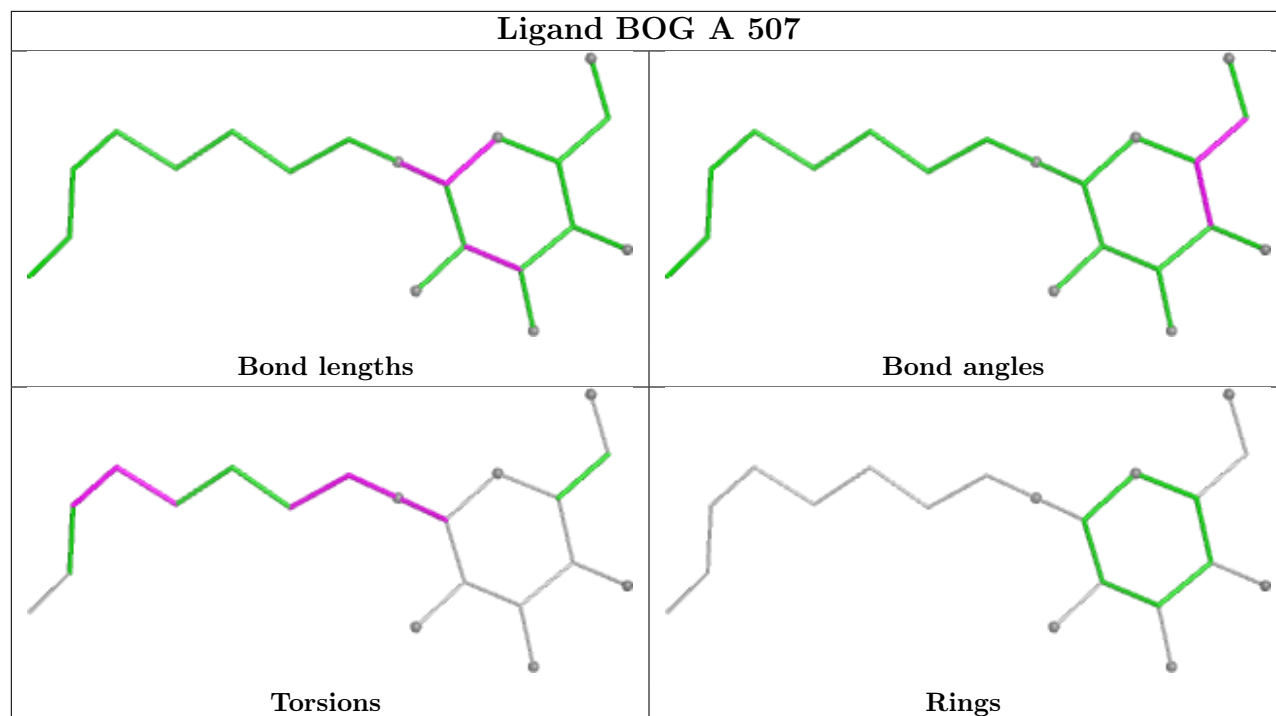
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



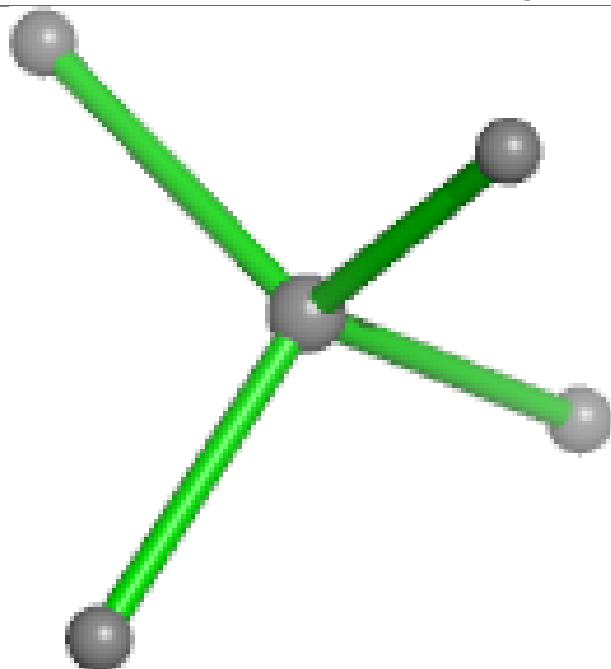




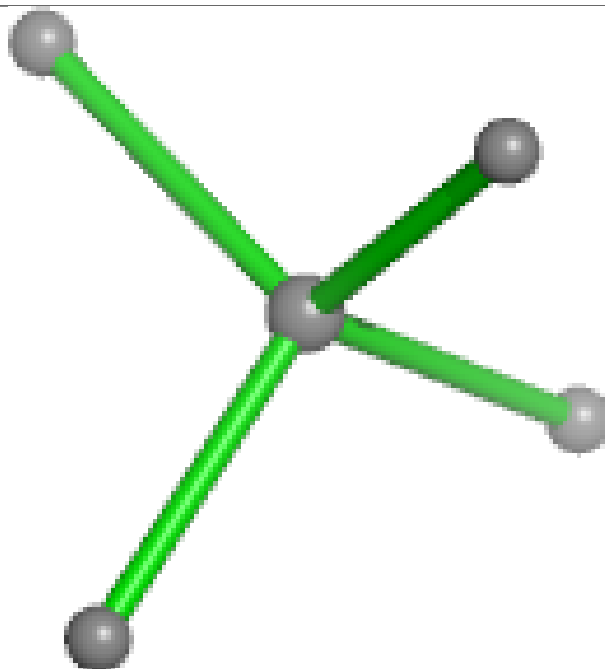




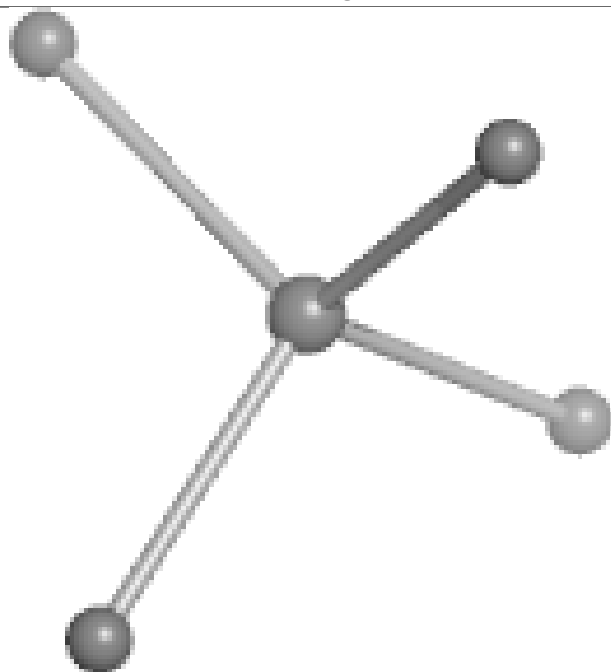
Ligand SO4 A 502



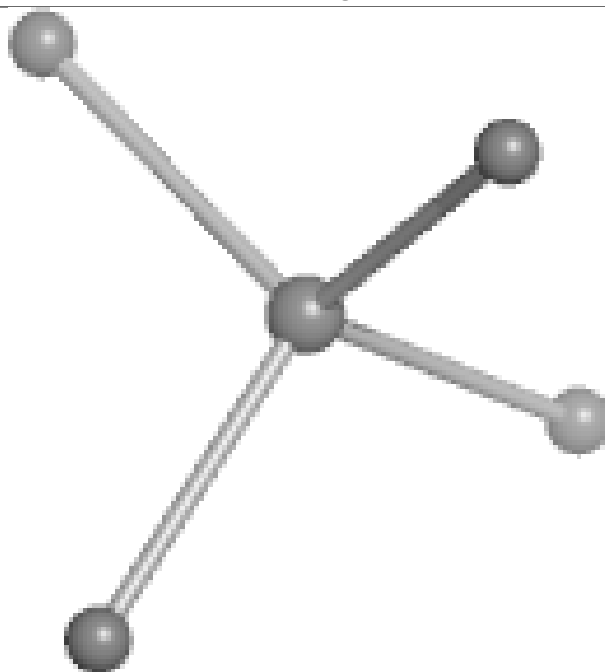
Bond lengths



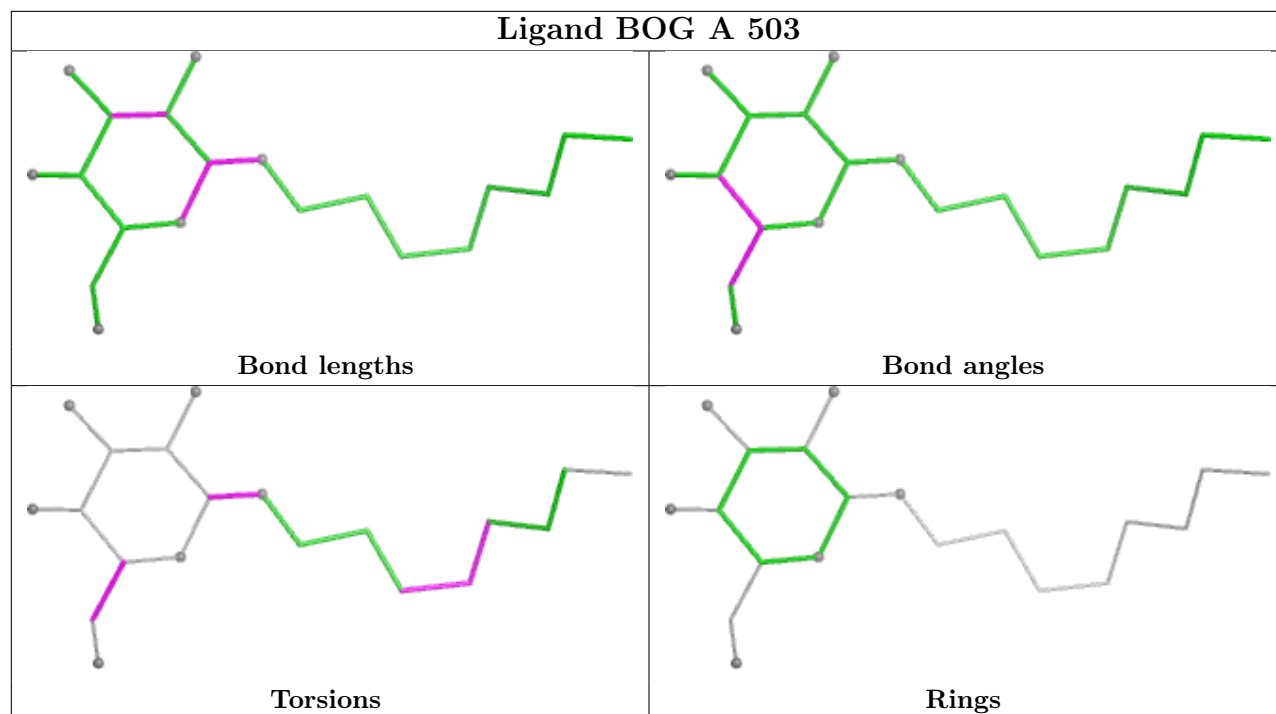
Bond angles



Torsions



Rings



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	455/474 (95%)	0.79	36 (7%) 18 13	32, 87, 138, 163	1 (0%)
1	B	457/474 (96%)	0.90	58 (12%) 8 6	59, 141, 187, 203	1 (0%)
All	All	912/948 (96%)	0.85	94 (10%) 12 9	32, 128, 172, 203	2 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	GLU	9.3
1	B	1	CYS	7.9
1	A	1	CYS	6.8
1	B	115	TYR	6.7
1	A	79	ILE	5.5
1	B	2	SER	4.9
1	B	116	GLY	4.8
1	A	218	ALA	4.3
1	B	77	TYR	4.0
1	A	2	SER	4.0
1	A	399	LEU	3.9
1	B	295	ALA	3.8
1	A	316	LEU	3.6
1	B	153	ALA	3.6
1	B	66	ALA	3.4
1	A	396	TYR	3.2
1	B	292	ALA	3.2
1	A	336	THR	3.2
1	B	349	ILE	3.2
1	A	115	TYR	3.1
1	A	221	ALA	3.1
1	B	185	TYR	3.1
1	B	314	SER	3.1
1	B	296	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	175	LEU	3.0
1	A	258	THR	3.0
1	B	382	GLN	2.9
1	B	140	LEU	2.9
1	B	87	ARG	2.9
1	B	340	LEU	2.9
1	B	343	SER	2.8
1	B	304	ALA	2.8
1	A	337	ALA	2.8
1	B	383	LEU	2.7
1	A	70	VAL	2.7
1	A	204	LEU	2.7
1	B	126	LEU	2.7
1	B	252	LEU	2.7
1	B	338	GLY	2.6
1	B	68	LEU	2.6
1	A	339	SER	2.6
1	B	96	ARG	2.6
1	B	313	LEU	2.6
1	A	296	PHE	2.6
1	B	111	ILE	2.6
1	B	274	ASP	2.6
1	A	83	ASP	2.5
1	A	411	TYR	2.5
1	B	397	TYR	2.5
1	B	149	ALA	2.5
1	B	341	ARG	2.5
1	B	444	LYS	2.5
1	B	93	SER	2.5
1	A	392	ALA	2.5
1	B	62	ASP	2.5
1	B	381	GLU	2.5
1	B	379	PHE	2.4
1	B	132	LEU	2.4
1	A	178	THR	2.4
1	B	251	GLY	2.4
1	B	198	VAL	2.4
1	A	313	LEU	2.3
1	B	400	ALA	2.3
1	B	402	LYS	2.3
1	B	336	THR	2.3
1	A	202	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	302	LEU	2.2
1	A	276	LEU	2.2
1	A	373	LEU	2.2
1	B	300	ILE	2.2
1	B	291	ALA	2.2
1	B	231	GLN	2.2
1	B	393	SER	2.2
1	A	157	LEU	2.2
1	A	414	LEU	2.2
1	B	221	ALA	2.2
1	B	337	ALA	2.2
1	A	425	GLN	2.2
1	A	158	VAL	2.2
1	B	3	LEU	2.2
1	A	261	PRO	2.1
1	A	84	LEU	2.1
1	A	151	ARG	2.1
1	B	34	PRO	2.1
1	B	135	LEU	2.1
1	B	233	ALA	2.1
1	B	375	ALA	2.1
1	A	140	LEU	2.0
1	A	412	LEU	2.0
1	B	316	LEU	2.0
1	B	342	ALA	2.0
1	B	347	ALA	2.0
1	B	315	GLY	2.0
1	A	394	ASP	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,

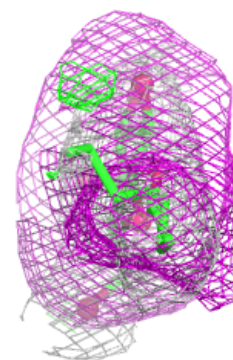
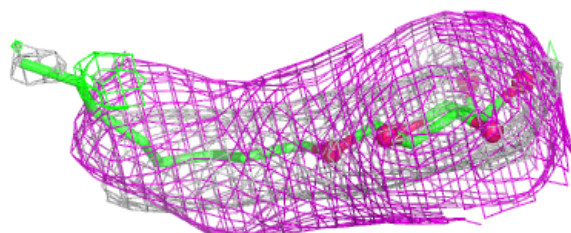
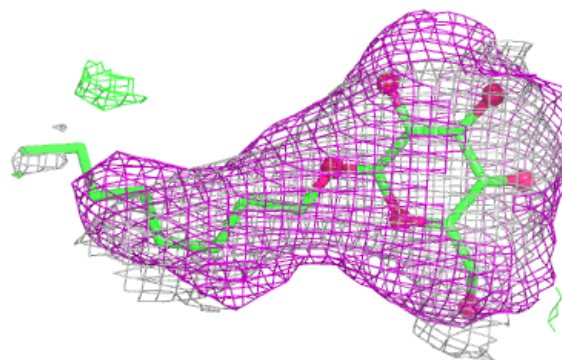
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BOG	A	503	20/20	0.55	0.20	94,111,140,149	0
4	BOG	A	511	20/20	0.57	0.19	135,135,135,135	0
4	BOG	A	510	20/20	0.59	0.23	111,111,111,111	0
4	BOG	A	512	20/20	0.59	0.15	123,123,123,123	0
4	BOG	A	513	20/20	0.59	0.17	101,101,101,101	0
4	BOG	A	509	20/20	0.62	0.14	119,120,122,122	0
4	BOG	A	507	20/20	0.64	0.15	122,127,140,144	0
4	BOG	A	506	20/20	0.72	0.13	75,140,169,179	0
2	PLM	A	501	17/18	0.76	0.25	97,97,97,97	0
4	BOG	A	505	20/20	0.79	0.15	78,111,142,142	0
4	BOG	A	504	20/20	0.82	0.18	64,111,131,133	0
4	BOG	A	508	18/20	0.83	0.15	98,100,102,103	0
3	SO4	A	502	5/5	0.87	0.12	104,112,120,125	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.

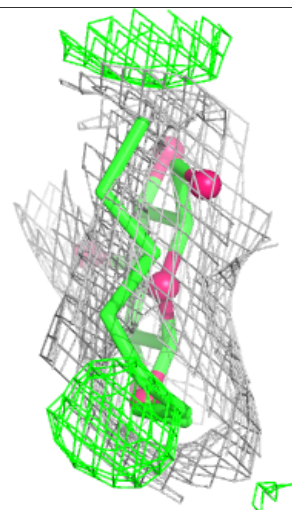
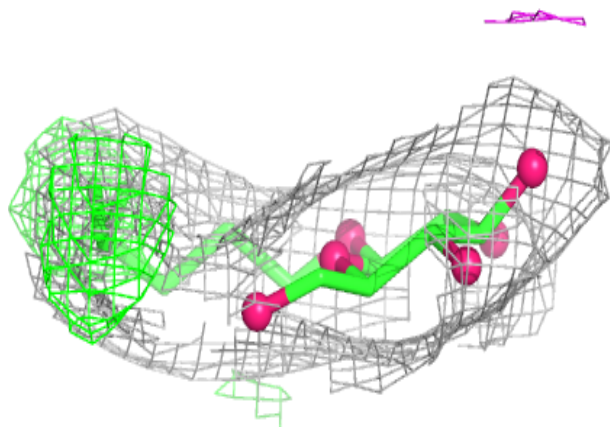
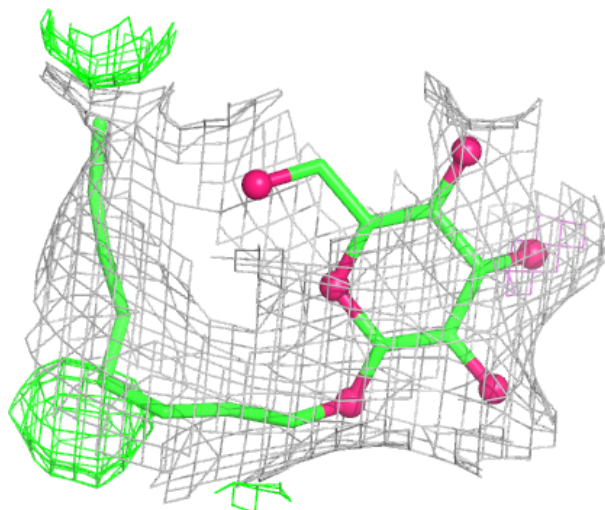
Electron density around BOG A 503:

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



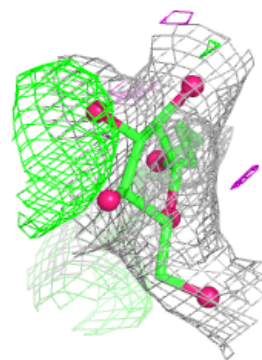
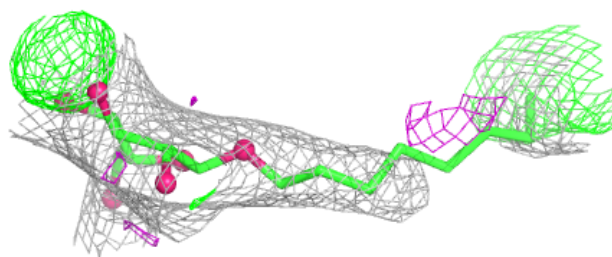
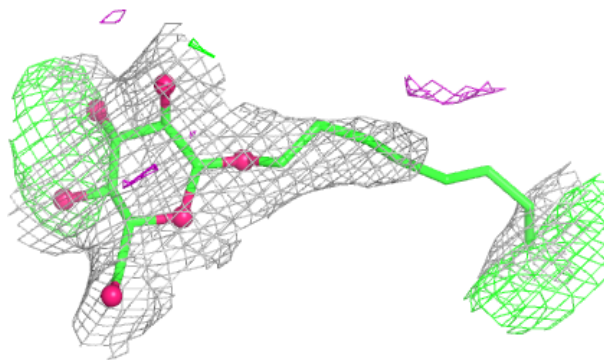
Electron density around BOG A 511:

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

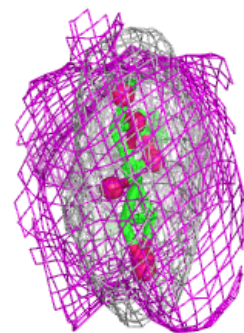
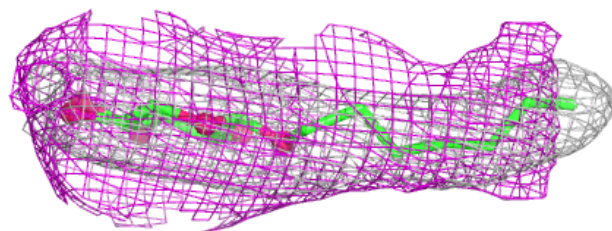
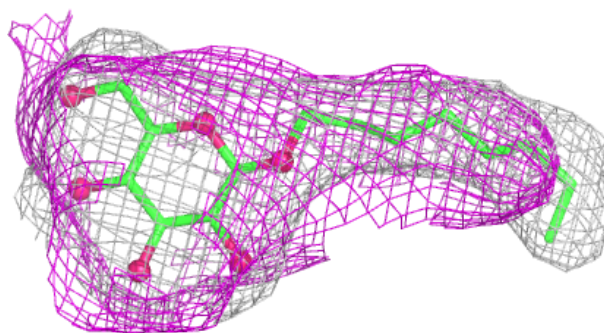


Electron density around BOG A 510:

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

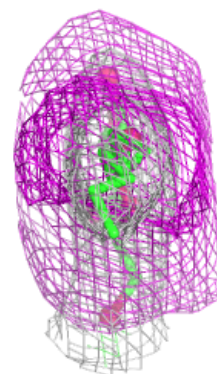
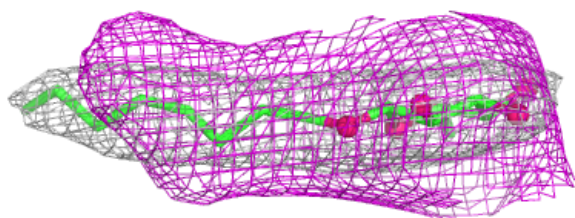
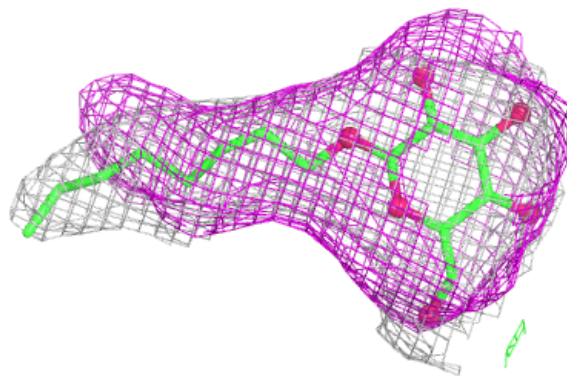
**Electron density around BOG A 512:**

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

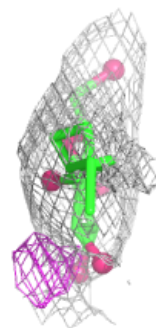
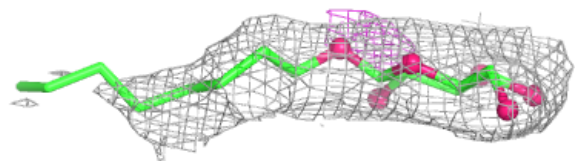
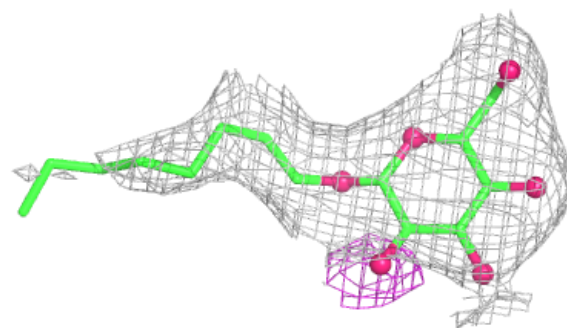


Electron density around BOG A 513:

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

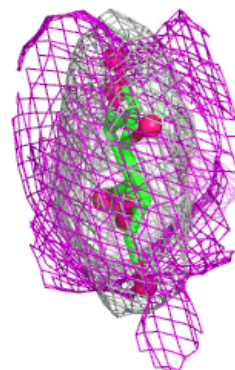
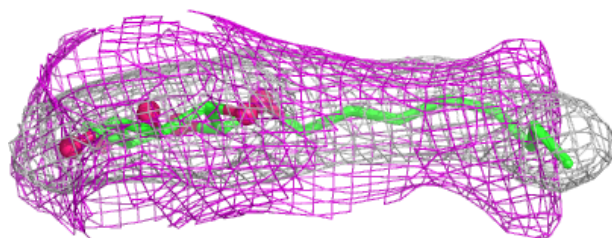
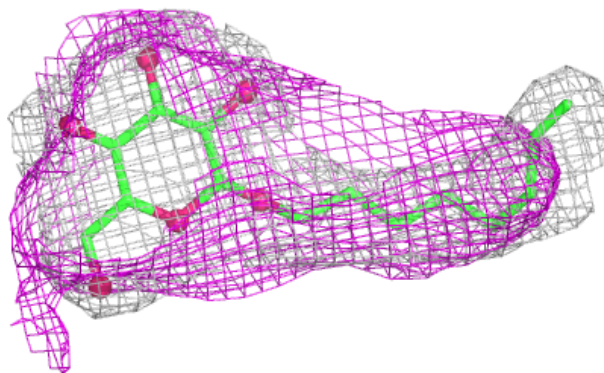
**Electron density around BOG A 509:**

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

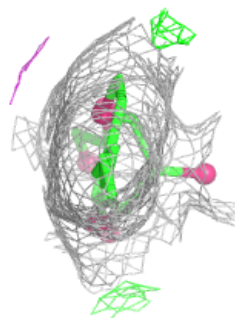
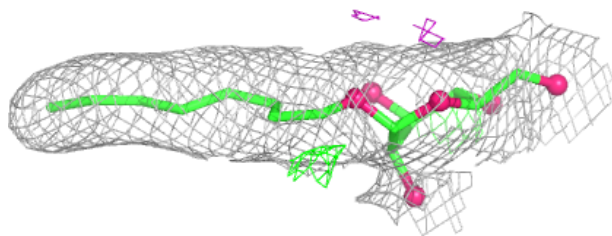
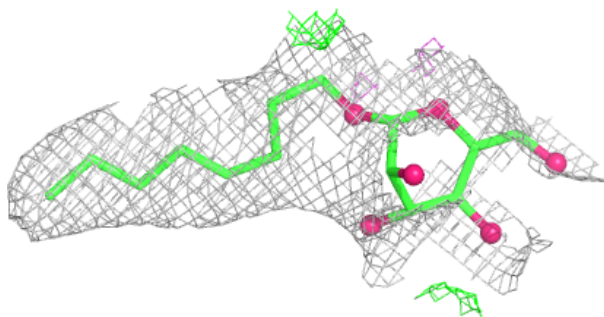


Electron density around BOG A 507:

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

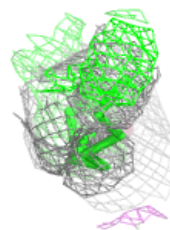
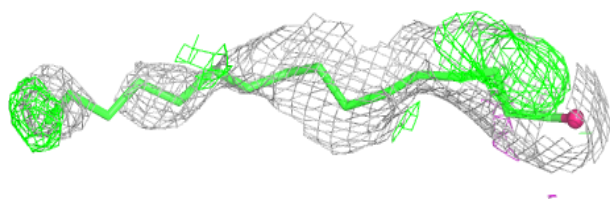
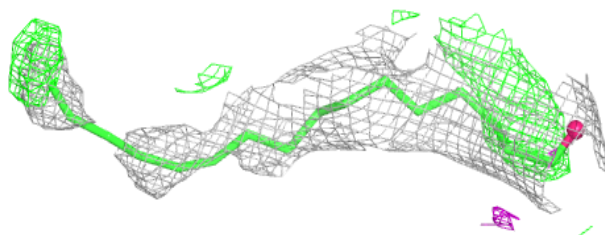
**Electron density around BOG A 506:**

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

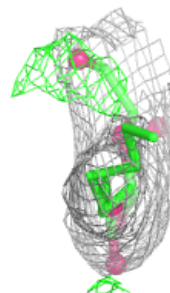
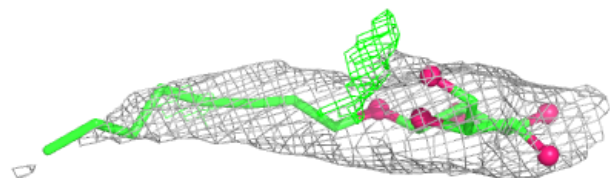
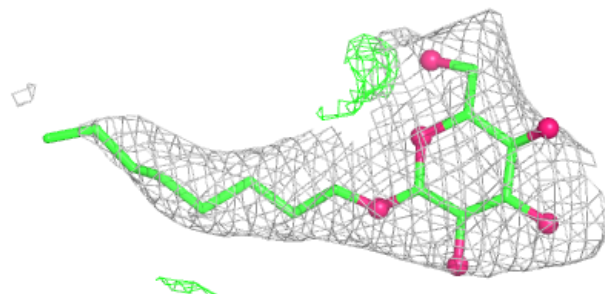


Electron density around PLM A 501:

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

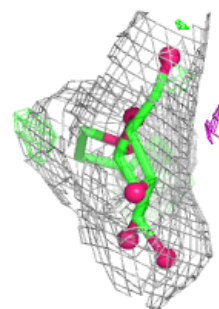
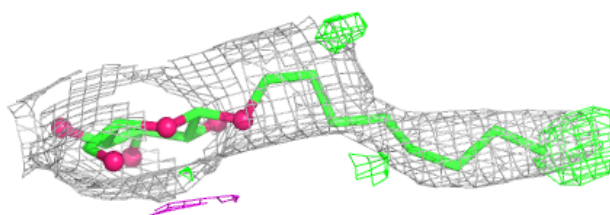
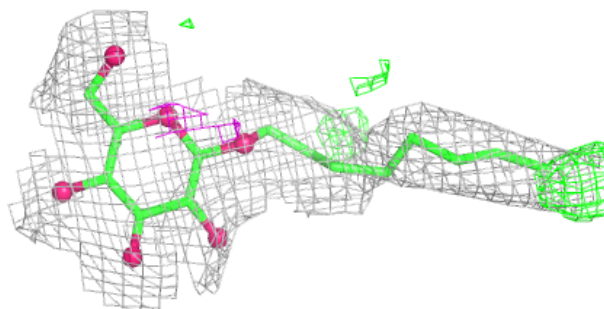
**Electron density around BOG A 505:**

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

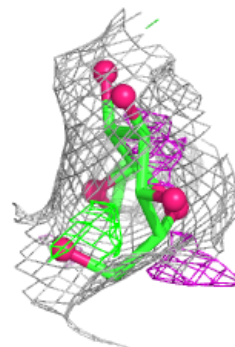
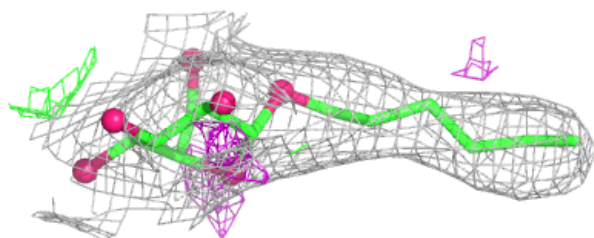
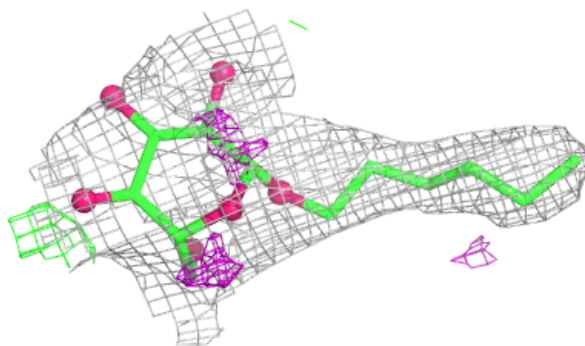


Electron density around BOG A 504:

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

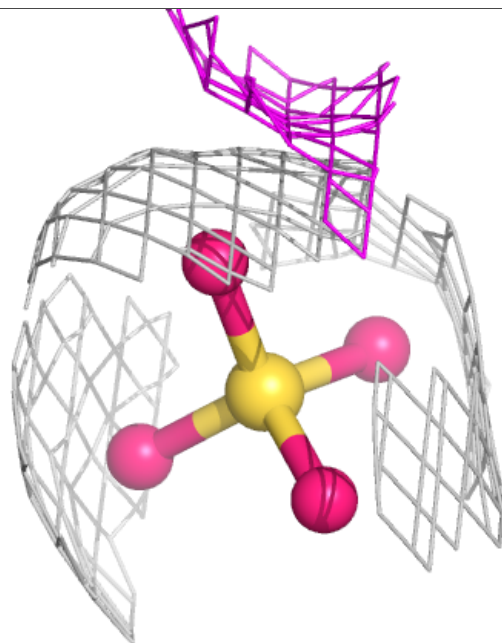
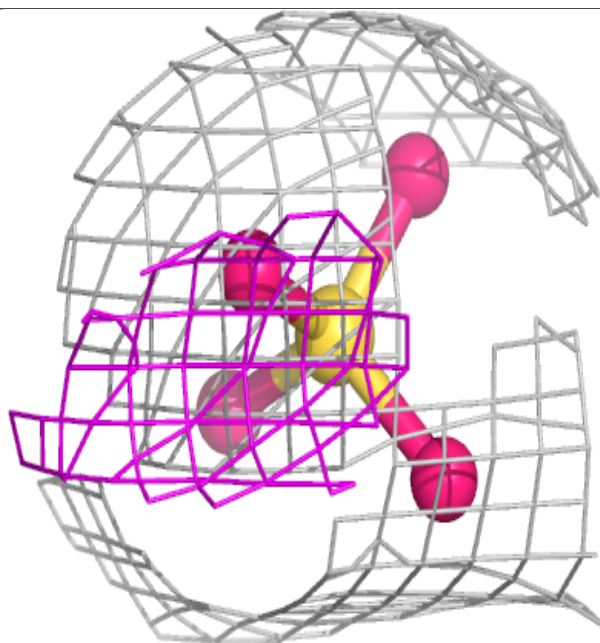
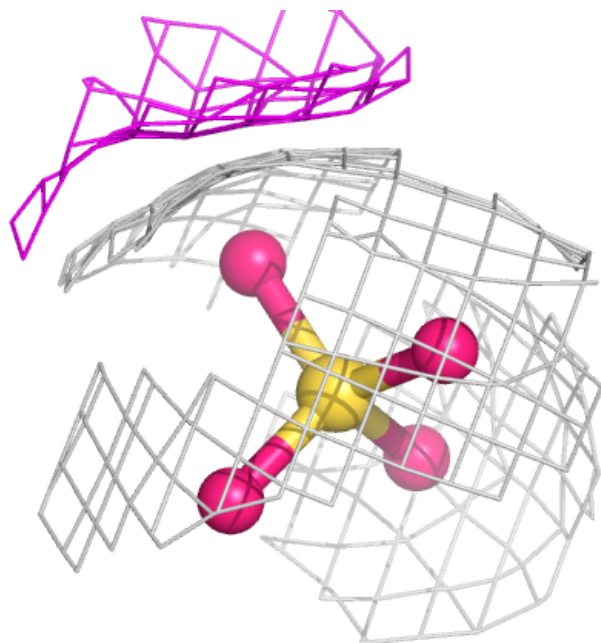
**Electron density around BOG A 508:**

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



Electron density around SO4 A 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.