



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 12:11 PM JST

PDB ID : 9V5V / pdb_00009v5v
Title : PfDXR - Mn²⁺ - SHOK166 ternary complex
Authors : Takada, S.; Sakamoto, Y.; Tanaka, N.
Deposited on : 2025-05-26
Resolution : 1.59 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 : 1.8.5 (274361), 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 : 9.0.010 (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

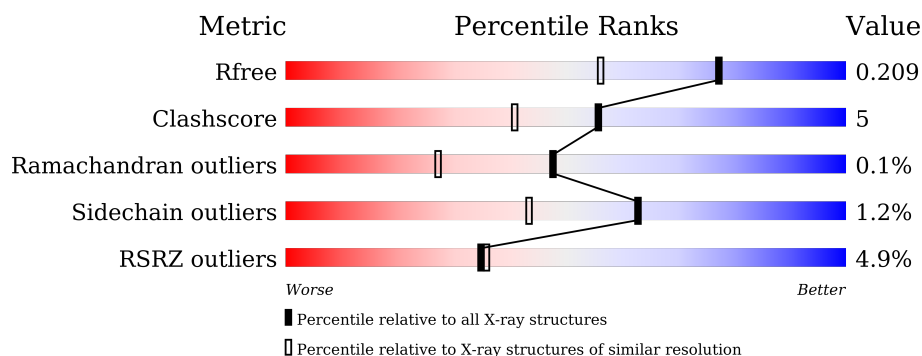
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	488	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>6% •</div> <div>16%</div> </div> </div>
1	B	488	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>7% •</div> <div>16%</div> </div> </div>

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	GOL	B	506	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7249 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.

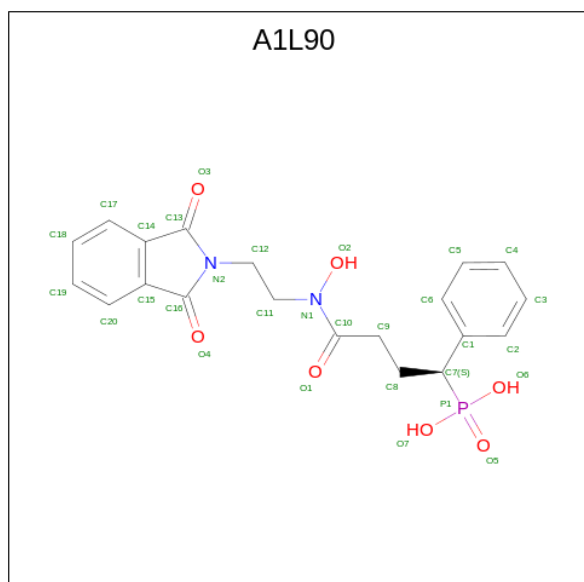
- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3285	2109	539	617	20			
1	B	411	Total	C	N	O	S	0	0	0
			3285	2109	539	617	20			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

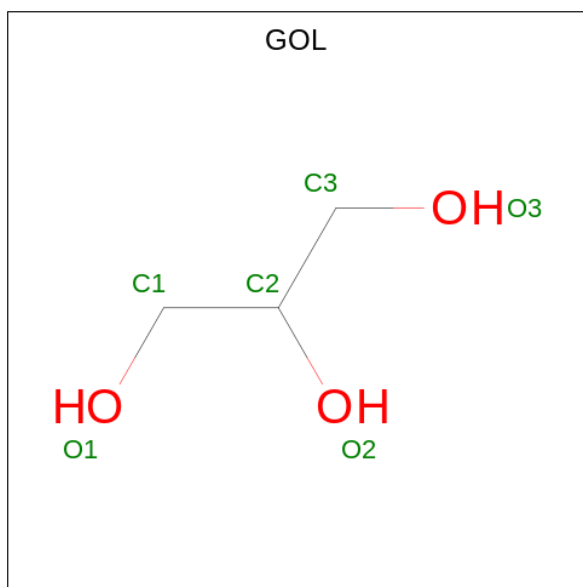
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is [(1 {S})-4-[2-[1,3-bis(oxidanylidene)isoindol-2-yl]ethyl-oxidanyl-amino]-4-oxidanylidene-1-phenyl-butyl]phosphonic acid (CCD ID: A1L90) (formula: C₂₀H₂₁N₂O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	20	2	7	1		
3	B	1	Total	C	N	O	P	0	0
			30	20	2	7	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Ca	0	0
			3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	273	Total	O	0	0
			273	273		
6	B	329	Total	O	0	0
			329	329		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.87Å 77.38Å 111.06Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	63.46 – 1.59 63.46 – 1.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (63.46-1.59) 99.9 (63.46-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.167 , 0.199 0.180 , 0.209	Depositor DCC
R_{free} test set	5967 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7249	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A1L90, GOL, MN

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	0.64	0/3348	1.09	8/4521 (0.2%)
1	B	0.67	1/3348 (0.0%)	1.10	6/4521 (0.1%)
All	All	0.66	1/6696 (0.0%)	1.09	14/9042 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	341	HIS	CE1-NE2	-5.21	1.27	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	464	MET	CG-SD-CE	-10.35	78.12	100.90
1	B	184	PHE	CA-CB-CG	8.12	121.92	113.80
1	B	152	LYS	CB-CA-C	6.56	120.61	109.53
1	A	231	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	286	THR	CA-CB-OG1	-5.88	100.79	109.60
1	A	136	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	126	ARG	CB-CA-C	-5.70	100.98	110.68
1	A	466	GLN	CB-CA-C	-5.70	101.94	110.88
1	A	234	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	B	279	MET	CG-SD-CE	-5.57	88.64	100.90
1	B	231	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	305	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	305	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	234	HIS	CB-CG-ND1	5.09	130.34	122.70

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	3285	0	3334	31	0
1	B	3285	0	3334	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	4	0
5	B	3	0	0	0	0
6	A	273	0	0	13	0
6	B	329	0	0	18	0
All	All	7249	0	6684	63	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 (63) 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:B:108:ASN:HB3	6:B:872:HOH:O	1.38	1.17
1:B:360:MET:HG3	6:B:893:HOH:O	1.44	1.17
1:B:480:ASP:HB2	6:B:604:HOH:O	1.71	0.90
1:A:360:MET:HG3	6:A:840:HOH:O	1.74	0.88
1:B:372:ASP:HB3	6:B:794:HOH:O	1.80	0.81
1:A:122:TYR:OH	1:A:126:ARG:NH1	2.23	0.72
1:B:279:MET:HE1	1:B:438:PHE:CZ	2.28	0.68
1:A:359:ASP:HB3	6:A:619:HOH:O	1.93	0.68
4:B:506:GOL:H12	6:B:608:HOH:O	1.95	0.66
1:A:234:HIS:CD2	6:A:653:HOH:O	2.48	0.66
1:B:393:LYS:HG2	6:B:673:HOH:O	1.94	0.66
1:B:480:ASP:CB	6:B:604:HOH:O	2.36	0.63
1:B:216:LYS:NZ	1:B:254:ASP:OD1	2.22	0.62
1:A:209:VAL:CG2	1:A:318:GLU:HG3	2.32	0.60
1:A:280:ASP:OD1	1:A:283:LYS:NZ	2.37	0.58
1:B:279:MET:CA	1:B:279:MET:HE3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:HIS:CE1	6:B:654:HOH:O	2.58	0.55
1:A:481:ILE:O	1:A:484:LYS:HG3	2.07	0.53
4:B:506:GOL:C3	6:B:608:HOH:O	2.56	0.53
1:A:234:HIS:CG	6:A:653:HOH:O	2.61	0.52
1:B:295:LYS:HB2	1:B:296:TRP:CE3	2.44	0.52
1:A:209:VAL:HG22	1:A:318:GLU:HG3	1.92	0.51
1:B:234:HIS:HD2	6:B:882:HOH:O	1.92	0.51
4:B:506:GOL:C1	6:B:608:HOH:O	2.54	0.51
1:A:209:VAL:HG23	1:A:318:GLU:OE2	2.10	0.50
1:A:273:PRO:CD	6:A:699:HOH:O	2.60	0.50
1:A:209:VAL:HG23	1:A:318:GLU:CD	2.37	0.50
1:A:234:HIS:CD2	6:A:808:HOH:O	2.65	0.49
1:A:185:GLN:HG3	6:A:821:HOH:O	2.11	0.49
1:A:209:VAL:HG23	1:A:318:GLU:CG	2.43	0.49
1:A:187:LEU:CD2	1:A:464:MET:HE2	2.43	0.48
1:B:372:ASP:CB	6:B:794:HOH:O	2.50	0.48
1:B:279:MET:HE3	1:B:279:MET:HA	1.96	0.48
1:B:205:LYS:HE2	1:B:302:ILE:HD11	1.96	0.47
1:B:84:GLY:HA3	1:B:181:ILE:HG23	1.96	0.47
1:B:216:LYS:HE3	1:B:252:LEU:O	2.14	0.47
1:B:449:GLU:HG2	6:B:835:HOH:O	2.14	0.47
1:A:187:LEU:HB2	6:A:615:HOH:O	2.15	0.46
1:B:165:MET:HE3	1:B:165:MET:HB2	1.63	0.46
1:B:234:HIS:CD2	6:B:882:HOH:O	2.68	0.45
1:A:295:LYS:HB2	1:A:296:TRP:CE3	2.51	0.45
1:B:84:GLY:CA	1:B:181:ILE:HG23	2.47	0.45
4:B:506:GOL:H32	6:B:608:HOH:O	2.16	0.45
1:A:241:LEU:O	6:A:601:HOH:O	2.19	0.45
1:B:480:ASP:CG	6:B:604:HOH:O	2.60	0.44
1:A:259:ILE:HD12	6:A:612:HOH:O	2.16	0.44
1:A:273:PRO:HD3	6:A:699:HOH:O	2.17	0.43
1:B:122:TYR:CZ	1:B:126:ARG:HD2	2.53	0.43
1:B:110:LYS:HD2	6:B:872:HOH:O	2.19	0.43
1:A:481:ILE:O	1:A:484:LYS:HE3	2.19	0.43
1:A:372:ASP:HB2	6:B:633:HOH:O	2.19	0.43
1:A:209:VAL:CG2	1:A:318:GLU:CG	2.97	0.42
1:A:234:HIS:HD2	6:A:808:HOH:O	2.00	0.42
1:B:113:TYR:CE1	1:B:181:ILE:HD13	2.55	0.42
1:B:181:ILE:HD12	1:B:185:GLN:HB3	2.00	0.42
1:A:138:LYS:HA	1:A:160:CYS:SG	2.60	0.42
1:A:113:TYR:HA	1:A:134:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:HIS:CD2	1:A:296:TRP:HZ3	2.39	0.41
1:A:484:LYS:HD2	1:A:485:HIS:N	2.35	0.41
1:A:360:MET:CG	6:A:840:HOH:O	2.51	0.41
1:B:254:ASP:O	1:B:255:ASN:HB2	2.21	0.40
1:B:113:TYR:CD1	1:B:113:TYR:C	3.00	0.40
1:A:340:ILE:HG12	1:A:355:MET:HG2	2.03	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	409/488 (84%)	397 (97%)	12 (3%)	0	100	100
1	B	409/488 (84%)	395 (97%)	13 (3%)	1 (0%)	43	24
All	All	818/976 (84%)	792 (97%)	25 (3%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	SER

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	378/449 (84%)	376 (100%)	2 (0%)	81	70
1	B	378/449 (84%)	371 (98%)	7 (2%)	50	27
All	All	756/898 (84%)	747 (99%)	9 (1%)	63	43

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

Mol	Chain	Res	Type
1	A	359	ASP
1	A	480	ASP
1	B	152	LYS
1	B	163	GLU
1	B	184	PHE
1	B	293	HIS
1	B	359	ASP
1	B	387	SER
1	B	460	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	A	224	ASN
1	A	234	HIS
1	A	260	ASN
1	A	261	ASN
1	A	276	ASN
1	A	293	HIS
1	A	328	ASN
1	A	377	ASN
1	A	407	GLN
1	A	483	ASN
1	B	105	ASN
1	B	136	HIS
1	B	185	GLN
1	B	234	HIS
1	B	253	GLN
1	B	255	ASN
1	B	293	HIS
1	B	452	ASN

5.3.3 RNA [i](#)

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](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	GOL	B	506	-	5,5,5	0.24	0	5,5,5	0.74	0
3	A1L90	B	502	2	31,32,32	1.64	7 (22%)	37,46,46	2.16	11 (29%)
4	GOL	A	503	-	5,5,5	0.27	0	5,5,5	0.90	0
3	A1L90	A	502	2	31,32,32	1.40	5 (16%)	37,46,46	2.40	11 (29%)

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	GOL	B	506	-	-	0/4/4/4	-
3	A1L90	B	502	2	-	3/24/40/40	0/3/3/3
4	GOL	A	503	-	-	2/4/4/4	-
3	A1L90	A	502	2	-	3/24/40/40	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1L90	P1-O5	4.93	1.57	1.49
3	B	502	A1L90	C13-N2	-4.11	1.34	1.39
3	B	502	A1L90	C10-N1	3.98	1.40	1.34
3	B	502	A1L90	O2-N1	-3.35	1.37	1.40
3	B	502	A1L90	P1-O7	-2.85	1.50	1.54
3	A	502	A1L90	C16-N2	-2.85	1.36	1.39
3	A	502	A1L90	P1-O7	-2.43	1.51	1.54
3	B	502	A1L90	C5-C6	2.23	1.43	1.38
3	B	502	A1L90	C14-C13	2.21	1.52	1.48
3	A	502	A1L90	C12-N2	2.18	1.52	1.47
3	B	502	A1L90	P1-C7	2.13	1.84	1.82
3	A	502	A1L90	C10-N1	2.04	1.37	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	A1L90	C15-C16-N2	5.88	110.06	105.88
3	A	502	A1L90	C15-C16-N2	5.87	110.05	105.88
3	A	502	A1L90	O3-C13-N2	5.24	129.91	124.81
3	A	502	A1L90	C16-N2-C13	-5.03	107.93	112.03
3	A	502	A1L90	C12-N2-C13	4.91	128.82	123.88
3	A	502	A1L90	C14-C13-N2	4.78	109.28	105.88
3	B	502	A1L90	O4-C16-N2	4.63	129.32	124.81
3	B	502	A1L90	O4-C16-C15	-4.14	120.62	128.68
3	A	502	A1L90	O3-C13-C14	-4.05	120.81	128.68
3	B	502	A1L90	C16-N2-C13	-3.53	109.16	112.03
3	B	502	A1L90	C17-C14-C13	3.40	135.17	129.63
3	B	502	A1L90	C14-C15-C16	-3.37	105.33	108.26
3	B	502	A1L90	C17-C14-C15	-3.34	117.31	121.07
3	A	502	A1L90	O5-P1-C7	-2.99	104.97	113.35
3	A	502	A1L90	C11-C12-N2	2.91	117.14	111.90
3	B	502	A1L90	C14-C13-N2	2.87	107.92	105.88
3	B	502	A1L90	O5-P1-C7	-2.53	106.26	113.35
3	A	502	A1L90	C15-C14-C13	-2.23	106.33	108.26
3	A	502	A1L90	C14-C15-C16	-2.13	106.41	108.26
3	A	502	A1L90	O7-P1-O6	2.08	113.24	107.64
3	B	502	A1L90	C12-C11-N1	-2.03	108.97	112.19
3	B	502	A1L90	C12-N2-C16	2.00	125.89	123.88

There are no chirality outliers.

All (8) torsion outliers are listed below:

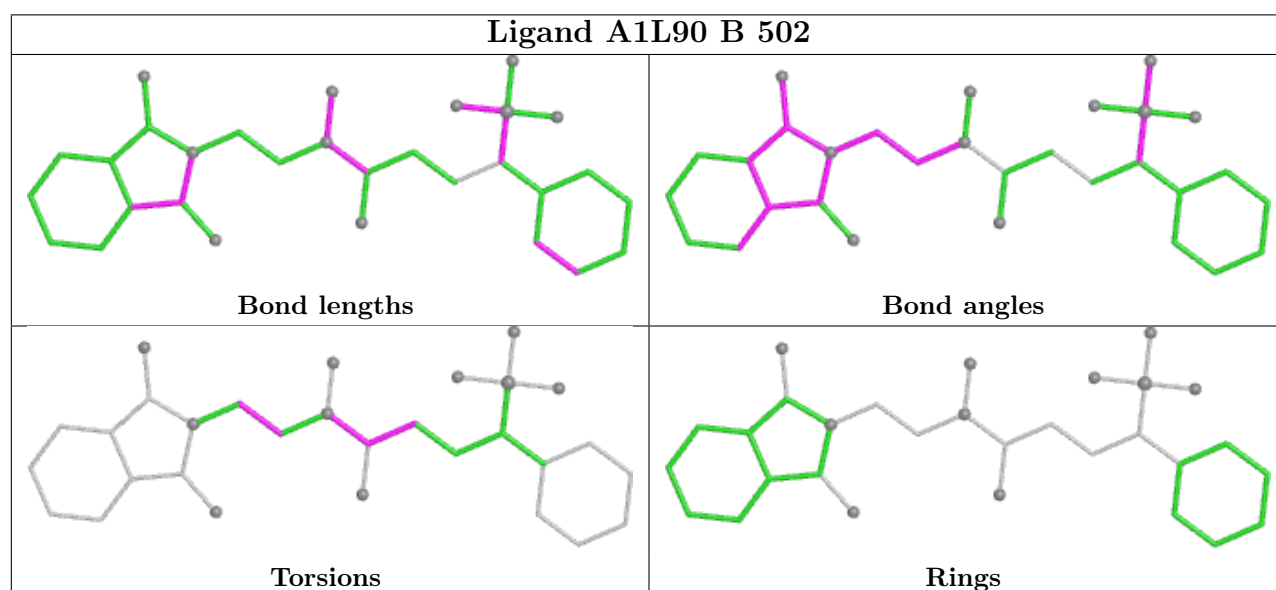
Mol	Chain	Res	Type	Atoms
3	A	502	A1L90	N1-C11-C12-N2
4	A	503	GOL	C1-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3
3	B	502	A1L90	N1-C11-C12-N2
3	A	502	A1L90	O1-C10-N1-O2
3	A	502	A1L90	N1-C10-C9-C8
3	B	502	A1L90	O1-C10-N1-O2
3	B	502	A1L90	N1-C10-C9-C8

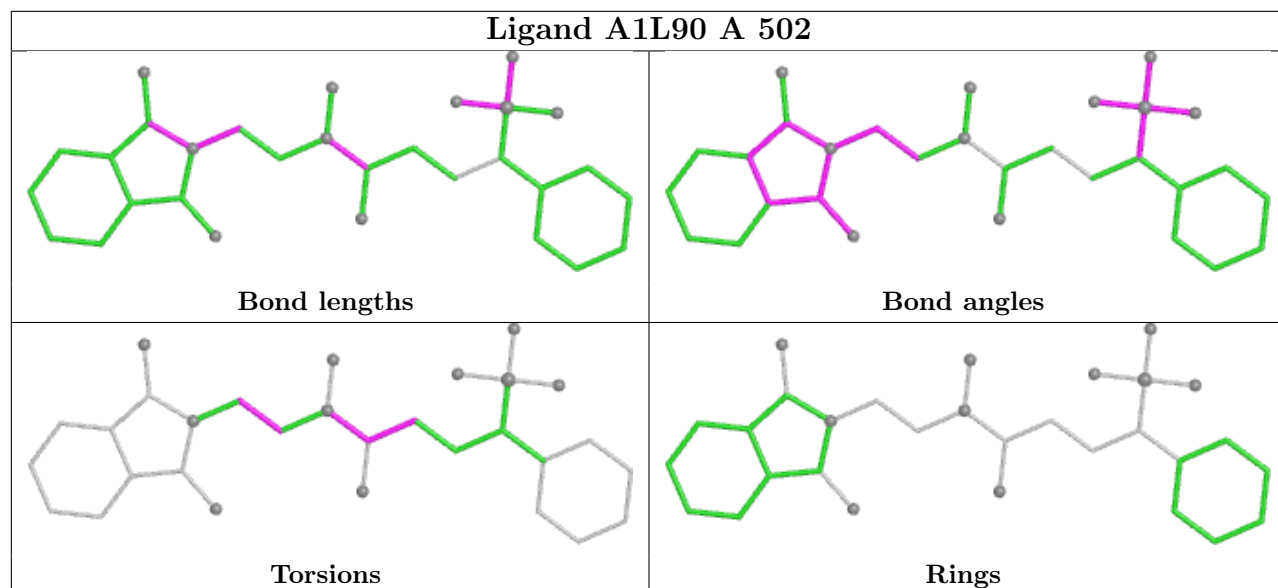
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	GOL	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/488 (84%)	0.27	25 (6%) 27 27	12, 22, 52, 83	0
1	B	411/488 (84%)	0.10	15 (3%) 46 48	12, 21, 41, 85	0
All	All	822/976 (84%)	0.18	40 (4%) 35 36	12, 21, 50, 85	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	TRP	5.1
1	B	296	TRP	4.8
1	B	184	PHE	4.6
1	A	293	HIS	3.7
1	A	295	LYS	3.6
1	B	293	HIS	3.6
1	B	213	PHE	3.6
1	A	292	LYS	3.4
1	A	184	PHE	3.3
1	A	188	TYR	3.3
1	B	292	LYS	3.3
1	B	76	LYS	3.3
1	A	294	PRO	3.3
1	B	294	PRO	3.2
1	B	295	LYS	3.1
1	B	485	HIS	3.0
1	A	76	LYS	3.0
1	A	151	ILE	2.9
1	A	152	LYS	2.9
1	A	185	GLN	2.7
1	A	485	HIS	2.6
1	A	122	TYR	2.6
1	A	144	LEU	2.6
1	A	160	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	192	TYR	2.4
1	A	155	LYS	2.4
1	B	152	LYS	2.4
1	A	359	ASP	2.3
1	A	106	VAL	2.3
1	A	147	LEU	2.3
1	B	192	TYR	2.3
1	A	148	VAL	2.3
1	A	291	LEU	2.3
1	A	486	ASN	2.3
1	B	153	ASP	2.2
1	B	486	ASN	2.1
1	B	460	SER	2.1
1	A	205	LYS	2.0
1	A	141	TYR	2.0
1	B	297	LYS	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	GOL	A	503	6/6	0.86	0.13	24,31,32,33	0
4	GOL	B	506	6/6	0.93	0.10	23,29,33,37	0
3	A1L90	A	502	30/30	0.95	0.11	17,24,59,63	0
3	A1L90	B	502	30/30	0.97	0.07	15,22,35,40	0
5	CA	B	504	1/1	0.97	0.06	25,25,25,25	0
5	CA	B	503	1/1	0.99	0.05	16,16,16,16	0
2	MN	B	501	1/1	0.99	0.03	13,13,13,13	0

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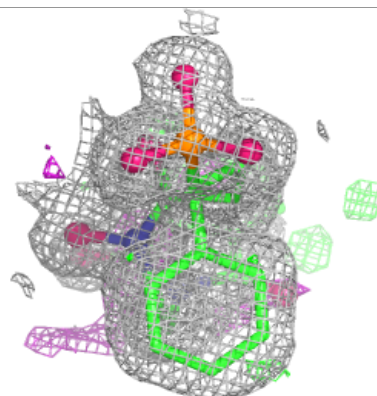
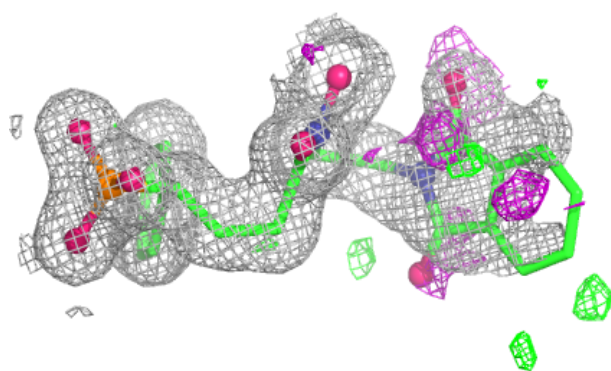
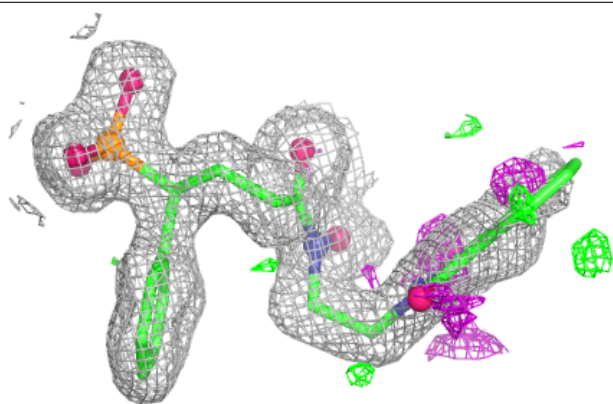
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	B	505	1/1	0.99	0.06	25,25,25,25	0
2	MN	A	501	1/1	1.00	0.02	15,15,15,15	0

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.

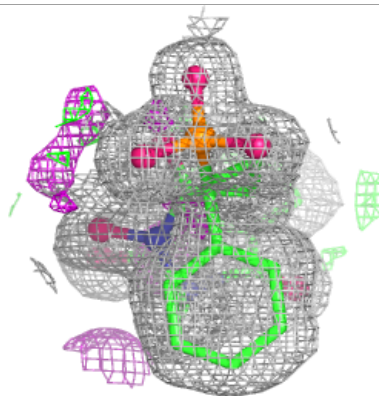
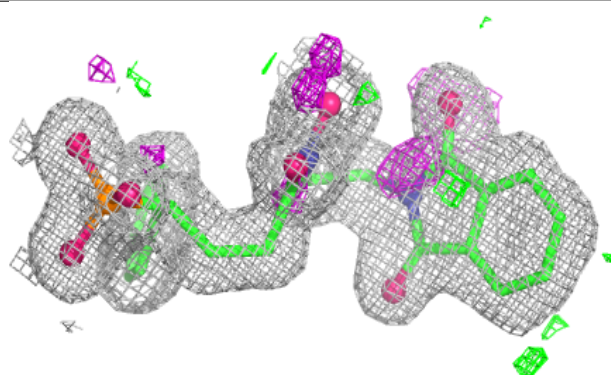
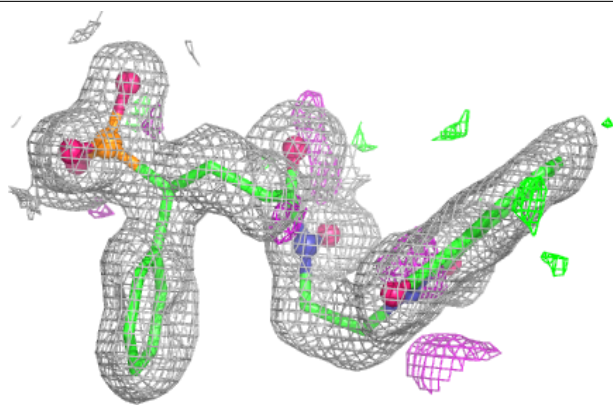
Electron density around A1L90 A 502:

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



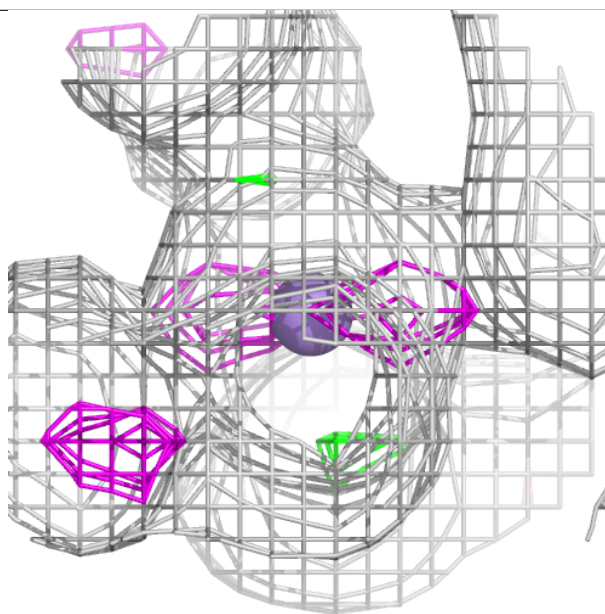
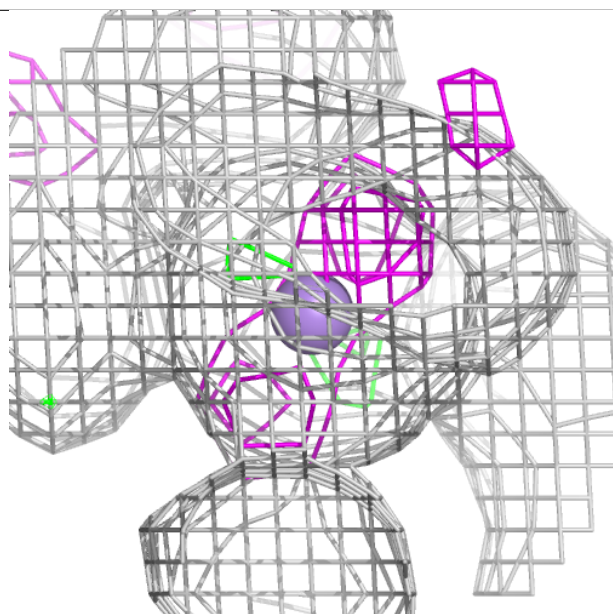
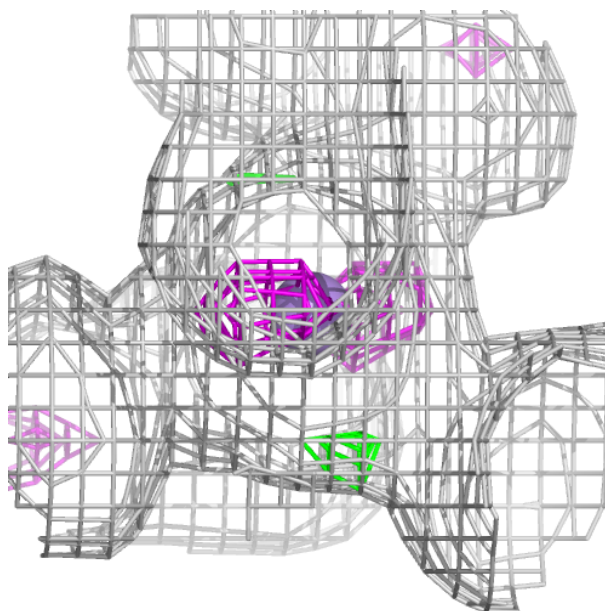
Electron density around A1L90 B 502:

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



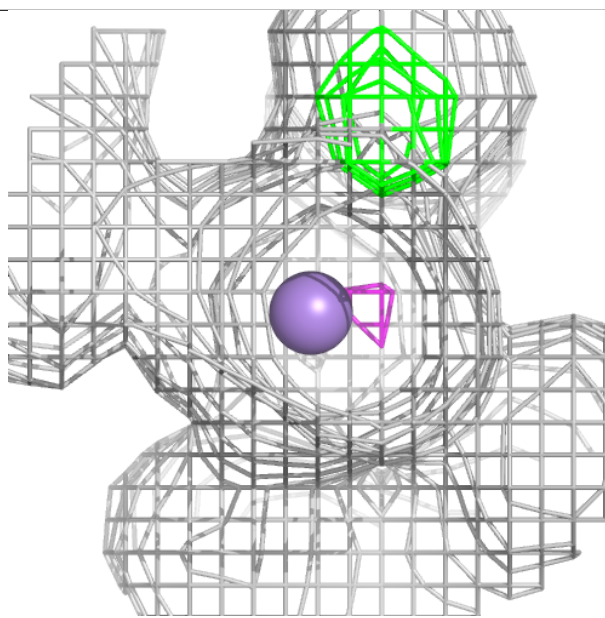
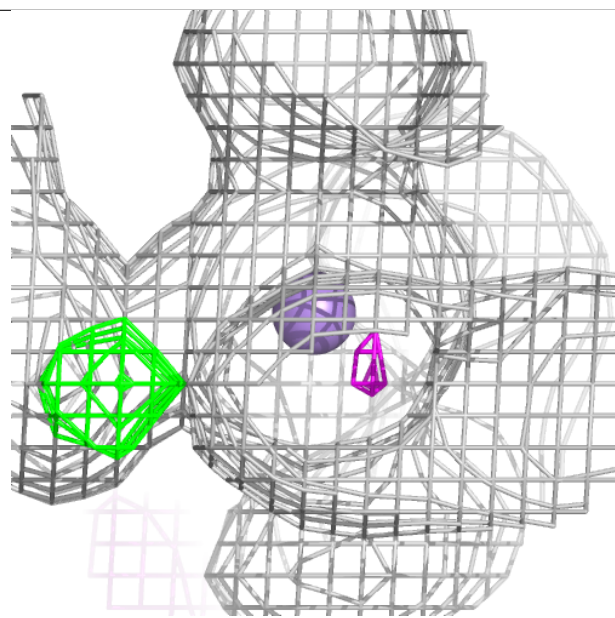
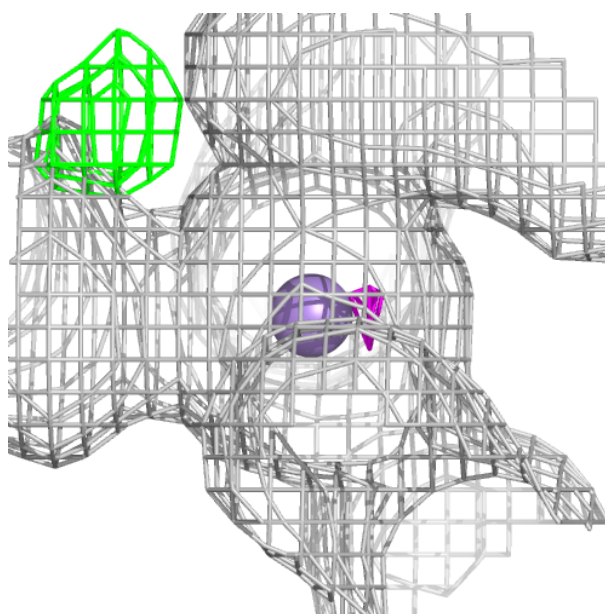
Electron density around MN B 501:

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



Electron density around MN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.