



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:08 AM UTC

PDB ID : 9JZ9 / pdb_00009jz9
Title : PfDXR - Mn²⁺ - MAMK218 ternary complex
Authors : Takada, S.; Sakamoto, Y.; Tanaka, N.
Deposited on : 2024-10-14
Resolution : 1.33 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

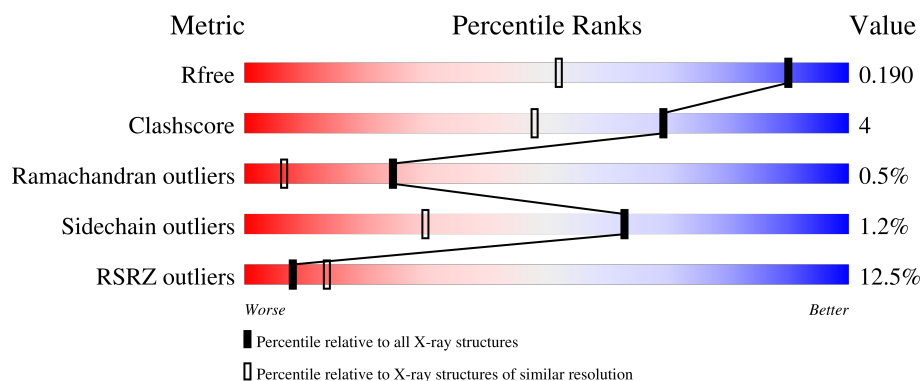
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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	13% 76% 7% 16%
1	B	488	8% 77% 7% 16%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7325 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.

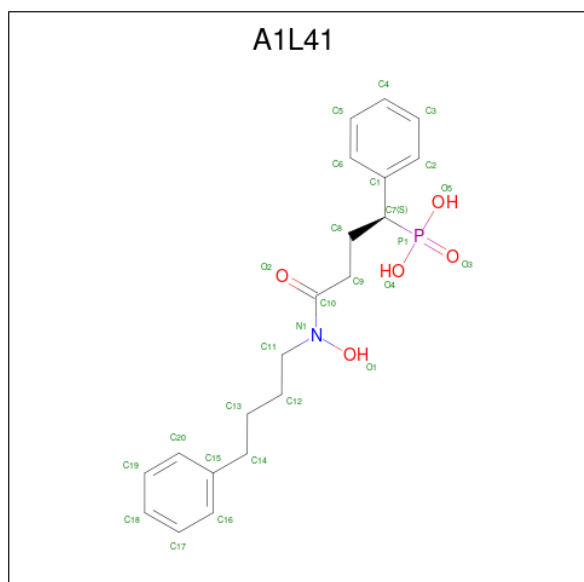
- Molecule 1 is a protein called 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	2	0
			3281	2107	536	618	20			
1	B	408	Total	C	N	O	S	0	2	0
			3281	2107	536	618	20			

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

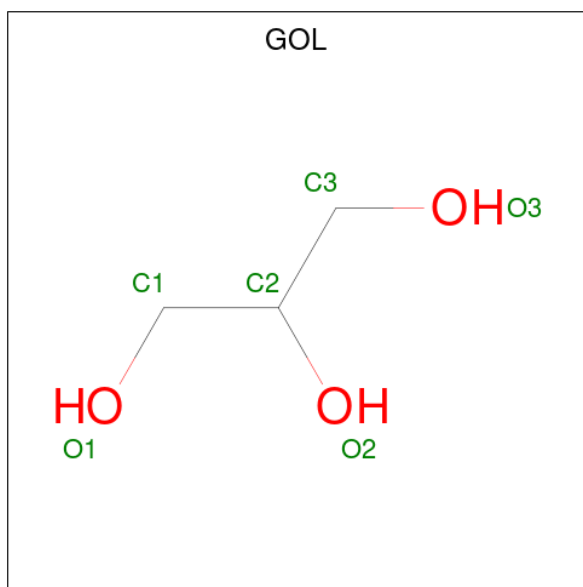
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is [(1 {S})-4-oxidanylidene-4-[oxidanyl(4-phenylbutyl)amino]-1-phenyl-butyl]phosphonic acid (CCD ID: A1L41) (formula: C₂₀H₂₆NO₅P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			37	30	1	5	1		
3	B	1	Total	C	N	O	P	0	1
			37	30	1	5	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	304	Total	O	0	0
			304	304		
6	B	368	Total	O	0	0
			368	368		

- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase, apicoplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.93Å 77.57Å 111.66Å 90.00° 93.20° 90.00°	Depositor
Resolution (Å)	46.04 – 1.33 46.04 – 1.33	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.04-1.33) 99.0 (46.04-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.169 , 0.190 0.169 , 0.190	Depositor DCC
R_{free} test set	10106 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7325	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: GOL, A1L41, MN, CA

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	0.73	1/3343 (0.0%)	1.09	5/4514 (0.1%)
1	B	0.76	0/3343	1.13	5/4514 (0.1%)
All	All	0.75	1/6686 (0.0%)	1.11	10/9028 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	HIS	ND1-CE1	5.31	1.37	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	MET	CG-SD-CE	8.07	118.66	100.90
1	B	131	GLU	CB-CG-CD	7.08	124.63	112.60
1	A	213	PHE	CB-CA-C	-6.52	99.96	110.79
1	B	231	ASP	CA-CB-CG	6.14	118.74	112.60
1	A	274	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	275	GLN	N-CA-C	5.76	118.34	111.71
1	A	305	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	466	GLN	N-CA-CB	-5.62	101.85	110.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	104	GLU	CB-CA-C	-5.00	100.70	109.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	PRO	Peptide
1	B	358	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3281	0	3317	23	0
1	B	3281	0	3317	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	37	0	0	2	0
3	B	37	0	0	3	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	B	3	0	0	0	0
6	A	304	0	0	6	0
6	B	368	0	0	9	0
All	All	7325	0	6650	47	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 4.

All (47) 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:328:ASN:HB2	6:A:813:HOH:O	1.32	1.27
1:B:361:GLN:HG3	6:B:653:HOH:O	1.49	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ASP:HB3	6:B:784:HOH:O	1.65	0.95
1:B:165:MET:HG3	6:B:765:HOH:O	1.75	0.85
1:B:296[A]:TRP:CD1	3:B:502[A]:A1L41:C17	2.60	0.84
1:B:217:LYS:HD3	6:B:625:HOH:O	1.77	0.83
1:A:296[A]:TRP:CD1	3:A:502[A]:A1L41:C17	2.74	0.70
1:B:191:MET:CE	1:B:192:TYR:CE1	2.74	0.70
1:A:122:TYR:OH	1:A:126:ARG:NH2	2.24	0.69
1:B:191:MET:HE3	1:B:192:TYR:CE1	2.28	0.68
1:B:393:LYS:HG2	6:B:612:HOH:O	1.93	0.68
1:B:372:ASP:CB	6:B:784:HOH:O	2.34	0.60
1:A:217:LYS:HD2	6:A:890:HOH:O	2.02	0.59
1:B:296[A]:TRP:HD1	3:B:502[A]:A1L41:C17	2.16	0.58
1:A:464:MET:HE3	1:A:467:ILE:HB	1.86	0.58
1:A:340:ILE:HG12	1:A:355:MET:HE3	1.86	0.57
1:B:84:GLY:HA3	1:B:181:ILE:HG23	1.87	0.56
1:B:359[B]:ASP:H	3:B:502[B]:A1L41:C19	2.19	0.55
1:A:464:MET:HE2	1:A:468:LEU:HG	1.89	0.54
1:A:213:PHE:CD1	6:A:870:HOH:O	2.53	0.53
1:A:484:LYS:HE3	1:A:485:HIS:HB2	1.92	0.52
1:B:131:GLU:HG2	6:B:624:HOH:O	2.09	0.51
1:A:340:ILE:CG1	1:A:355:MET:HE3	2.41	0.51
1:B:83:PHE:CD2	6:B:955:HOH:O	2.62	0.50
1:B:204:ASN:OD1	1:B:207:SER:OG	2.23	0.48
1:A:182:ASP:HA	1:A:204:ASN:ND2	2.28	0.47
1:A:481:ILE:O	1:A:484:LYS:HG3	2.14	0.47
1:A:84:GLY:HA3	1:A:181:ILE:HG23	1.96	0.47
1:B:84:GLY:CA	1:B:181:ILE:HG23	2.45	0.47
1:A:184:PHE:O	1:A:188:TYR:HB2	2.15	0.46
1:A:213:PHE:CG	6:A:870:HOH:O	2.67	0.46
6:A:741:HOH:O	1:B:393:LYS:HE2	2.17	0.44
1:B:191:MET:HE2	1:B:192:TYR:CE1	2.51	0.44
1:B:454:GLN:HE22	1:B:469:GLN:HE22	1.64	0.43
1:B:191:MET:CE	1:B:192:TYR:HE1	2.30	0.43
1:B:113:TYR:OH	1:B:136:HIS:CD2	2.71	0.43
1:A:76:LYS:HB3	1:A:77:PRO:CD	2.49	0.42
1:B:208:ILE:HD11	6:B:876:HOH:O	2.20	0.42
1:B:296[B]:TRP:HD1	1:B:298:MET:HG2	1.85	0.42
1:A:296[A]:TRP:HD1	3:A:502[A]:A1L41:C17	2.29	0.42
1:B:254:ASP:O	1:B:255:ASN:HB2	2.20	0.42
1:A:227:ILE:HD12	1:A:252:LEU:CD1	2.51	0.41
1:A:76:LYS:HB3	1:A:77:PRO:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:HH11	1:A:126:ARG:HG3	1.86	0.41
1:A:464:MET:HE3	1:A:464:MET:O	2.19	0.41
1:A:114:VAL:HG22	1:A:121:LEU:HD22	2.03	0.41
1:A:434:LYS:CE	6:A:861:HOH:O	2.69	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	405/488 (83%)	394 (97%)	9 (2%)	2 (0%)	24	6
1	B	405/488 (83%)	393 (97%)	10 (2%)	2 (0%)	24	6
All	All	810/976 (83%)	787 (97%)	19 (2%)	4 (0%)	24	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	SER
1	B	183	SER
1	B	342	SER
1	A	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	377/449 (84%)	372 (99%)	5 (1%)	61	26
1	B	377/449 (84%)	373 (99%)	4 (1%)	65	33
All	All	754/898 (84%)	745 (99%)	9 (1%)	63	30

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

Mol	Chain	Res	Type
1	A	105	ASN
1	A	181	ILE
1	A	349	LYS
1	A	411	LYS
1	A	484	LYS
1	B	76	LYS
1	B	145	LYS
1	B	152	LYS
1	B	163	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	124	GLN
1	A	220	ASN
1	A	260	ASN
1	A	261	ASN
1	A	407	GLN
1	A	428	ASN
1	A	452	ASN
1	A	454	GLN
1	A	483	ASN
1	B	105	ASN
1	B	108	ASN
1	B	136	HIS
1	B	185	GLN
1	B	244	ASN
1	B	253	GLN
1	B	260	ASN
1	B	328	ASN
1	B	407	GLN
1	B	420	ASN
1	B	469	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	A	503	-	5,5,5	0.33	0	5,5,5	0.81	0
3	A1L41	B	502[A]	-	27,28,28	2.86	6 (22%)	28,37,37	2.53	8 (28%)
3	A1L41	B	502[B]	-	27,28,28	2.84	6 (22%)	28,37,37	2.75	9 (32%)
4	GOL	B	506	-	5,5,5	0.37	0	5,5,5	0.83	0
3	A1L41	A	502[B]	-	27,28,28	3.20	11 (40%)	28,37,37	2.30	4 (14%)
3	A1L41	A	502[A]	-	27,28,28	3.34	11 (40%)	28,37,37	2.16	5 (17%)

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	A	503	-	-	0/4/4/4	-
3	A1L41	B	502[A]	-	-	5/26/26/26	0/2/2/2
3	A1L41	B	502[B]	-	-	6/26/26/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	506	-	-	0/4/4/4	-
3	A1L41	A	502[B]	-	-	5/26/26/26	0/2/2/2
3	A1L41	A	502[A]	-	-	4/26/26/26	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[A]	A1L41	C11-N1	-10.06	1.30	1.46
3	A	502[A]	A1L41	O1-N1	9.75	1.47	1.40
3	A	502[B]	A1L41	O1-N1	9.75	1.47	1.40
3	B	502[B]	A1L41	C11-N1	-9.54	1.31	1.46
3	A	502[A]	A1L41	C11-N1	-9.44	1.31	1.46
3	A	502[B]	A1L41	C11-N1	-7.92	1.33	1.46
3	B	502[A]	A1L41	O1-N1	6.59	1.45	1.40
3	B	502[B]	A1L41	O1-N1	6.59	1.45	1.40
3	B	502[B]	A1L41	C12-C11	-5.24	1.30	1.51
3	A	502[A]	A1L41	C12-C11	-5.14	1.31	1.51
3	A	502[B]	A1L41	C12-C11	-5.08	1.31	1.51
3	B	502[A]	A1L41	C12-C11	-4.92	1.32	1.51
3	A	502[A]	A1L41	P1-O3	4.50	1.57	1.49
3	A	502[B]	A1L41	P1-O3	4.50	1.57	1.49
3	A	502[A]	A1L41	P1-C7	4.03	1.87	1.81
3	A	502[B]	A1L41	P1-C7	4.03	1.87	1.81
3	B	502[A]	A1L41	C5-C6	3.64	1.45	1.38
3	B	502[B]	A1L41	C5-C6	3.64	1.45	1.38
3	A	502[A]	A1L41	C1-C7	-3.55	1.46	1.52
3	A	502[B]	A1L41	C1-C7	-3.55	1.46	1.52
3	B	502[A]	A1L41	P1-O3	3.52	1.55	1.49
3	B	502[B]	A1L41	P1-O3	3.52	1.55	1.49
3	A	502[A]	A1L41	P1-O5	-3.11	1.49	1.54
3	A	502[B]	A1L41	P1-O5	-3.11	1.49	1.54
3	B	502[A]	A1L41	P1-O5	-3.10	1.49	1.54
3	B	502[B]	A1L41	P1-O5	-3.10	1.49	1.54
3	A	502[A]	A1L41	C3-C2	2.82	1.43	1.38
3	A	502[B]	A1L41	C3-C2	2.82	1.43	1.38
3	A	502[A]	A1L41	C5-C6	2.76	1.43	1.38
3	A	502[B]	A1L41	C5-C6	2.76	1.43	1.38
3	A	502[A]	A1L41	P1-O4	-2.50	1.50	1.54
3	A	502[B]	A1L41	P1-O4	-2.50	1.50	1.54
3	A	502[A]	A1L41	O2-C10	-2.01	1.18	1.23
3	A	502[B]	A1L41	O2-C10	-2.01	1.18	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502[A]	A1L41	C12-C11-N1	8.69	129.01	111.11
3	B	502[B]	A1L41	C12-C11-N1	8.64	128.91	111.11
3	A	502[B]	A1L41	C12-C11-N1	8.41	128.43	111.11
3	A	502[A]	A1L41	C12-C11-N1	8.11	127.81	111.11
3	B	502[B]	A1L41	O1-N1-C11	6.18	128.23	113.76
3	A	502[B]	A1L41	O1-N1-C11	5.52	126.69	113.76
3	B	502[A]	A1L41	C5-C6-C1	-5.32	114.28	120.65
3	B	502[B]	A1L41	C5-C6-C1	-5.32	114.28	120.65
3	B	502[A]	A1L41	O1-N1-C11	5.13	125.77	113.76
3	A	502[A]	A1L41	O1-N1-C11	4.58	124.49	113.76
3	B	502[A]	A1L41	C4-C5-C6	3.17	124.14	120.24
3	B	502[B]	A1L41	C4-C5-C6	3.17	124.14	120.24
3	B	502[A]	A1L41	C4-C3-C2	-3.06	116.46	120.24
3	B	502[B]	A1L41	C4-C3-C2	-3.06	116.46	120.24
3	A	502[A]	A1L41	C3-C4-C5	2.92	123.86	119.87
3	A	502[B]	A1L41	C3-C4-C5	2.92	123.86	119.87
3	B	502[B]	A1L41	C18-C19-C20	-2.87	116.70	120.24
3	B	502[A]	A1L41	C6-C1-C7	-2.70	116.29	120.73
3	B	502[B]	A1L41	C6-C1-C7	-2.70	116.29	120.73
3	A	502[A]	A1L41	C4-C3-C2	-2.61	117.02	120.24
3	A	502[B]	A1L41	C4-C3-C2	-2.61	117.02	120.24
3	B	502[A]	A1L41	C3-C2-C1	2.53	123.67	120.65
3	B	502[B]	A1L41	C3-C2-C1	2.53	123.67	120.65
3	B	502[A]	A1L41	C8-C9-C10	-2.32	110.34	113.39
3	B	502[B]	A1L41	C8-C9-C10	-2.32	110.34	113.39
3	A	502[A]	A1L41	C13-C14-C15	-2.09	105.86	113.67

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502[A]	A1L41	C12-C11-N1-C10
3	A	502[A]	A1L41	C12-C11-N1-O1
3	A	502[B]	A1L41	C12-C11-N1-C10
3	A	502[B]	A1L41	C12-C11-N1-O1
3	B	502[A]	A1L41	C12-C11-N1-C10
3	B	502[A]	A1L41	C12-C11-N1-O1
3	B	502[B]	A1L41	C12-C11-N1-C10
3	B	502[B]	A1L41	C12-C11-N1-O1
3	B	502[A]	A1L41	C11-C12-C13-C14
3	A	502[A]	A1L41	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	502[B]	A1L41	C11-C12-C13-C14
3	A	502[B]	A1L41	C11-C12-C13-C14
3	B	502[B]	A1L41	C12-C13-C14-C15
3	B	502[A]	A1L41	N1-C10-C9-C8
3	B	502[B]	A1L41	N1-C10-C9-C8
3	A	502[B]	A1L41	C12-C13-C14-C15
3	A	502[A]	A1L41	O2-C10-N1-O1
3	A	502[B]	A1L41	O2-C10-N1-O1
3	B	502[A]	A1L41	O2-C10-N1-O1
3	B	502[B]	A1L41	O2-C10-N1-O1

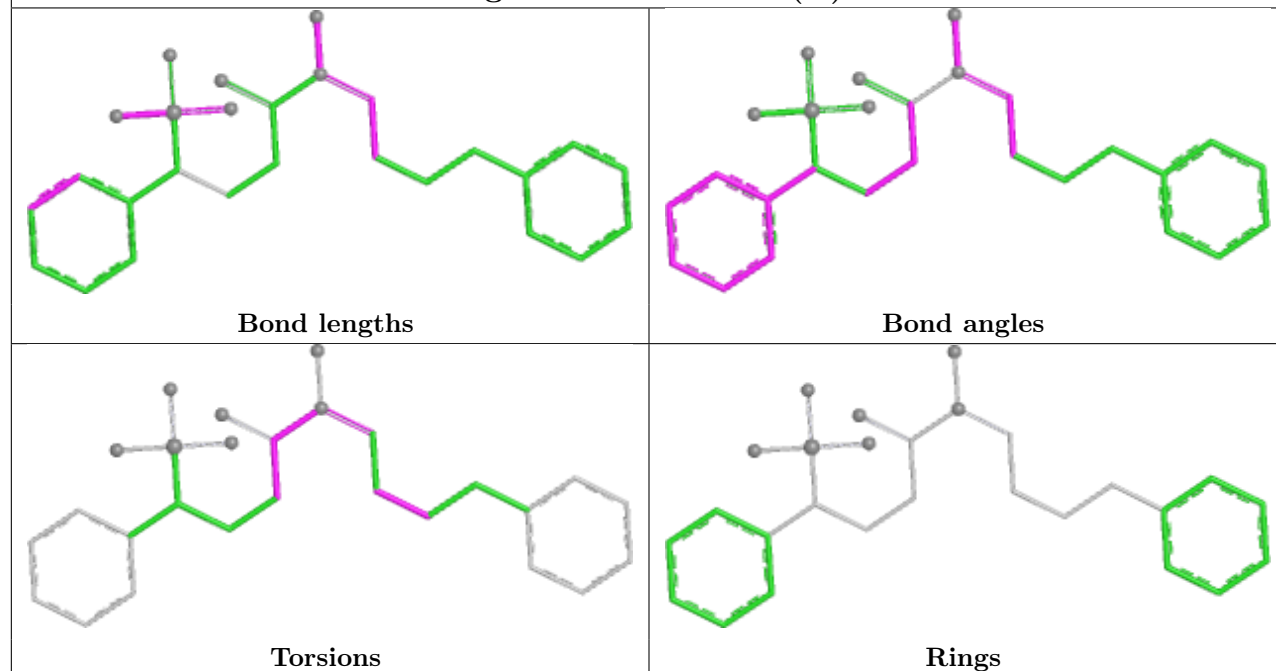
There are no ring outliers.

3 monomers are involved in 5 short contacts:

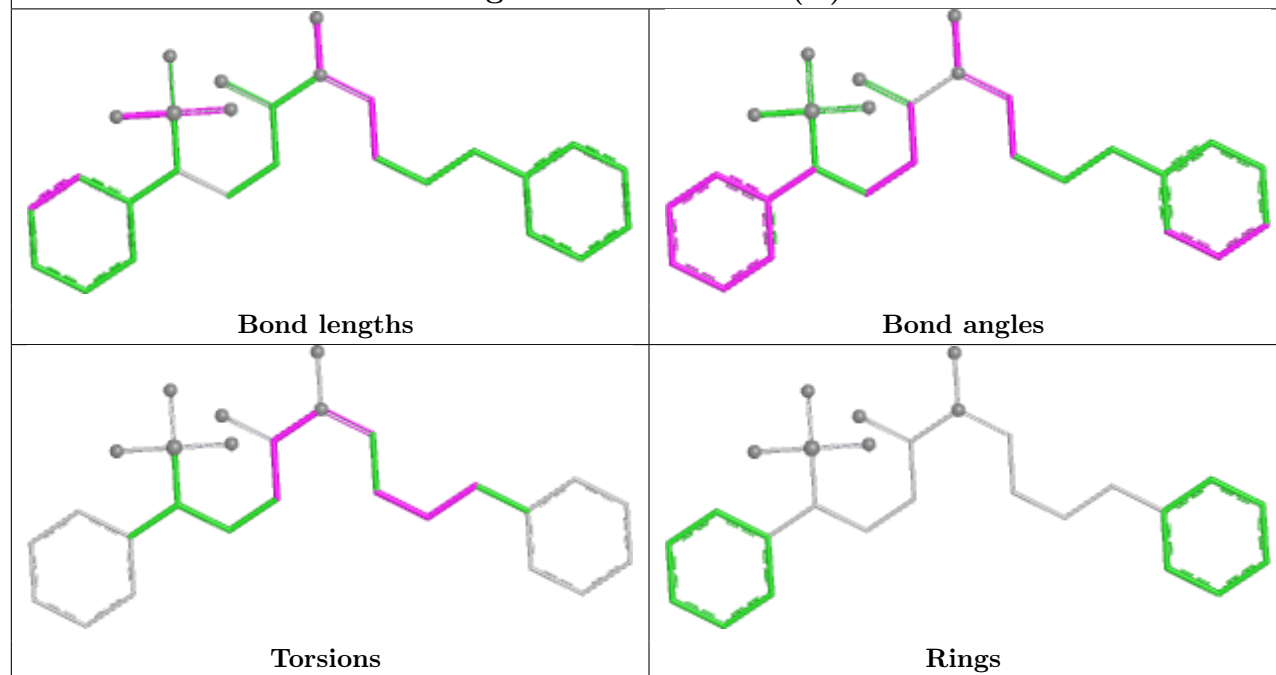
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502[A]	A1L41	2	0
3	B	502[B]	A1L41	1	0
3	A	502[A]	A1L41	2	0

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.

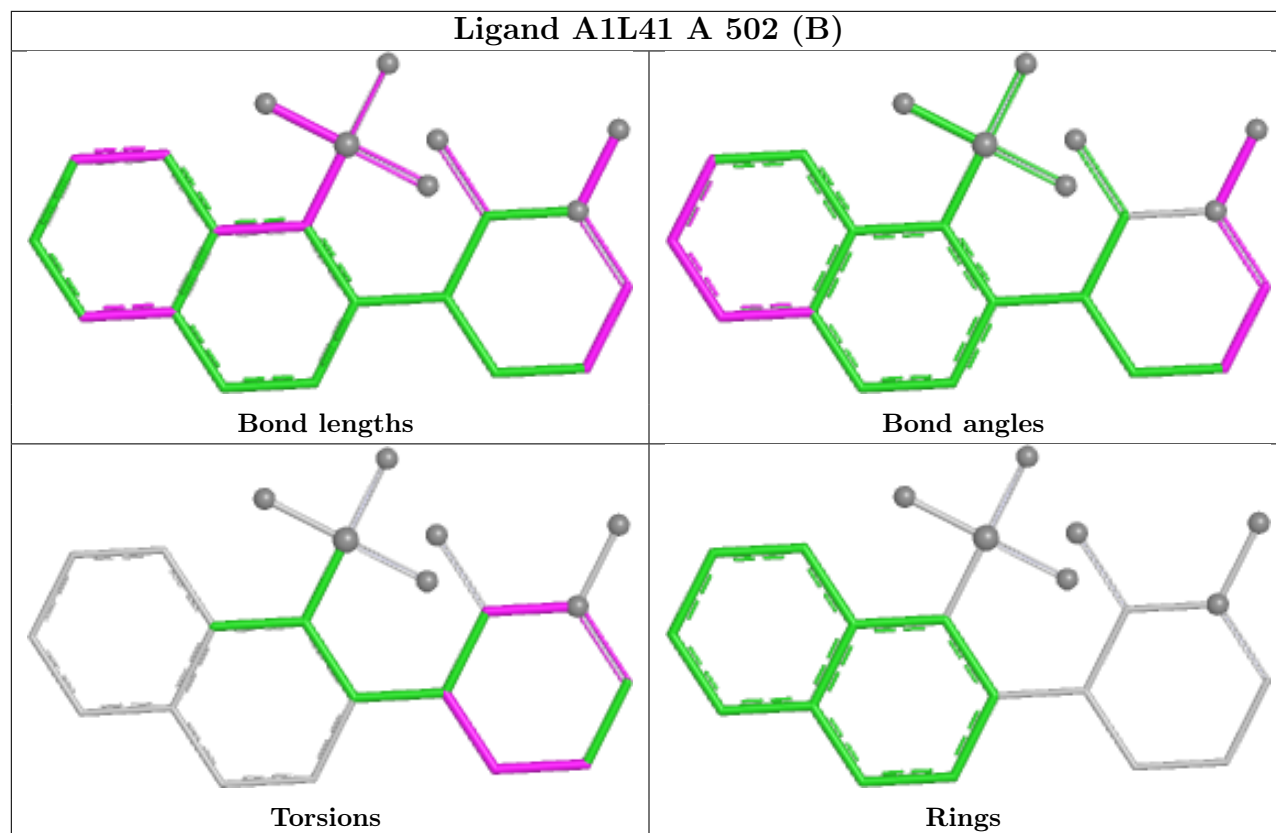
Ligand A1L41 B 502 (A)



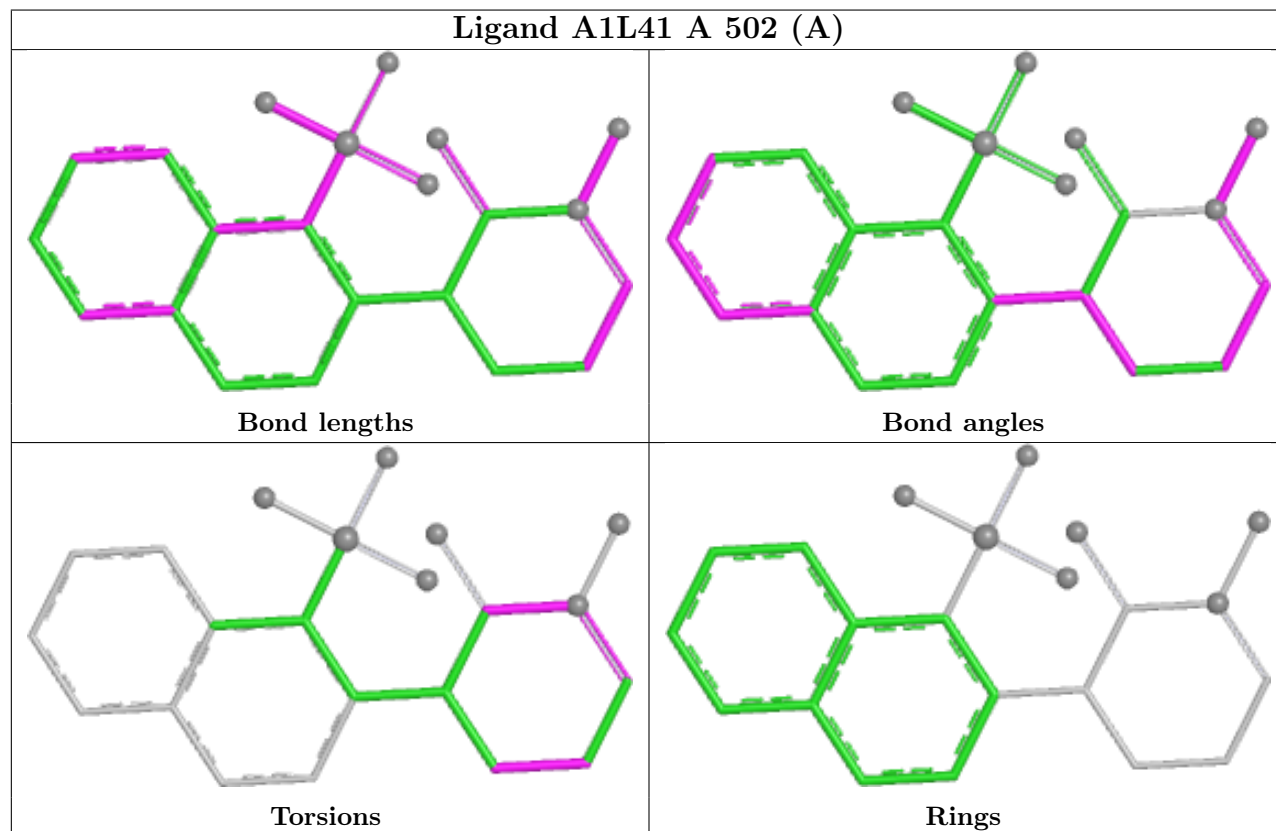
Ligand A1L41 B 502 (B)



Ligand A1L41 A 502 (B)



Ligand A1L41 A 502 (A)



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	408/488 (83%)	0.84	63 (15%) 5 10	10, 19, 50, 88	2 (0%)
1	B	408/488 (83%)	0.58	39 (9%) 13 20	10, 17, 38, 58	2 (0%)
All	All	816/976 (83%)	0.71	102 (12%) 8 13	10, 18, 46, 88	4 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	PHE	9.9
1	A	296[A]	TRP	9.7
1	B	296[A]	TRP	8.9
1	B	184	PHE	7.1
1	A	182	ASP	5.7
1	A	188	TYR	5.5
1	A	213	PHE	5.5
1	B	182	ASP	5.1
1	A	359[A]	ASP	4.7
1	A	144	LEU	4.4
1	A	173	SER	4.4
1	A	192	TYR	4.3
1	A	157	ILE	4.2
1	A	151	ILE	4.2
1	A	183	SER	4.1
1	A	203	ALA	4.1
1	A	147	LEU	3.9
1	A	148	VAL	3.8
1	B	188	TYR	3.8
1	A	160	CYS	3.7
1	A	158	ILE	3.6
1	A	186	GLY	3.6
1	A	122	TYR	3.5
1	A	118	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	150	ASN	3.5
1	A	484	LYS	3.5
1	B	192	TYR	3.4
1	B	151	ILE	3.4
1	B	292	LYS	3.4
1	A	129	LEU	3.3
1	A	140	VAL	3.3
1	B	152	LYS	3.3
1	B	183	SER	3.3
1	B	459	ASN	3.3
1	B	213	PHE	3.3
1	A	485	HIS	3.2
1	A	221	ILE	3.2
1	A	76	LYS	3.2
1	B	147	LEU	3.1
1	B	153	ASP	3.0
1	B	113	TYR	3.0
1	A	292	LYS	3.0
1	A	113	TYR	3.0
1	A	141	TYR	3.0
1	A	159	LEU	3.0
1	A	137	ASP	2.9
1	B	76	LYS	2.9
1	A	152	LYS	2.9
1	A	297	LYS	2.9
1	A	135	ILE	2.8
1	A	486	ASN	2.8
1	A	290	ALA	2.8
1	A	154	TYR	2.8
1	B	462	ASP	2.8
1	A	119	ASN	2.8
1	A	133	LEU	2.7
1	A	185	GLN	2.7
1	A	291	LEU	2.7
1	A	181	ILE	2.7
1	A	114	VAL	2.6
1	A	149	LYS	2.6
1	A	172	ASN	2.6
1	B	203	ALA	2.6
1	A	274	PHE	2.6
1	B	173	SER	2.6
1	B	461	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	77	PRO	2.6
1	B	468	LEU	2.5
1	B	172	ASN	2.5
1	B	359[A]	ASP	2.5
1	B	115	ASN	2.4
1	B	290	ALA	2.4
1	A	456	VAL	2.4
1	B	377	ASN	2.4
1	A	145	LYS	2.4
1	B	460	SER	2.4
1	A	121	LEU	2.4
1	A	187	LEU	2.3
1	A	204	ASN	2.3
1	B	126	ARG	2.3
1	B	204	ASN	2.3
1	B	486	ASN	2.3
1	B	279	MET	2.2
1	B	282	LEU	2.2
1	A	139	SER	2.2
1	A	142	GLU	2.2
1	A	115	ASN	2.2
1	A	88	SER	2.2
1	A	156	PRO	2.2
1	B	449	GLU	2.2
1	B	105	ASN	2.2
1	B	485	HIS	2.1
1	A	153	ASP	2.1
1	B	297	LYS	2.1
1	B	150	ASN	2.1
1	B	181	ILE	2.1
1	A	458	GLU	2.1
1	A	106	VAL	2.1
1	A	155	LYS	2.1
1	B	458	GLU	2.0
1	A	143	GLU	2.0
1	A	136	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

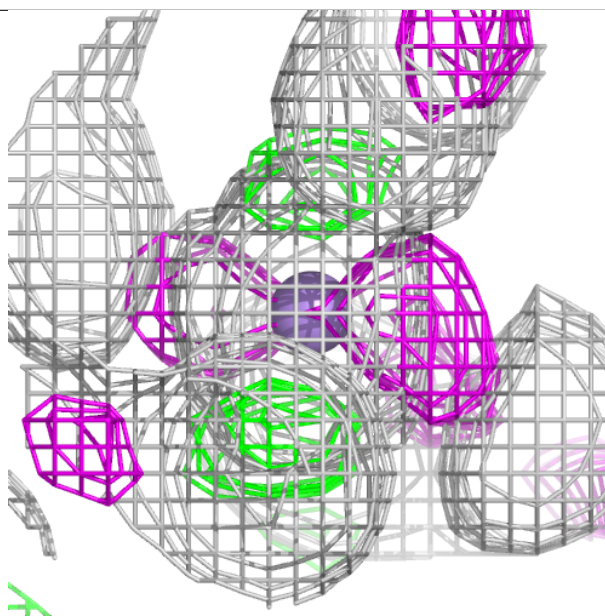
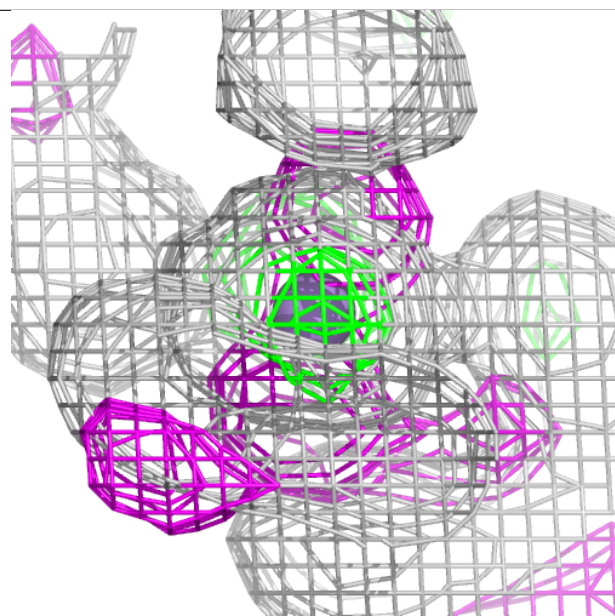
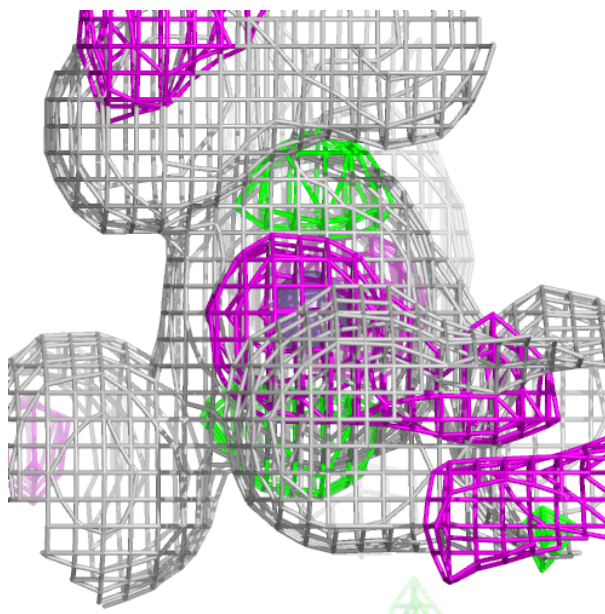
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	506	6/6	0.88	0.13	21,27,31,34	0
4	GOL	A	503	6/6	0.89	0.13	20,28,31,35	0
5	CA	B	504	1/1	0.92	0.10	23,23,23,23	0
2	MN	B	501	1/1	0.98	0.04	11,11,11,11	0
3	A1L41	A	502[A]	27/27	0.98	0.08	12,16,42,43	10
3	A1L41	A	502[B]	27/27	0.98	0.08	12,16,20,22	10
5	CA	B	505	1/1	0.98	0.12	24,24,24,24	0
3	A1L41	B	502[A]	27/27	0.99	0.08	11,15,57,59	10
5	CA	B	503	1/1	0.99	0.04	12,12,12,12	0
3	A1L41	B	502[B]	27/27	0.99	0.08	11,15,23,25	10
2	MN	A	501	1/1	0.99	0.02	11,11,11,11	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.

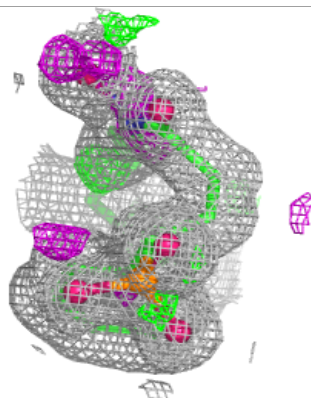
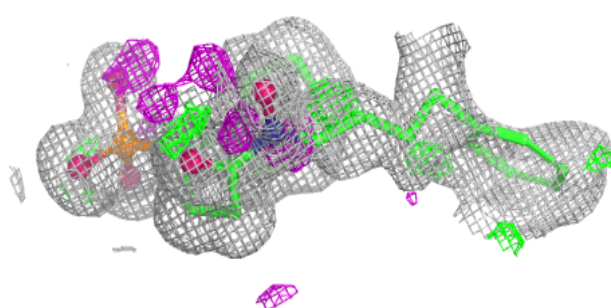
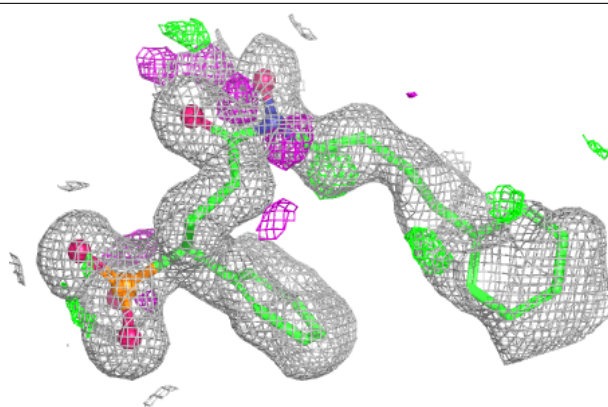
Electron density around MN B 501:

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

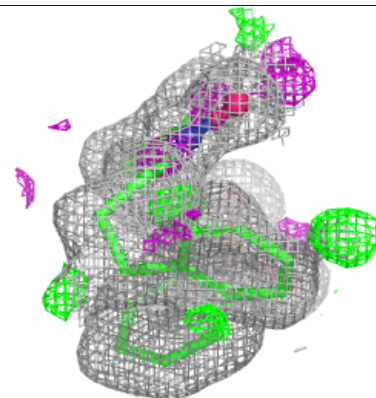
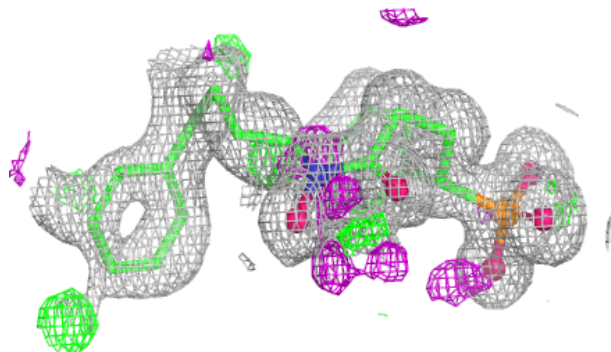
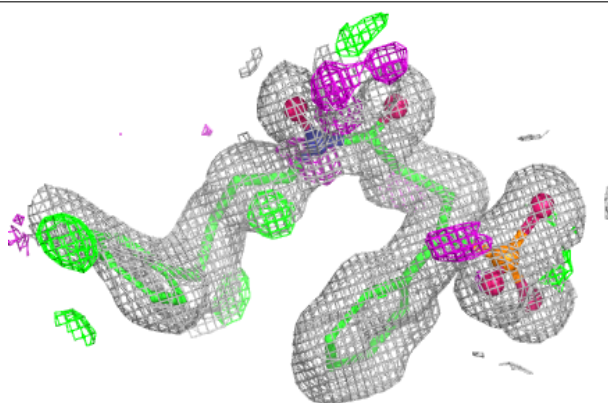


Electron density around A1L41 A 502 (A):

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

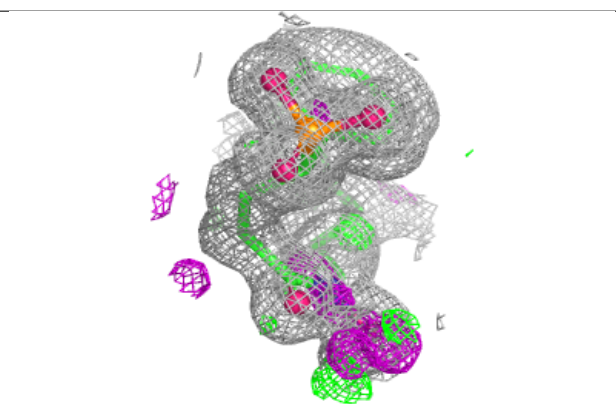
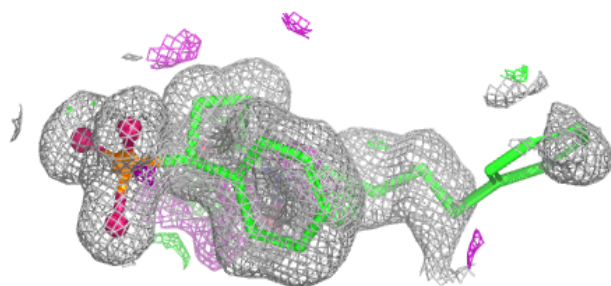
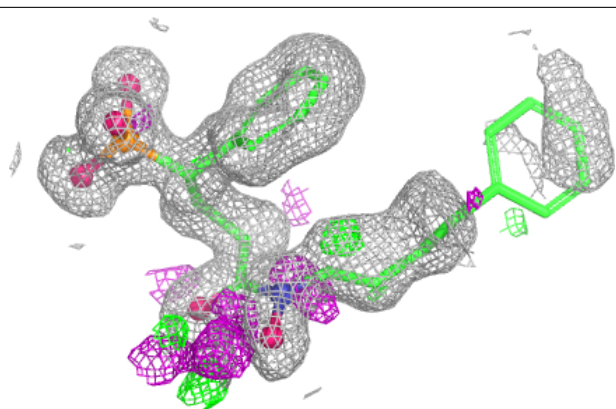
**Electron density around A1L41 A 502 (B):**

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

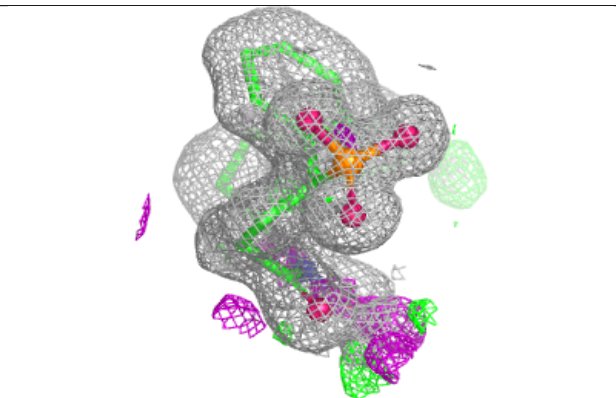
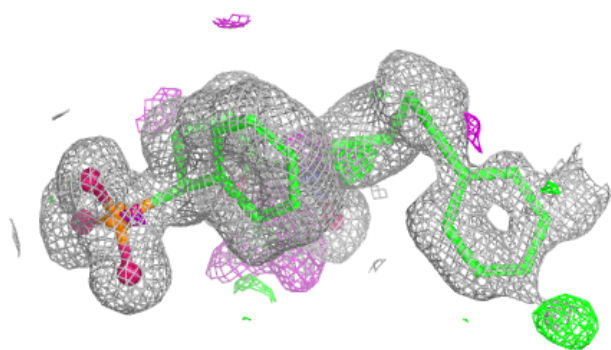
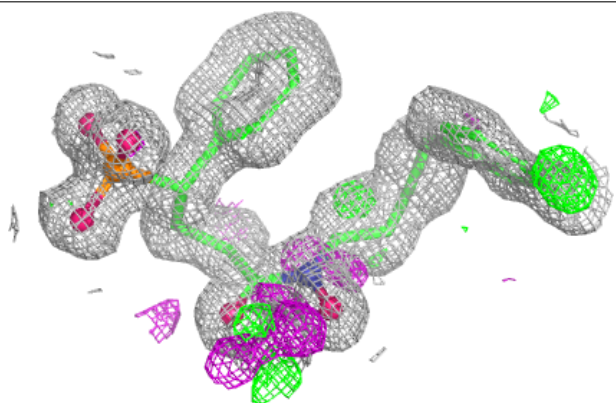


Electron density around A1L41 B 502 (A):

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

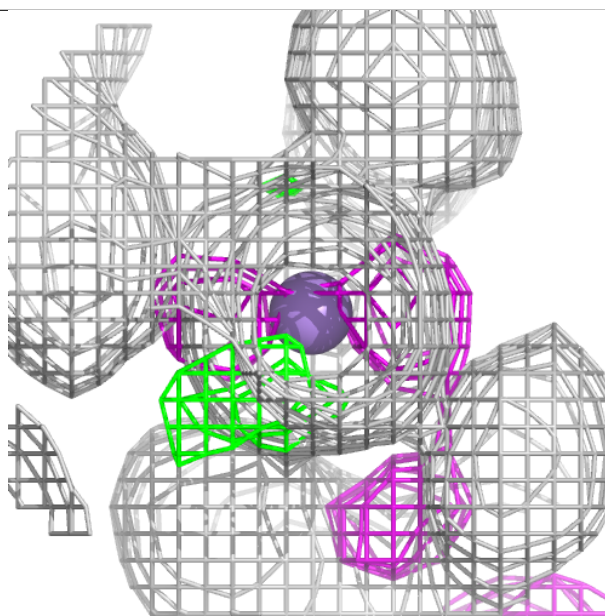
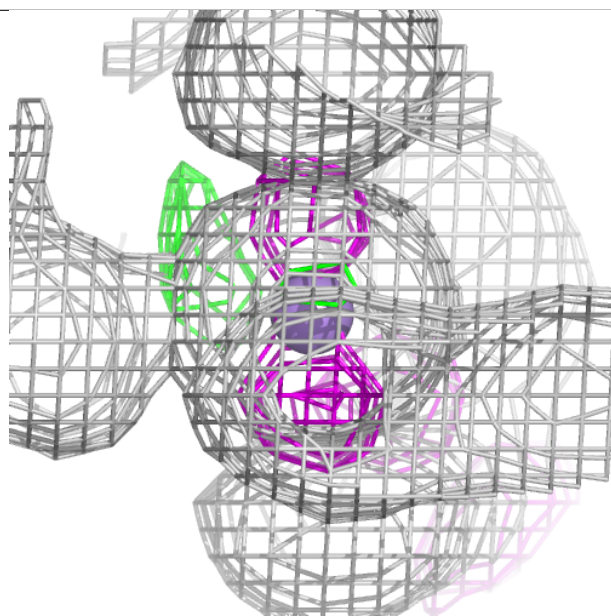
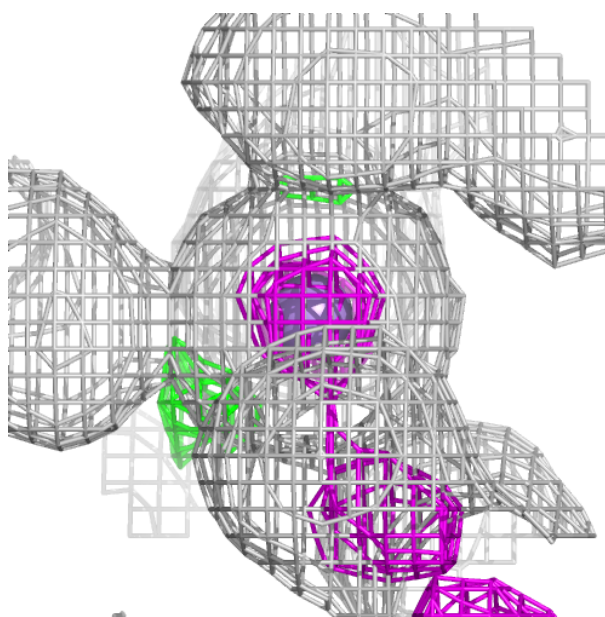
**Electron density around A1L41 B 502 (B):**

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



Electron density around 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.