



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 PM UTC

PDB ID : 9GH9 / pdb_00009gh9
Title : A novel aminotransferase from Streptomyces sp.
Authors : De Rose, S.A.; Isupov, M.N.; Patti, S.
Deposited on : 2024-08-15
Resolution : 1.49 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

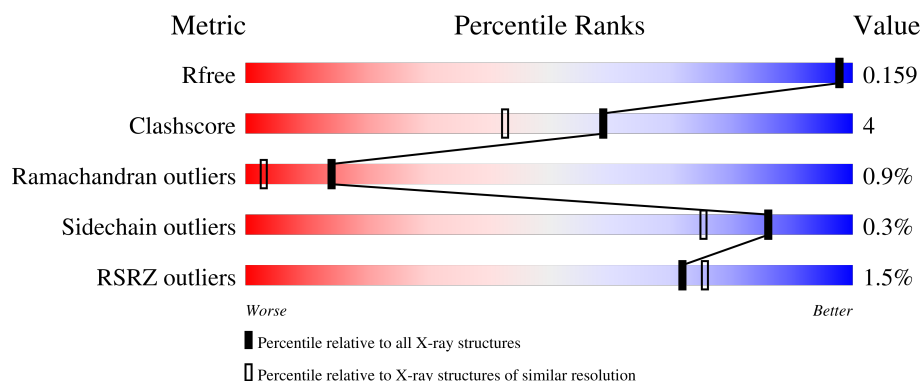
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	465	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>••</div> </div> </div>
1	B	465	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</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
1	LLP	A	289[B]	-	X	-	-
2	EDO	A	504	-	X	-	-
2	EDO	B	508	-	-	X	-
4	SO4	A	508	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15886 atoms, of which 7292 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.

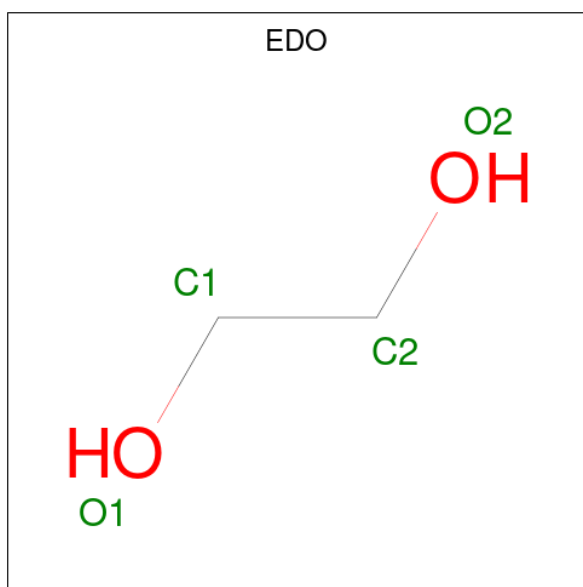
- Molecule 1 is a protein called Aspartate aminotransferase family protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	453	Total	C	H	N	O	P	S	111	21	0
			7228	2344	3576	611	685	1	11			
1	B	453	Total	C	H	N	O	P	S	111	26	0
			7306	2364	3628	617	685	1	11			

There are 12 discrepancies between the modelled and reference sequences:

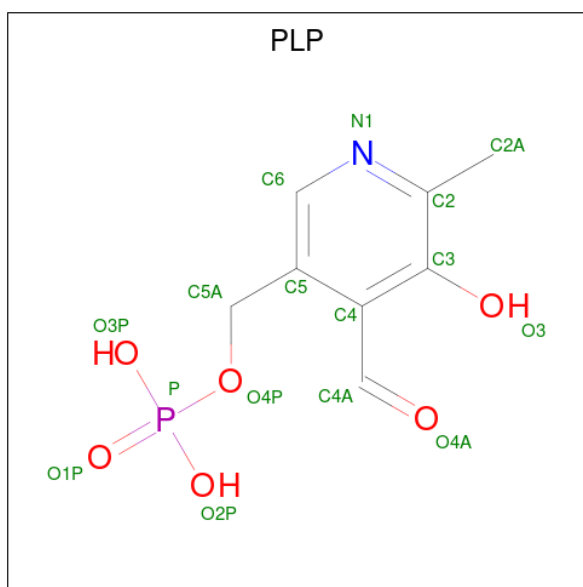
Chain	Residue	Modelled	Actual	Comment	Reference
A	460	HIS	-	expression tag	UNP A0AA46ZEV9
A	461	HIS	-	expression tag	UNP A0AA46ZEV9
A	462	HIS	-	expression tag	UNP A0AA46ZEV9
A	463	HIS	-	expression tag	UNP A0AA46ZEV9
A	464	HIS	-	expression tag	UNP A0AA46ZEV9
A	465	HIS	-	expression tag	UNP A0AA46ZEV9
B	460	HIS	-	expression tag	UNP A0AA46ZEV9
B	461	HIS	-	expression tag	UNP A0AA46ZEV9
B	462	HIS	-	expression tag	UNP A0AA46ZEV9
B	463	HIS	-	expression tag	UNP A0AA46ZEV9
B	464	HIS	-	expression tag	UNP A0AA46ZEV9
B	465	HIS	-	expression tag	UNP A0AA46ZEV9

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



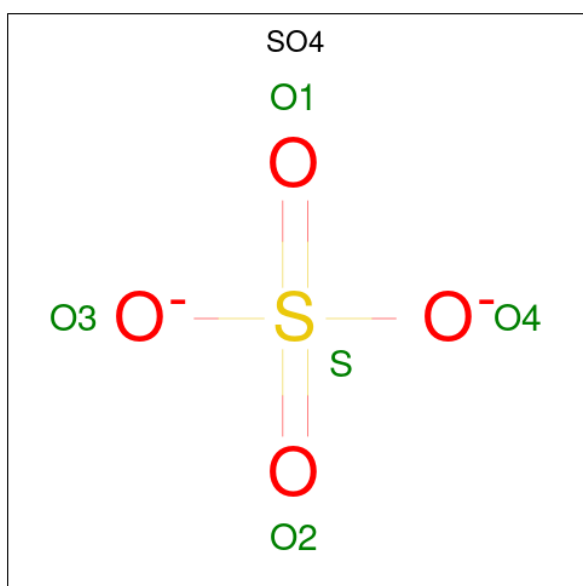
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			10	2	6	2		
2	A	1	Total	C	H	O	2	0
			10	2	6	2		
2	A	1	Total	C	H	O	2	0
			10	2	6	2		
2	A	1	Total	C	H	O	2	0
			10	2	6	2		
2	B	1	Total	C	H	O	2	0
			10	2	6	2		
2	B	1	Total	C	H	O	2	0
			10	2	6	2		
2	B	1	Total	C	H	O	2	0
			10	2	6	2		
2	B	1	Total	C	H	O	2	0
			10	2	6	2		
2	B	1	Total	C	H	O	2	0
			10	2	6	2		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	4	0
			24	8	8	1	6	1		
3	B	1	Total	C	H	N	O	P	4	0
			24	8	8	1	6	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

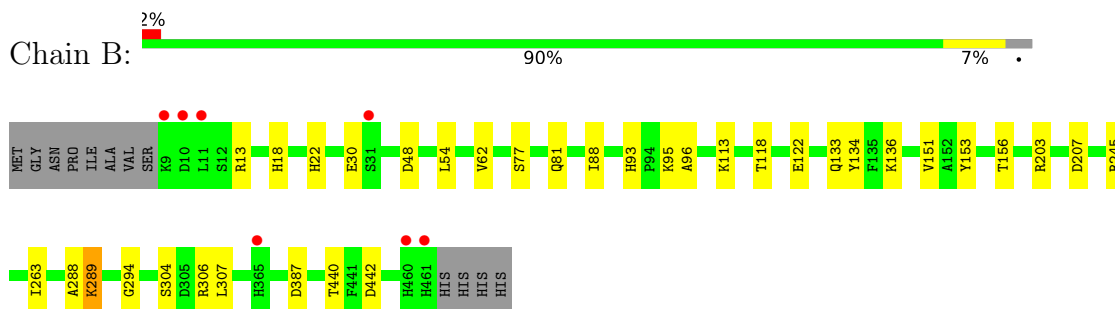
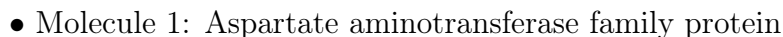
Continued from previous page...

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	609	Total	O	0	0
			609	609		
5	B	560	Total	O	0	0
			560	560		

- Molecule 1: Aspartate aminotransferase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	78.32Å 176.10Å 60.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.85 – 1.49 60.85 – 1.49	Depositor EDS
% Data completeness (in resolution range)	81.4 (60.85-1.49) 81.4 (60.85-1.49)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.129 , 0.159 0.129 , 0.159	Depositor DCC
R_{free} test set	5566 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	14.3	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.2	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	0.98	EDS
Total number of atoms	15886	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: EDO, SO4, LLP, PLP

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	0/3787	1.04	3/5149 (0.1%)
1	B	0.74	0/3826	1.03	4/5197 (0.1%)
All	All	0.73	0/7613	1.03	7/10346 (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	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	450	THR	CA-CB-OG1	-6.21	100.29	109.60
1	B	387	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	378	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	30	GLU	CB-CA-C	-5.47	102.30	110.88
1	B	442	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	48	ASP	CA-CB-CG	5.15	117.75	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306[A]	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	306[B]	ARG	Sidechain

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	3652	3576	3521	24	1
1	B	3678	3628	3580	36	1
2	A	20	30	27	8	0
2	B	28	42	39	12	0
3	A	16	8	6	1	0
3	B	16	8	6	1	0
4	A	10	0	0	2	0
4	B	5	0	0	0	0
5	A	609	0	0	16	1
5	B	560	0	0	9	0
All	All	8594	7292	7179	64	2

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 (64) 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:203[B]:ARG:HD2	1:B:245[B]:ARG:CD	2.01	0.88
2:A:501:EDO:H22	5:A:993:HOH:O	1.77	0.84
1:B:203[B]:ARG:CD	1:B:245[B]:ARG:CD	2.57	0.83
1:A:78[B]:LYS:HE2	5:A:913:HOH:O	1.81	0.81
1:B:203[B]:ARG:HD2	1:B:245[B]:ARG:HD3	1.66	0.78
1:B:13[B]:ARG:HD3	5:B:668:HOH:O	1.87	0.75
1:A:70[B]:THR:OG1	1:B:81[B]:GLN:OE1	2.03	0.74
1:B:306[A]:ARG:NH1	5:B:602:HOH:O	2.21	0.73
4:A:508:SO4:O2	5:A:601:HOH:O	2.14	0.64
1:A:313[A]:GLN:CD	5:A:639:HOH:O	2.39	0.63
1:B:306[A]:ARG:CD	5:B:602:HOH:O	2.47	0.63
1:B:306[A]:ARG:CZ	5:B:602:HOH:O	2.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLN:HE21	2:B:508:EDO:H21	1.67	0.60
2:A:501:EDO:H12	5:A:981:HOH:O	2.01	0.59
4:A:508:SO4:O4	5:A:602:HOH:O	2.16	0.59
1:B:263:ILE:HG13	1:B:289[A]:LLP:O3	2.04	0.58
1:B:13[B]:ARG:CD	5:B:668:HOH:O	2.50	0.58
1:A:263:ILE:HG13	1:A:289[A]:LLP:O3	2.03	0.58
1:A:118[B]:THR:HB	1:B:118[B]:THR:HG21	1.86	0.57
2:A:505:EDO:H21	5:A:1046:HOH:O	2.05	0.56
5:A:685:HOH:O	1:B:136:LYS:HE2	2.06	0.56
1:A:77[B]:SER:HB2	1:B:77[B]:SER:HB2	1.87	0.55
1:A:118[B]:THR:HG21	1:B:118[B]:THR:OG1	2.07	0.55
1:A:304[B]:SER:OG	1:A:307:LEU:HG	2.07	0.55
1:A:317[B]:THR:HG23	1:A:319:LEU:HG	1.89	0.54
1:B:95:LYS:NZ	2:B:501:EDO:H22	2.23	0.53
1:B:81[B]:GLN:NE2	5:B:604:HOH:O	2.28	0.53
1:A:215:PHE:HA	2:A:504:EDO:H12	1.91	0.53
1:B:62:VAL:CG1	1:B:294:GLY:HA3	2.39	0.53
1:A:49:GLN:NE2	5:A:607:HOH:O	2.32	0.52
1:B:304[B]:SER:OG	1:B:307:LEU:HG	2.10	0.52
1:B:153:TYR:HE2	3:B:503:PLP:C4A	2.23	0.52
5:A:665:HOH:O	1:B:118[B]:THR:HG23	2.10	0.51
1:B:95:LYS:HZ2	2:B:501:EDO:H22	1.77	0.50
5:A:665:HOH:O	1:B:118[B]:THR:CG2	2.59	0.49
1:B:113[B]:LYS:NZ	5:B:606:HOH:O	2.36	0.49
1:A:167:PRO:HD3	2:A:505:EDO:H11	1.94	0.49
2:A:501:EDO:C1	5:A:981:HOH:O	2.61	0.49
2:B:501:EDO:H12	5:B:999:HOH:O	2.12	0.48
1:A:70[A]:THR:HG23	5:A:1043:HOH:O	2.14	0.47
1:A:30:GLU:HG3	5:A:619:HOH:O	2.14	0.47
1:B:118[B]:THR:HG22	1:B:122:GLU:OE1	2.14	0.47
1:B:289[A]:LLP:O3	1:B:289[A]:LLP:NZ	2.47	0.47
1:A:153:TYR:HE2	3:A:502:PLP:C4A	2.27	0.47
1:A:62:VAL:CG1	1:A:294:GLY:HA3	2.45	0.47
1:A:118[B]:THR:CB	1:B:118[B]:THR:HG21	2.44	0.47
1:B:203[B]:ARG:CD	1:B:245[B]:ARG:HD2	2.43	0.47
1:B:18:HIS:NE2	2:B:506:EDO:H21	2.30	0.46
1:B:54[B]:LEU:HD11	1:B:440:THR:HG23	1.98	0.46
1:A:102[B]:ARG:NH1	1:A:338:LEU:HD13	2.32	0.44
1:A:89:TRP:CD1	1:B:22:HIS:HB2	2.53	0.43
1:A:204:TRP:HD1	2:A:503:EDO:H21	1.84	0.43
1:B:93:HIS:CE1	1:B:96:ALA:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:CD	2:A:505:EDO:H11	2.49	0.42
1:A:118[B]:THR:CG2	1:B:118[B]:THR:HG21	2.48	0.42
1:A:358[B]:PHE:HZ	5:A:666:HOH:O	2.02	0.42
1:B:133:GLN:NE2	2:B:508:EDO:C2	2.83	0.41
2:B:508:EDO:C1	5:B:904:HOH:O	2.69	0.41
1:B:133:GLN:HE21	2:B:508:EDO:C2	2.32	0.41
1:A:460:HIS:CD2	5:A:905:HOH:O	2.74	0.40
1:B:134:TYR:OH	2:B:505:EDO:H11	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:OH	1:B:30[A]:GLU:OE2[1_554]	1.74	0.46
5:A:898:HOH:O	5:A:898:HOH:O[2_555]	2.13	0.07

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	470/465 (101%)	447 (95%)	19 (4%)	4 (1%)	14	3
1	B	475/465 (102%)	455 (96%)	16 (3%)	4 (1%)	16	4
All	All	945/930 (102%)	902 (95%)	35 (4%)	8 (1%)	14	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	A	288	ALA
1	B	151	VAL
1	B	288	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	88	ILE
1	A	88	ILE
1	B	156	THR
1	A	156	THR

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	385/376 (102%)	382 (99%)	3 (1%)	73	54
1	B	390/376 (104%)	390 (100%)	0	100	100
All	All	775/752 (103%)	772 (100%)	3 (0%)	86	71

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102[A]	ARG
1	A	102[B]	ARG
1	A	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	133	GLN
1	A	316	ASN
1	A	362	GLN
1	A	438	GLN
1	B	79	GLN
1	B	133	GLN
1	B	438	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	A	289[A]	-	23,24,25	0.58	0	25,32,34	1.33	3 (12%)
1	LLP	B	289[A]	-	23,24,25	0.66	0	25,32,34	1.31	3 (12%)
1	LLP	B	289[B]	-	23,8,25	12.04	1 (4%)	25,8,34	5.12	5 (20%)
1	LLP	A	289[B]	-	23,8,25	11.95	1 (4%)	25,8,34	5.16	5 (20%)

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
1	LLP	A	289[A]	-	-	4/16/17/19	0/1/1/1
1	LLP	B	289[A]	-	-	3/16/17/19	0/1/1/1
1	LLP	B	289[B]	-	-	3/16/7/19	0/1/0/1
1	LLP	A	289[B]	-	-	4/16/7/19	0/1/0/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289[B]	LLP	C4'-NZ	57.63	3.20	1.27
1	A	289[B]	LLP	C4'-NZ	57.26	3.18	1.27

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289[B]	LLP	CE-NZ-C4'	-22.94	45.26	118.72
1	B	289[B]	LLP	CE-NZ-C4'	-22.92	45.30	118.72
1	A	289[B]	LLP	C4-C4'-NZ	9.99	170.11	124.04
1	B	289[B]	LLP	C4-C4'-NZ	9.71	168.85	124.04
1	B	289[A]	LLP	OP4-C5'-C5	3.38	115.69	109.36
1	B	289[B]	LLP	OP4-C5'-C5	3.38	115.69	109.36
1	B	289[A]	LLP	CD-CE-NZ	3.23	119.38	110.83
1	A	289[A]	LLP	CD-CE-NZ	3.21	119.32	110.83
1	A	289[A]	LLP	OP4-C5'-C5	2.78	114.57	109.36
1	A	289[B]	LLP	OP4-C5'-C5	2.78	114.57	109.36
1	A	289[A]	LLP	C3-C4-C5	-2.77	116.05	118.28
1	A	289[B]	LLP	C3-C4-C5	-2.77	116.05	118.28
1	A	289[B]	LLP	CD-CE-NZ	2.41	117.22	110.83
1	B	289[A]	LLP	O3-C3-C2	2.29	122.34	117.58
1	B	289[B]	LLP	O3-C3-C2	2.29	122.34	117.58
1	B	289[B]	LLP	CD-CE-NZ	2.01	116.15	110.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	289[A]	LLP	O-C-CA-CB
1	A	289[A]	LLP	CG-CD-CE-NZ
1	A	289[B]	LLP	C4-C4'-NZ-CE
1	A	289[B]	LLP	O-C-CA-CB
1	B	289[A]	LLP	O-C-CA-CB
1	B	289[A]	LLP	CG-CD-CE-NZ
1	B	289[B]	LLP	C4-C4'-NZ-CE
1	B	289[B]	LLP	O-C-CA-CB
1	A	289[A]	LLP	C4-C4'-NZ-CE
1	A	289[B]	LLP	CD-CE-NZ-C4'
1	B	289[B]	LLP	CD-CE-NZ-C4'
1	A	289[A]	LLP	C-CA-CB-CG
1	A	289[B]	LLP	C-CA-CB-CG
1	B	289[A]	LLP	C4-C4'-NZ-CE

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	289[A]	LLP	1	0
1	B	289[A]	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	$\# Z > 2$
2	EDO	A	505	-	3,3,3	0.78	0	2,2,2	1.41	0
2	EDO	B	505	-	3,3,3	0.51	0	2,2,2	0.30	0
2	EDO	A	501	-	3,3,3	1.17	0	2,2,2	0.72	0
3	PLP	B	503	-	16,16,16	0.72	0	20,23,23	1.33	3 (15%)
2	EDO	A	506	-	3,3,3	0.30	0	2,2,2	0.29	0
2	EDO	B	501	-	3,3,3	0.11	0	2,2,2	0.41	0
2	EDO	B	507	-	3,3,3	0.20	0	2,2,2	0.35	0
2	EDO	B	508	-	3,3,3	1.24	0	2,2,2	0.14	0
4	SO4	A	508	-	4,4,4	0.40	0	6,6,6	0.68	0
4	SO4	A	507	-	4,4,4	0.56	0	6,6,6	0.41	0
2	EDO	A	504	-	3,3,3	1.79	2 (66%)	2,2,2	0.41	0
2	EDO	B	504	-	3,3,3	0.12	0	2,2,2	0.39	0
4	SO4	B	509	-	4,4,4	0.68	0	6,6,6	0.33	0
2	EDO	B	506	-	3,3,3	0.14	0	2,2,2	0.29	0
2	EDO	A	503	-	3,3,3	0.37	0	2,2,2	0.35	0
3	PLP	A	502	-	16,16,16	0.61	0	20,23,23	1.24	3 (15%)
2	EDO	B	502	-	3,3,3	1.00	0	2,2,2	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	B	505	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	501	-	-	1/1/1/1	-
3	PLP	B	503	-	-	0/8/8/8	0/1/1/1
2	EDO	A	506	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	B	507	-	-	1/1/1/1	-
2	EDO	B	508	-	-	1/1/1/1	-
2	EDO	A	504	-	-	1/1/1/1	-
2	EDO	B	504	-	-	1/1/1/1	-
2	EDO	B	506	-	-	0/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
3	PLP	A	502	-	-	0/8/8/8	0/1/1/1
2	EDO	B	502	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	504	EDO	O1-C1	-2.14	1.31	1.42
2	A	504	EDO	O2-C2	-2.02	1.31	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	PLP	O3-C3-C2	3.51	124.86	117.58
3	A	502	PLP	O2P-P-O4P	-3.22	98.27	106.67
3	B	503	PLP	C4-C3-C2	-2.79	118.58	120.14
3	B	503	PLP	O2P-P-O4P	-2.43	100.34	106.67
3	A	502	PLP	C4-C3-C2	-2.37	118.81	120.14
3	A	502	PLP	O3-C3-C2	2.34	122.44	117.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	504	EDO	O1-C1-C2-O2
2	B	507	EDO	O1-C1-C2-O2
2	A	503	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2
2	B	508	EDO	O1-C1-C2-O2
2	A	504	EDO	O1-C1-C2-O2
2	A	506	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

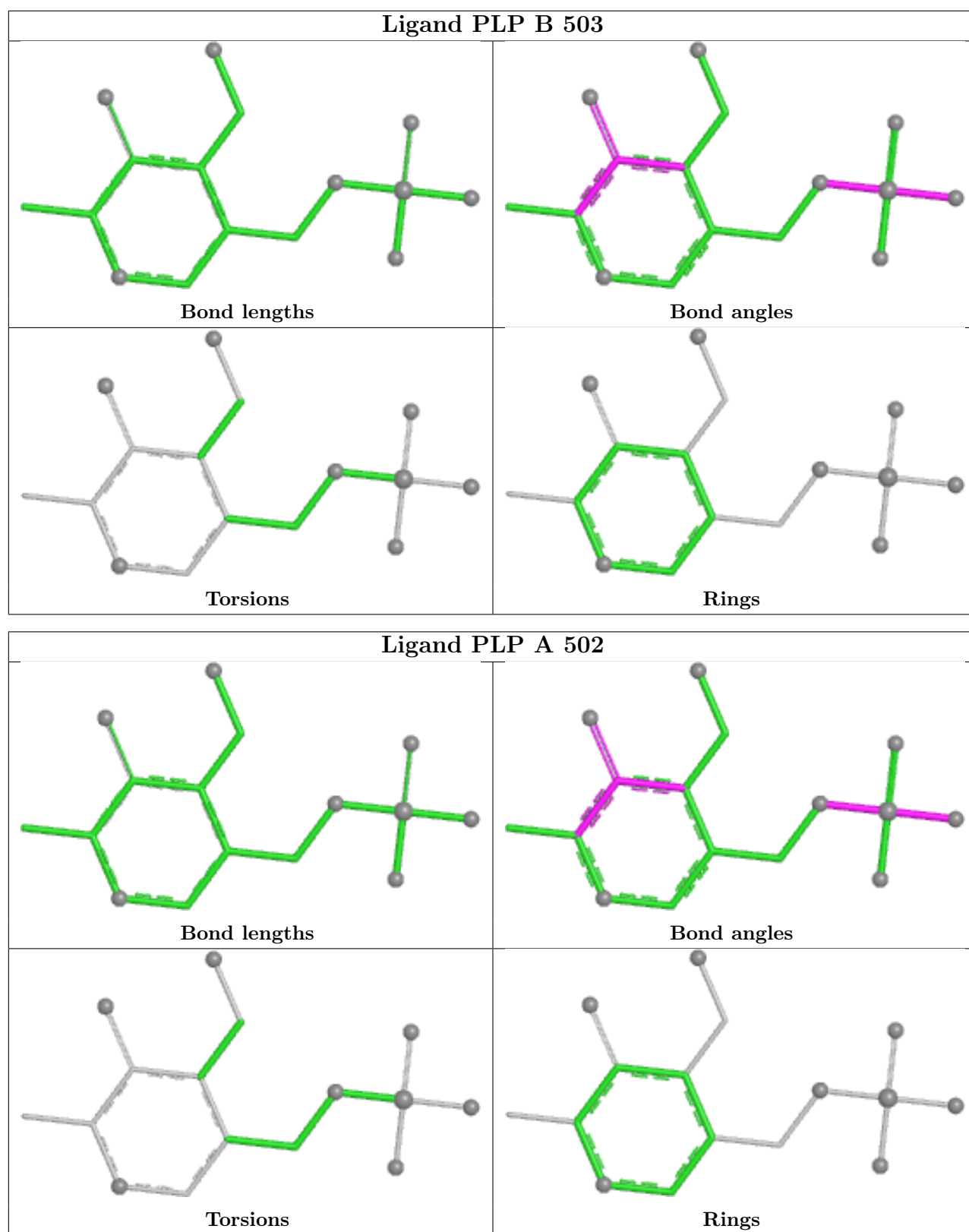
Mol	Chain	Res	Type	Atoms
2	A	501	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	EDO	3	0
2	B	505	EDO	3	0
2	A	501	EDO	3	0
3	B	503	PLP	1	0
2	B	501	EDO	3	0
2	B	508	EDO	4	0
4	A	508	SO4	2	0
2	A	504	EDO	1	0
2	B	504	EDO	1	0
2	B	506	EDO	1	0
2	A	503	EDO	1	0
3	A	502	PLP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/465 (97%)	-0.74	7 (1%) 72 75	5, 12, 25, 91	17 (3%)
1	B	452/465 (97%)	-0.67	7 (1%) 72 75	6, 13, 27, 85	22 (4%)
All	All	904/930 (97%)	-0.71	14 (1%) 72 75	5, 13, 26, 91	39 (4%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	4.1
1	B	11	LEU	4.1
1	A	460	HIS	3.8
1	A	461	HIS	2.9
1	B	460	HIS	2.9
1	B	461	HIS	2.8
1	B	9	LYS	2.8
1	B	10	ASP	2.7
1	A	9	LYS	2.5
1	B	365[A]	HIS	2.4
1	A	13	ARG	2.1
1	A	10	ASP	2.1
1	A	12	SER	2.1
1	B	31	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	LLP	A	289[A]	24/25	0.98	0.06	5,11,14,18	26
1	LLP	A	289[B]	9/25	0.98	0.06	10,10,11,12	3
1	LLP	B	289[A]	24/25	0.98	0.06	6,11,15,20	26
1	LLP	B	289[B]	9/25	0.98	0.06	9,10,12,13	3

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

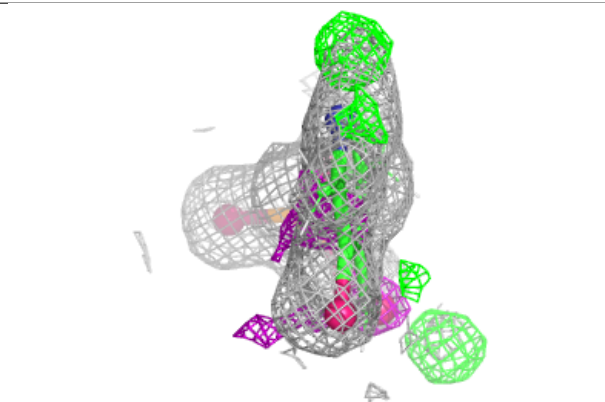
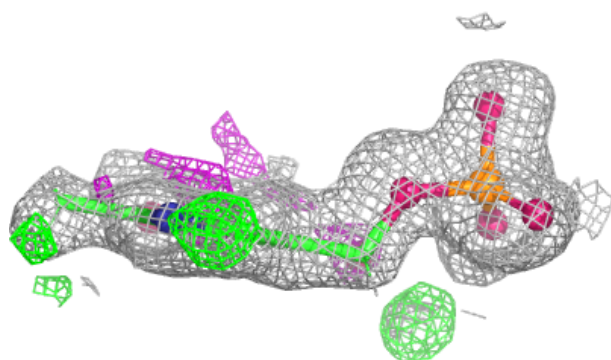
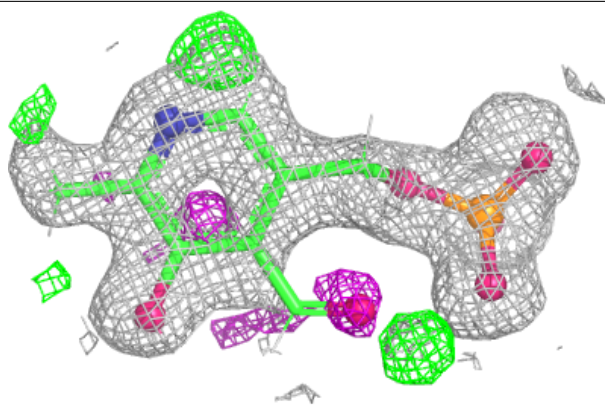
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	505	4/4	0.80	0.14	34,35,54,54	2
2	EDO	B	504	4/4	0.81	0.18	18,19,20,21	10
2	EDO	B	506	4/4	0.81	0.15	34,48,55,56	2
2	EDO	B	507	4/4	0.81	0.12	33,36,40,44	2
2	EDO	A	506	4/4	0.82	0.17	42,46,54,59	2
2	EDO	A	503	4/4	0.84	0.14	31,34,43,48	2
2	EDO	A	504	4/4	0.85	0.36	23,26,30,32	2
2	EDO	A	505	4/4	0.87	0.21	19,24,37,41	2
2	EDO	B	501	4/4	0.90	0.09	33,36,45,45	2
2	EDO	B	502	4/4	0.91	0.09	24,26,27,28	2
2	EDO	A	501	4/4	0.93	0.09	25,32,34,37	2
2	EDO	B	508	4/4	0.93	0.08	25,27,34,36	2
4	SO4	A	507	5/5	0.93	0.10	24,27,35,36	5
4	SO4	B	509	5/5	0.93	0.09	21,26,28,30	5
4	SO4	A	508	5/5	0.94	0.11	21,22,37,38	5
3	PLP	A	502	16/16	0.94	0.11	15,21,28,43	24
3	PLP	B	503	16/16	0.95	0.11	15,18,27,37	24

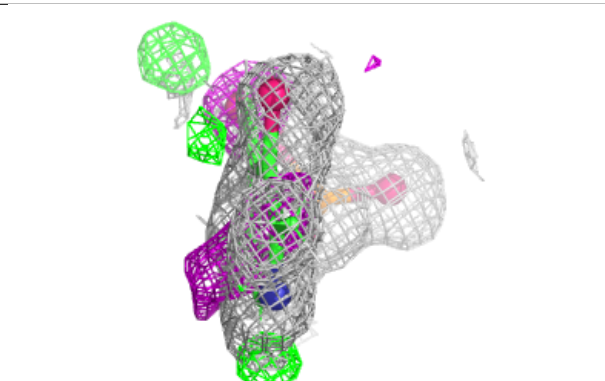
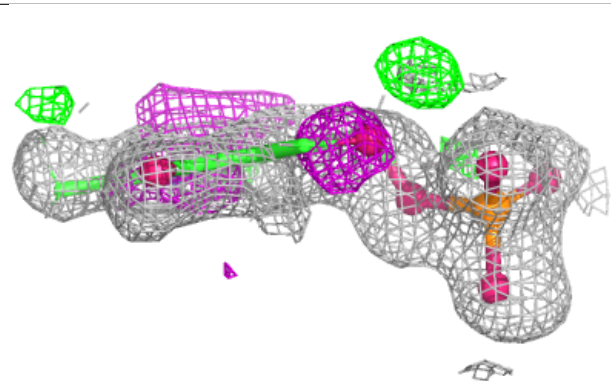
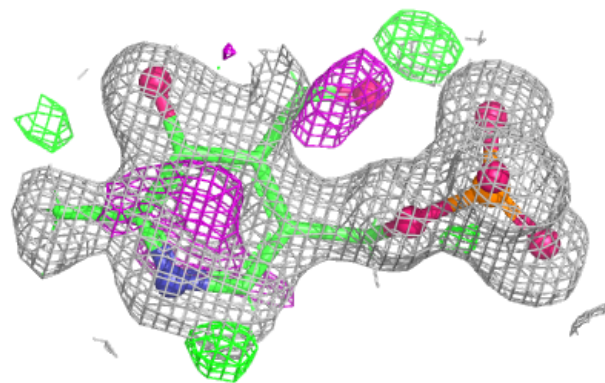
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PLP 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 PLP B 503:**

$2mF_o-DF_c$ (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.