



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:55 AM UTC

PDB ID : 7LPF / pdb_00007lpf
Title : The internal aldimine form of the wild-type Salmonella typhimurium Tryptophan Synthase in complex with inhibitor N-(4'-trifluoromethoxybenzenesulfonyl)-2-amino-1-ethylphosphate (F9F) at the enzyme alpha-site and sodium ion at the metal coordination site at 1.10 Angstrom resolution
Authors : Hilario, E.; Dunn, M.F.; Mueller, L.J.
Deposited on : 2021-02-11
Resolution : 1.10 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](#) ①) 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

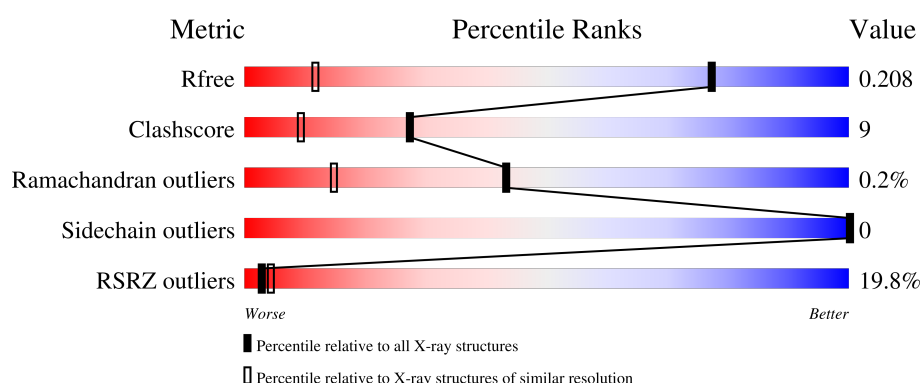
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	268	28% 87% 13%
2	B	397	14% 88% 11% .

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
3	F9F	A	301	-	-	X	-
4	PEG	A	302	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6031 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.

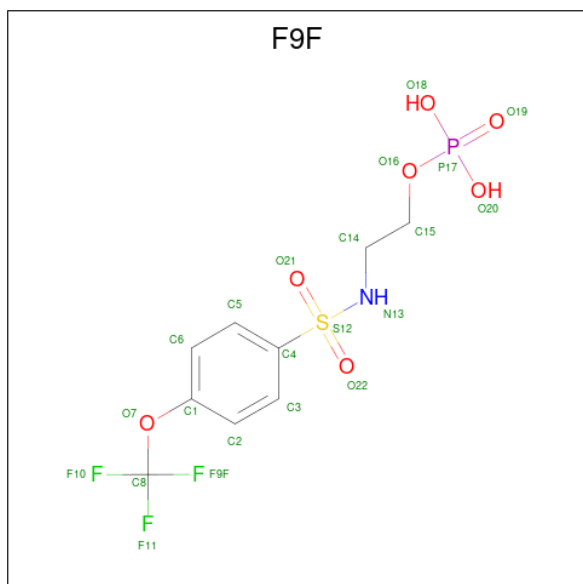
- Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	12	0
			2086	1316	366	395	9			

- Molecule 2 is a protein called Tryptophan synthase beta chain.

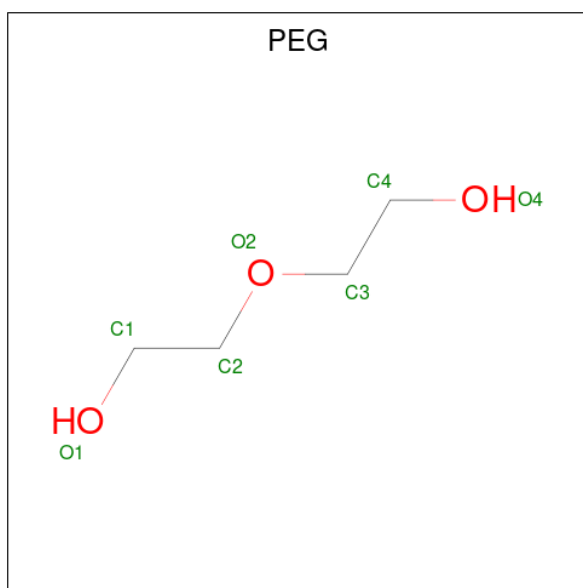
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	393	Total	C	N	O	S	0	16	0
			3107	1947	546	592	22			

- Molecule 3 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (CCD ID: F9F) (formula: C₉H₁₁F₃NO₇PS) (labeled as "Ligand of Interest" by depositor).



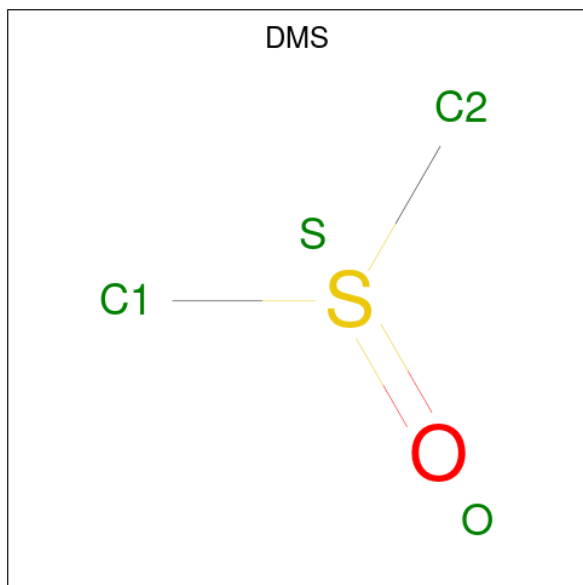
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	P	S	0	0
			22	9	3	1	7	1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



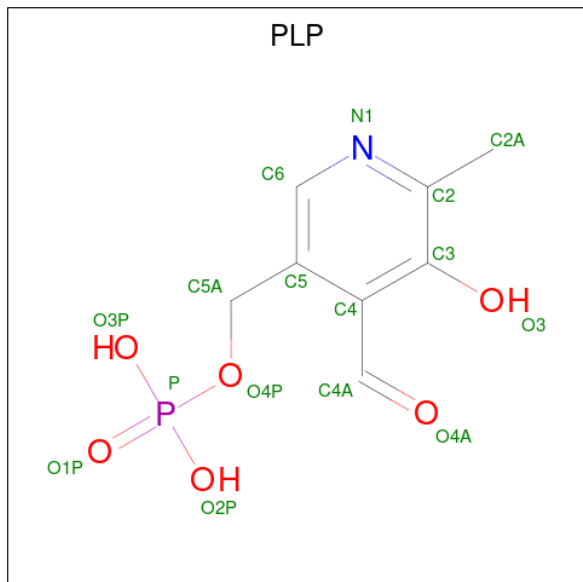
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



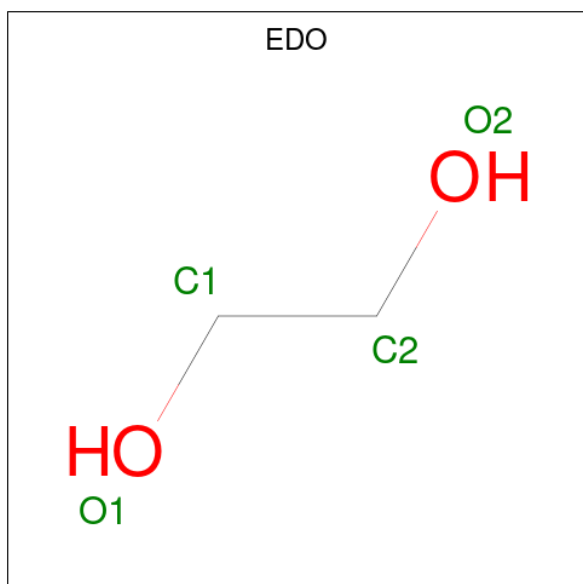
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 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
6	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Na 1	0	0

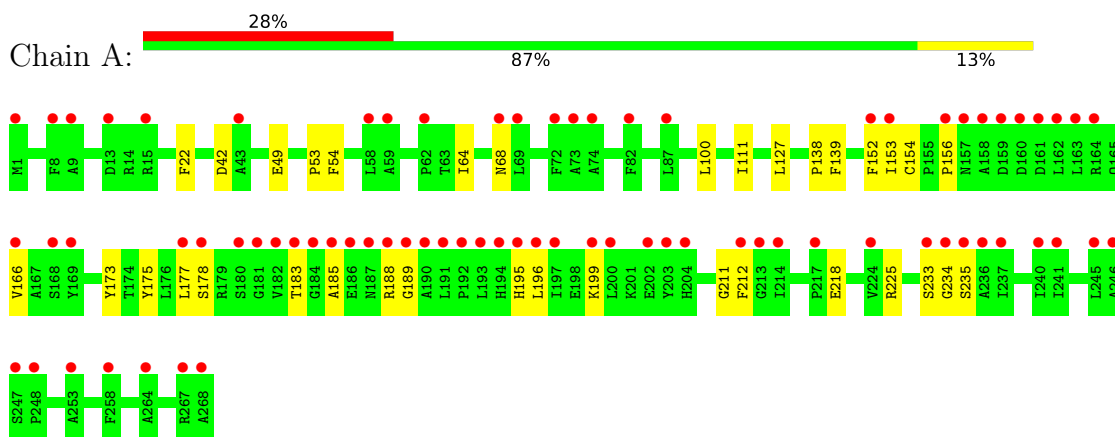
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	296	Total 301	O 301	0	4
9	B	469	Total 480	O 480	0	11

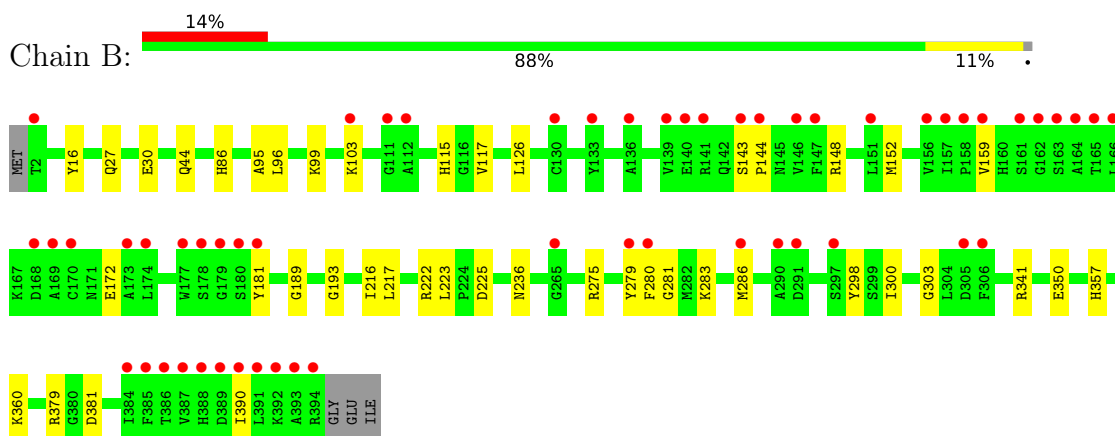
3 Residue-property plots

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: Tryptophan synthase alpha chain



• Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.23Å 59.18Å 67.33Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	28.52 – 1.10 28.52 – 1.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (28.52-1.10) 96.3 (28.52-1.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.172 , 0.199 0.180 , 0.208	Depositor DCC
R_{free} test set	13730 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	7.2	Xtriage
Anisotropy	1.776	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6031	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.45% 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: EDO, PLP, F9F, NA, PEG, DMS

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	0.94	0/2127	1.14	1/2891 (0.0%)
2	B	0.95	0/3166	1.04	1/4272 (0.0%)
All	All	0.94	0/5293	1.08	2/7163 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	PHE	CA-CB-CG	-6.04	107.76	113.80
2	B	357	HIS	CA-CB-CG	-5.27	108.53	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2086	0	2049	49	0
2	B	3107	0	3054	42	0
3	A	22	0	9	18	0
4	A	7	0	10	10	0
5	A	4	0	6	0	0
5	B	4	0	6	1	0
6	B	15	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	6	0	0
8	B	1	0	0	0	0
9	A	301	0	0	11	0
9	B	480	0	0	13	0
All	All	6031	0	5146	95	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 9.

All (95) 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:234[B]:GLY:O	3:A:301:F9F:P17	2.03	1.17
1:A:218:GLU:HG3	9:A:615:HOH:O	1.50	1.07
1:A:234[B]:GLY:O	3:A:301:F9F:O19	1.73	1.05
1:A:234[B]:GLY:O	3:A:301:F9F:O20	1.76	1.03
1:A:178:SER:OG	1:A:211[B]:GLY:O	1.84	0.94
1:A:234[A]:GLY:HA3	9:A:416:HOH:O	1.70	0.91
1:A:173[A]:TYR:OH	9:A:401:HOH:O	1.76	0.86
2:B:217:LEU:HD11	9:B:927:HOH:O	1.76	0.83
1:A:234[B]:GLY:HA3	9:A:416:HOH:O	1.83	0.79
4:A:302:PEG:H32	2:B:283:LYS:HZ3	1.47	0.78
1:A:42[B]:ASP:OD1	9:A:402:HOH:O	2.05	0.74
2:B:181[B]:TYR:CE2	9:B:638:HOH:O	2.40	0.74
1:A:49[B]:GLU:OE1	3:A:301:F9F:S12	2.46	0.72
2:B:217:LEU:HG	9:B:774:HOH:O	1.90	0.71
1:A:64:ILE:HD11	9:A:416:HOH:O	1.90	0.71
2:B:27:GLN:O	2:B:30:GLU:HG3	1.92	0.70
3:A:301:F9F:H151	9:A:416:HOH:O	1.90	0.70
4:A:302:PEG:H21	2:B:16:TYR:OH	1.93	0.69
1:A:153:ILE:HG23	1:A:177:LEU:HG	1.76	0.68
2:B:181[B]:TYR:CZ	9:B:638:HOH:O	2.47	0.67
2:B:117:VAL:HG13	2:B:152[A]:MET:HE1	1.77	0.66
1:A:53:PRO:HA	1:A:68:ASN:HD22	1.62	0.65
1:A:175:TYR:CE2	3:A:301:F9F:H5	2.32	0.64
2:B:44:GLN:HG3	9:B:718:HOH:O	1.98	0.64
1:A:154[B]:CYS:SG	1:A:166:VAL:HG11	2.38	0.64
1:A:153:ILE:HD11	3:A:301:F9F:H6	1.80	0.63
4:A:302:PEG:H32	2:B:283:LYS:NZ	2.11	0.63
1:A:234[B]:GLY:CA	9:A:416:HOH:O	2.42	0.63
2:B:217:LEU:HD21	9:B:927:HOH:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49[B]:GLU:OE1	3:A:301:F9F:O22	2.16	0.62
1:A:49[B]:GLU:CD	3:A:301:F9F:O21	2.42	0.62
1:A:49[B]:GLU:OE1	3:A:301:F9F:O21	2.19	0.61
2:B:99:LYS:HZ1	2:B:126:LEU:HD13	1.68	0.58
1:A:185:ALA:O	1:A:188:ARG:NH1	2.37	0.58
1:A:53:PRO:HA	1:A:68:ASN:ND2	2.18	0.57
1:A:153:ILE:CG2	1:A:177:LEU:HG	2.33	0.57
1:A:234[B]:GLY:C	9:A:416:HOH:O	2.48	0.55
2:B:148:ARG:O	2:B:152[A]:MET:HE3	2.06	0.55
2:B:216[B]:ILE:HG22	2:B:222:ARG:O	2.07	0.53
1:A:138:PRO:HG2	4:A:302:PEG:H11	1.90	0.53
1:A:100:LEU:C	1:A:100:LEU:HD13	2.34	0.53
2:B:341[A]:ARG:HD2	9:B:541:HOH:O	2.08	0.53
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.45	0.51
2:B:223:LEU:HD23	9:B:774:HOH:O	2.10	0.51
1:A:225[B]:ARG:HB2	1:A:225[B]:ARG:CZ	2.40	0.50
2:B:148:ARG:C	2:B:152[A]:MET:HE3	2.37	0.50
2:B:99:LYS:NZ	2:B:126:LEU:HD13	2.27	0.49
2:B:143:SER:OG	2:B:144:PRO:HD3	2.13	0.48
1:A:156:PRO:HA	1:A:196:LEU:HD11	1.96	0.48
1:A:22:PHE:HA	1:A:49[B]:GLU:O	2.13	0.48
2:B:216[A]:ILE:HG23	9:B:774:HOH:O	2.13	0.48
2:B:99:LYS:HE3	2:B:126:LEU:HD22	1.96	0.47
1:A:139:PHE:HE1	4:A:302:PEG:C1	2.28	0.47
2:B:96:LEU:HD23	2:B:99:LYS:HE2	1.97	0.47
2:B:103:LYS:NZ	2:B:181[A]:TYR:O	2.44	0.47
2:B:95:ALA:C	2:B:99:LYS:HZ3	2.22	0.46
2:B:379[B]:ARG:NH2	9:B:751[B]:HOH:O	2.12	0.46
2:B:159:VAL:HG13	2:B:172[A]:GLU:HG3	1.97	0.46
1:A:178:SER:HB3	1:A:189:GLY:HA3	1.98	0.46
1:A:183:THR:CG2	3:A:301:F9F:H142	2.46	0.45
1:A:153:ILE:HD13	1:A:175:TYR:HB3	1.98	0.45
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.46	0.45
3:A:301:F9F:H3	9:A:497:HOH:O	2.15	0.45
1:A:111:ILE:CD1	4:A:302:PEG:H31	2.47	0.45
4:A:302:PEG:H22	4:A:302:PEG:H42	1.71	0.45
2:B:159:VAL:CG1	2:B:172[A]:GLU:HG3	2.48	0.44
1:A:211[A]:GLY:O	1:A:212:PHE:HB2	2.18	0.44
2:B:222:ARG:HH22	2:B:225:ASP:CG	2.26	0.44
1:A:234[B]:GLY:C	3:A:301:F9F:O19	2.54	0.44
2:B:303:GLY:HA3	2:B:350:GLU:OE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:ARG:NH2	9:B:510:HOH:O	2.51	0.43
1:A:195:HIS:O	1:A:199:LYS:HG2	2.17	0.43
2:B:95:ALA:C	2:B:99:LYS:NZ	2.76	0.43
2:B:379[B]:ARG:HD2	2:B:381:ASP:OD1	2.18	0.43
5:B:403:DMS:H11	9:B:608:HOH:O	2.17	0.43
2:B:103:LYS:NZ	2:B:181[B]:TYR:O	2.40	0.43
1:A:175:TYR:HE2	3:A:301:F9F:O22	2.02	0.42
1:A:49[B]:GLU:CD	3:A:301:F9F:S12	3.02	0.42
2:B:279:TYR:HB3	2:B:286[B]:MET:HE1	2.02	0.42
2:B:360[A]:LYS:HG3	9:B:653:HOH:O	2.18	0.42
1:A:233[B]:SER:O	3:A:301:F9F:O20	2.38	0.42
1:A:139:PHE:HE1	4:A:302:PEG:H12	1.83	0.42
1:A:127:LEU:HD11	1:A:153:ILE:HD11	2.01	0.42
1:A:175:TYR:CE2	3:A:301:F9F:O22	2.73	0.42
1:A:22:PHE:HA	1:A:49[A]:GLU:O	2.19	0.41
1:A:111:ILE:HD11	4:A:302:PEG:H31	2.01	0.41
1:A:218:GLU:O	1:A:218:GLU:CD	2.63	0.41
2:B:298:TYR:CD2	2:B:298:TYR:C	2.99	0.41
2:B:193:GLY:HA2	2:B:280:PHE:O	2.21	0.40
1:A:183:THR:HG21	3:A:301:F9F:H142	2.02	0.40
2:B:16:TYR:O	2:B:281:GLY:HA2	2.22	0.40
2:B:86:HIS:CE1	2:B:236:ASN:HB3	2.55	0.40
1:A:49[A]:GLU:CD	9:A:401:HOH:O	2.65	0.40
1:A:54:PHE:H	1:A:68:ASN:HD22	1.69	0.40
4:A:302:PEG:H12	2:B:16:TYR:HE1	1.85	0.40

There are no symmetry-related clashes.

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	278/268 (104%)	269 (97%)	7 (2%)	2 (1%)	18 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	407/397 (102%)	398 (98%)	9 (2%)	0	100	100
All	All	685/665 (103%)	667 (97%)	16 (2%)	2 (0%)	43	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235[A]	SER
1	A	235[B]	SER

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	212/208 (102%)	212 (100%)	0	100	100
2	B	322/311 (104%)	322 (100%)	0	100	100
All	All	534/519 (103%)	534 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	68	ASN
1	A	109	ASN
1	A	165	GLN
1	A	250	GLN
2	B	160	HIS

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](#)

Of 7 ligands modelled in this entry, 1 is 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	$\# Z > 2$
6	PLP	B	401	2	15,15,16	1.11	1 (6%)	21,22,23	1.33	3 (14%)
4	PEG	A	302	-	6,6,6	0.30	0	5,5,5	0.45	0
3	F9F	A	301	-	22,22,22	0.40	0	32,33,33	0.56	0
5	DMS	A	303	-	3,3,3	0.20	0	3,3,3	0.10	0
7	EDO	B	402	-	3,3,3	0.47	0	2,2,2	0.38	0
5	DMS	B	403	-	3,3,3	0.23	0	3,3,3	0.22	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
4	PEG	A	302	-	-	3/4/4/4	-
6	PLP	B	401	2	-	0/6/6/8	0/1/1/1
3	F9F	A	301	-	-	8/20/20/20	0/1/1/1
7	EDO	B	402	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	PLP	C4A-C4	-2.79	1.46	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	401	PLP	O4P-C5A-C5	3.13	115.23	109.36
6	B	401	PLP	C6-C5-C4	-2.82	115.78	118.10
6	B	401	PLP	O3P-P-O4P	-2.03	101.38	106.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	PEG	C4-C3-O2-C2
4	A	302	PEG	O2-C3-C4-O4
4	A	302	PEG	O1-C1-C2-O2
3	A	301	F9F	C3-C4-S12-O21
3	A	301	F9F	C5-C4-S12-O21
3	A	301	F9F	C6-C1-O7-C8
3	A	301	F9F	C14-N13-S12-O22
3	A	301	F9F	C3-C4-S12-N13
3	A	301	F9F	C2-C1-O7-C8
3	A	301	F9F	N13-C14-C15-O16
3	A	301	F9F	C5-C4-S12-N13

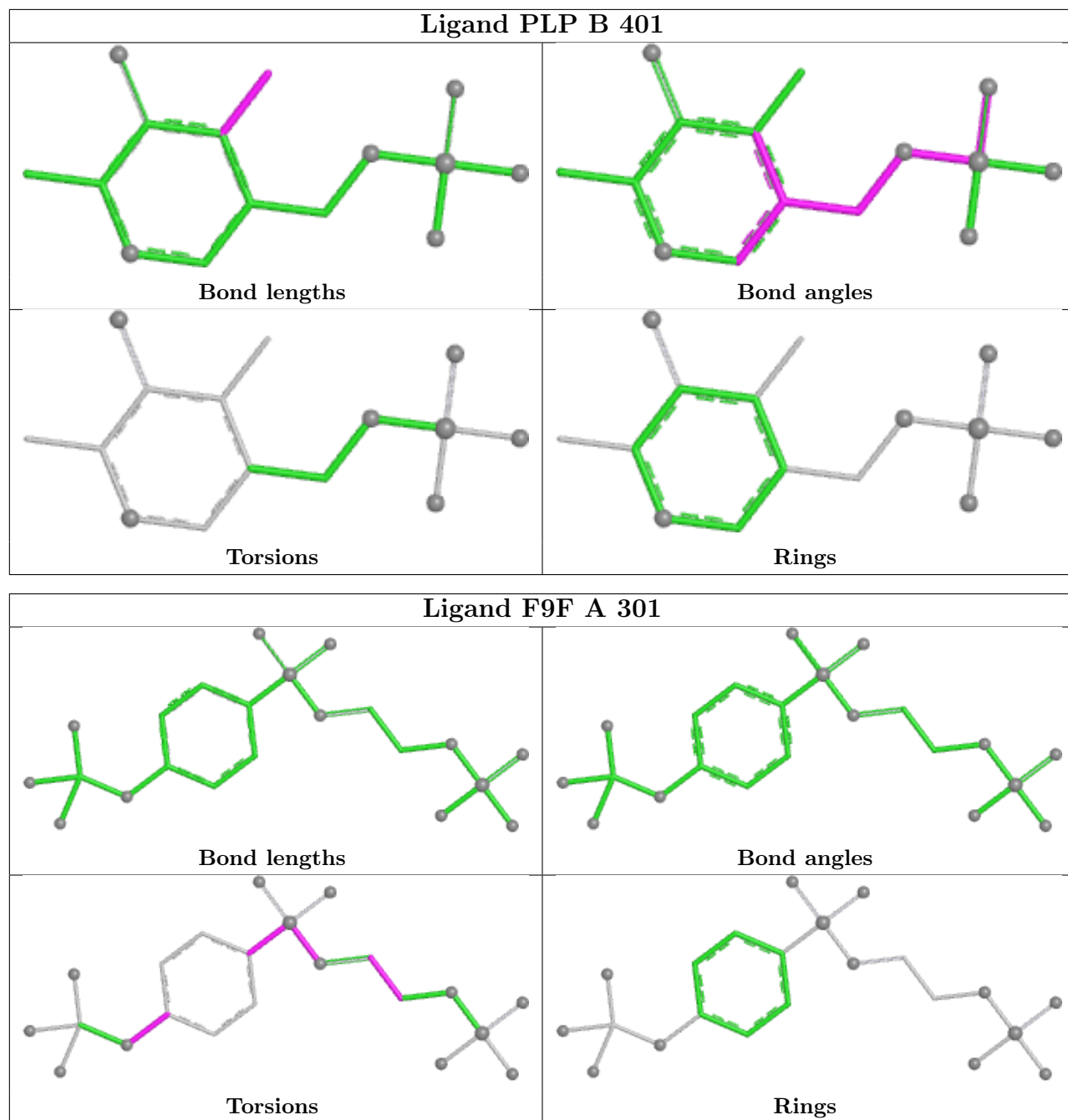
There are no ring outliers.

3 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	PEG	10	0
3	A	301	F9F	18	0
5	B	403	DMS	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 ⓘ

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 ⓘ

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	268/268 (100%)	1.65	76 (28%) ⓘ ⓘ	6, 17, 41, 71	12 (4%)
2	B	393/397 (98%)	0.90	55 (13%) ⓘ ⓘ	5, 12, 25, 62	16 (4%)
All	All	661/665 (99%)	1.20	131 (19%) ⓘ ⓘ	5, 14, 34, 71	28 (4%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	9.5
1	A	191	LEU	8.2
2	B	286[A]	MET	7.2
2	B	385	PHE	7.0
1	A	190	ALA	6.4
2	B	391	LEU	6.1
1	A	182	VAL	6.0
1	A	157	ASN	6.0
1	A	158	ALA	5.6
2	B	393	ALA	5.5
1	A	185	ALA	5.3
1	A	58	LEU	4.7
2	B	390	ILE	4.7
1	A	192	PRO	4.7
2	B	181[A]	TYR	4.5
1	A	183	THR	4.4
1	A	203	TYR	4.4
2	B	386	THR	4.4
1	A	268	ALA	4.3
2	B	174	LEU	4.3
1	A	169	TYR	4.3
1	A	212	PHE	4.2
2	B	392	LYS	4.1
1	A	194	HIS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	214	ILE	4.0
1	A	195	HIS	4.0
1	A	245	LEU	3.9
1	A	156	PRO	3.9
1	A	87[A]	LEU	3.9
1	A	159	ASP	3.8
1	A	213	GLY	3.8
2	B	159	VAL	3.8
2	B	179	GLY	3.7
2	B	139	VAL	3.6
1	A	196	LEU	3.6
2	B	177	TRP	3.6
2	B	388	HIS	3.6
2	B	170	CYS	3.6
2	B	2	THR	3.6
1	A	177	LEU	3.5
1	A	181	GLY	3.5
1	A	224	VAL	3.4
1	A	62	PRO	3.4
2	B	158	PRO	3.4
1	A	184	GLY	3.4
1	A	162	LEU	3.4
1	A	246	ALA	3.3
1	A	234[A]	GLY	3.3
2	B	147	PHE	3.3
1	A	237	ILE	3.2
2	B	157	ILE	3.2
2	B	291	ASP	3.1
2	B	162	GLY	3.1
1	A	186	GLU	3.0
1	A	168	SER	3.0
1	A	247	SER	3.0
2	B	178[A]	SER	3.0
1	A	187	ASN	3.0
1	A	189	GLY	2.9
2	B	143	SER	2.9
1	A	15	ARG	2.9
2	B	280	PHE	2.9
1	A	160	ASP	2.8
2	B	165	THR	2.8
1	A	43	ALA	2.8
1	A	152	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	188	ARG	2.8
1	A	163	LEU	2.8
1	A	197	ILE	2.8
2	B	136	ALA	2.8
1	A	200	LEU	2.8
1	A	74	ALA	2.7
2	B	163	SER	2.7
2	B	387	VAL	2.7
2	B	141	ARG	2.7
2	B	173	ALA	2.7
1	A	180	SER	2.7
2	B	166	LEU	2.7
2	B	164	ALA	2.7
1	A	178	SER	2.6
1	A	73	ALA	2.6
1	A	1	MET	2.6
2	B	133	TYR	2.6
1	A	68	ASN	2.5
2	B	144	PRO	2.5
1	A	236	ALA	2.5
2	B	306	PHE	2.5
2	B	156	VAL	2.5
2	B	384	ILE	2.5
2	B	279	TYR	2.5
1	A	248	PRO	2.4
1	A	161	ASP	2.4
2	B	168	ASP	2.4
2	B	112	ALA	2.4
1	A	267	ARG	2.4
2	B	151	LEU	2.4
1	A	164	ARG	2.4
1	A	9	ALA	2.4
1	A	253	ALA	2.4
2	B	169	ALA	2.4
1	A	217	PRO	2.4
1	A	8	PHE	2.4
2	B	180	SER	2.4
1	A	13	ASP	2.3
1	A	264	ALA	2.3
2	B	290	ALA	2.3
2	B	146	VAL	2.3
1	A	241	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	305	ASP	2.3
1	A	204	HIS	2.2
2	B	161	SER	2.2
1	A	153	ILE	2.2
2	B	111	GLY	2.2
2	B	130	CYS	2.2
1	A	82	PHE	2.2
1	A	233[A]	SER	2.2
2	B	389	ASP	2.2
1	A	202	GLU	2.2
2	B	103	LYS	2.1
1	A	69	LEU	2.1
2	B	394	ARG	2.1
1	A	166	VAL	2.1
2	B	297	SER	2.1
1	A	199	LYS	2.1
1	A	59	ALA	2.1
1	A	72	PHE	2.0
1	A	258	PHE	2.0
1	A	240	ILE	2.0
2	B	140	GLU	2.0
2	B	265	GLY	2.0
1	A	235[A]	SER	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.

Continued on next page...

Continued from previous page...

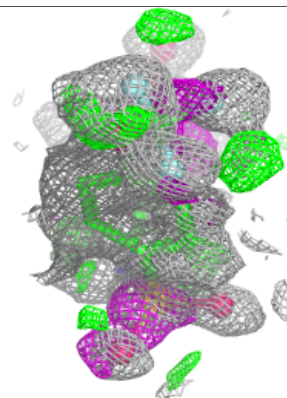
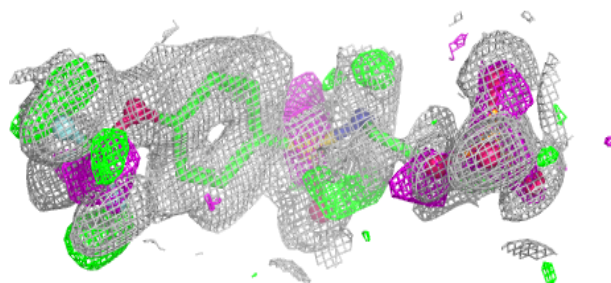
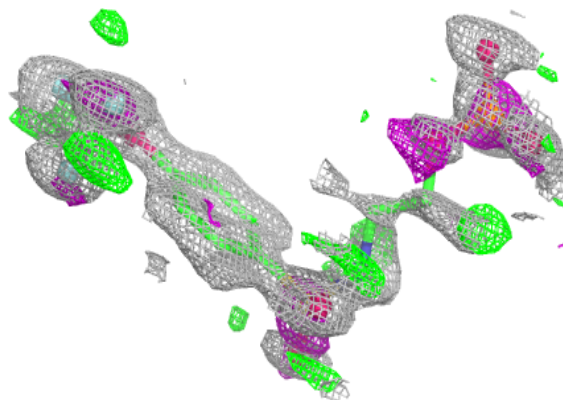
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	B	402	4/4	0.86	0.15	16,25,25,36	0
5	DMS	A	303	4/4	0.90	0.16	37,38,39,42	0
4	PEG	A	302	7/7	0.92	0.16	23,28,35,40	0
3	F9F	A	301	22/22	0.94	0.13	18,20,26,28	0
5	DMS	B	403	4/4	0.95	0.13	20,23,25,28	0
6	PLP	B	401	15/16	0.99	0.05	9,10,12,13	0
8	NA	B	404	1/1	0.99	0.05	13,13,13,13	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.

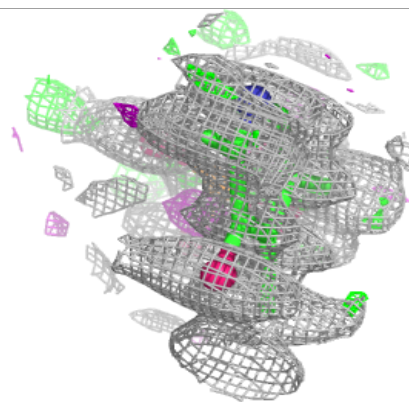
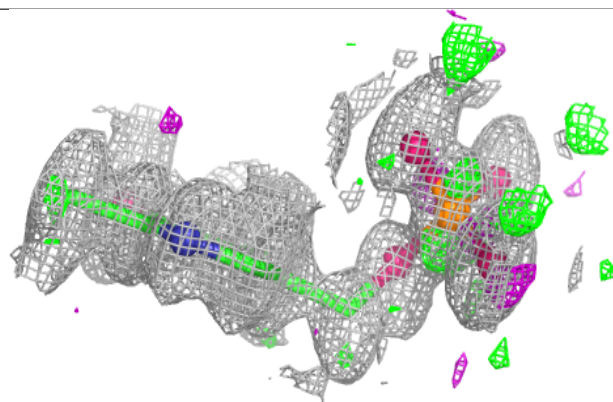
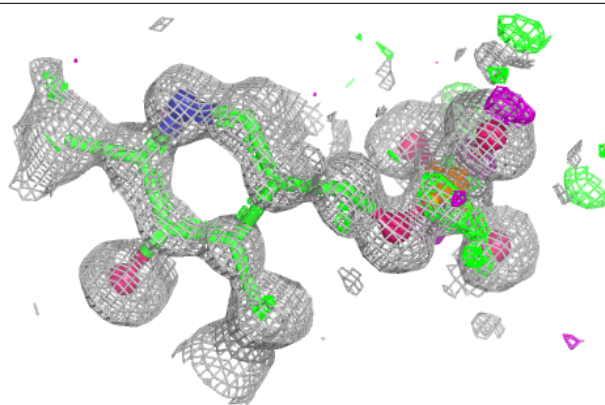
Electron density around F9F A 301:

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



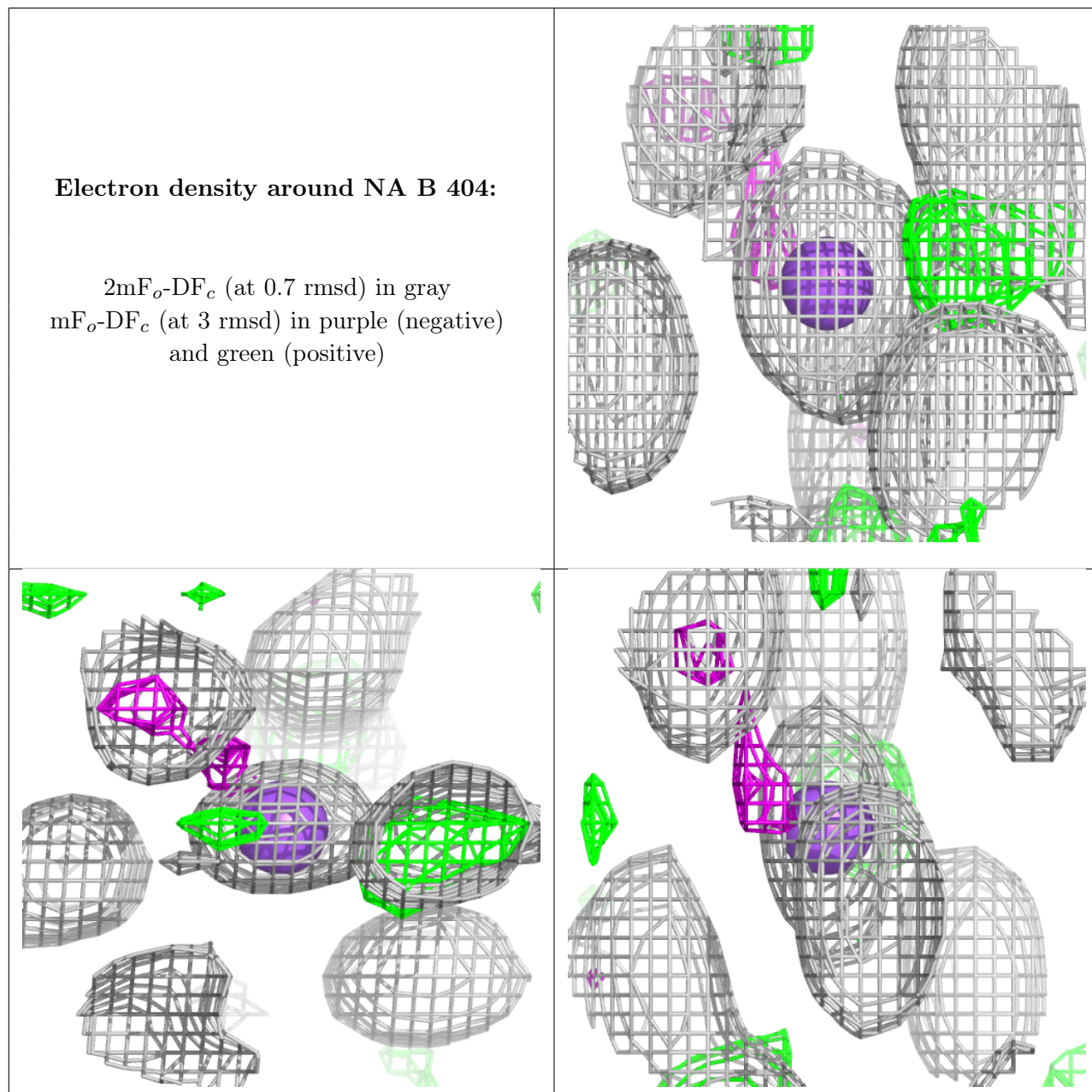
Electron density around PLP B 401:

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



Electron density around NA B 404:

$2mF_o-DF_c$ (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.