

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 12:51 AM EDT

PDB ID : 7M2L

Title	:	The internal aldimine form of the wild-type Salmonella Typhimurium Trypto-
		phan Synthase in complex with N-(4'-trifluoromethoxybenzoyl)-2-amino-1-e
		thylphosphate (F6F) inhibitor at the alpha-and beta-site, sodium ion at the
		metal coordination site, and another F6F molecule at the enzyme beta-site at
		1.60 Angstrom resolution. Two of the beta-Q114 rotamer conformations allows
		a hydrogen bond to form with the PLP oxygen at the position 3 in the ring
Authors	:	Hilario, E.; Dunn, M.F.; Mueller, L.J.
Deposited on	:	2021-03-16
Resolution	:	1.60 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 (i) 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:

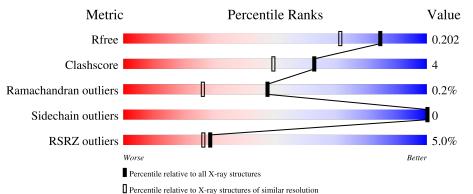
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

Overall quality at a glance (i) 1

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	$\begin{array}{l} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range({\rm \AA})}) \end{array}$			
R_{free}	130704	3398 (1.60-1.60)			
Clashscore	141614	3665(1.60-1.60)			
Ramachandran outliers	138981	3564 (1.60-1.60)			
Sidechain outliers	138945	3563 (1.60-1.60)			
RSRZ outliers	127900	3321 (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	А	268	9% 87%	12% •					
2	В	397	2% 94%	5% •					

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)

Parkinson et al. (1996) :

: 2.35.1



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	EDO	В	506	-	-	Х	-
6	PGE	В	503	-	-	Х	-



7M2L

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 5667 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.

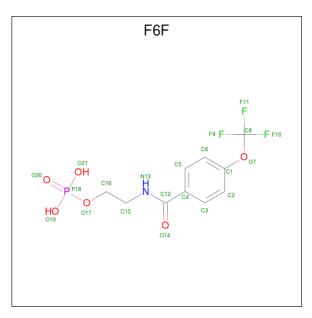
• Molecule 1 is a protein called Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	265	Total	C 1944	N 227	0	S	0	1	0
			1953	1244	337	364	8			

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	395	Total 3073	C 1929	N 542	O 583	S 19	0	12	0

• Molecule 3 is 2-{[4-(TRIFLUOROMETHOXY)BENZOYL]AMINO}ETHYL DIHYDRO-GEN PHOSPHATE (three-letter code: F6F) (formula: C₁₀H₁₁F₃NO₆P) (labeled as "Ligand of Interest" by depositor).

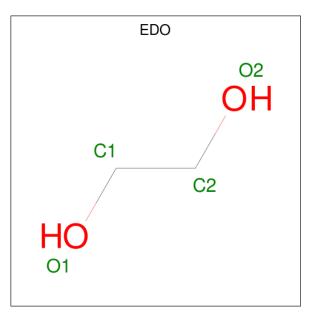


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	А	1	Total 21			N 1		Р 1	0	0



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	В	1	Total 21	C 10	F 3	N 1	O 6	Р 1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



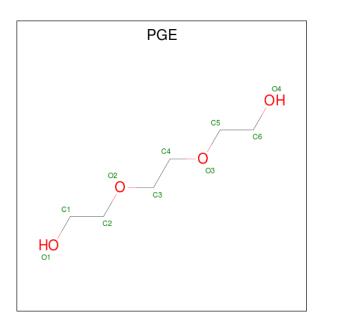
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Cl 1 1	0	0
5	В	4	Total Cl 5 5	0	1

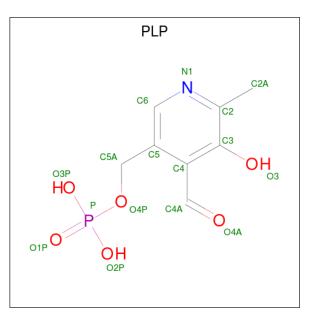
• Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
6	В	1	Total 10	С 6	0 4	0	0

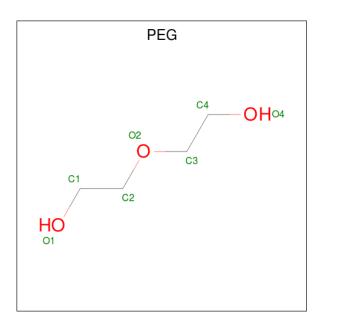
• Molecule 7 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	В	1	Total	С	Ν	0	Р	0	0
	D	1	15	8	1	5	1	0	0

• Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	В	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 7 & 4 \end{array}$	O 3	0	0

• Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	В	2	Total Na 2 2	0	0

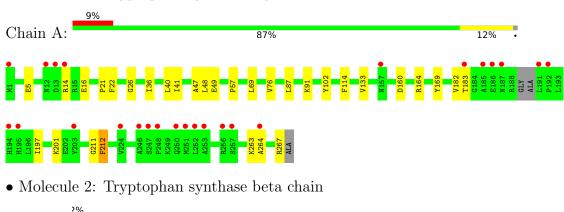
• Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	147	Total O 149 149	0	2
10	В	382	Total O 394 394	0	12

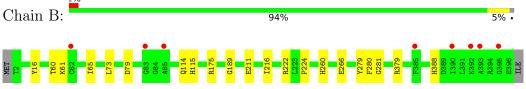


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Tryptophan synthase alpha chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	183.52Å 58.60Å 67.10Å	Depositor
a, b, c, α , β , γ	90.00° 95.18° 90.00°	Depositor
Resolution (Å)	39.41 - 1.60	Depositor
Resolution (A)	39.41 - 1.60	EDS
% Data completeness	98.9 (39.41-1.60)	Depositor
(in resolution range)	99.0 (39.41-1.60)	EDS
R _{merge}	0.04	Depositor
R _{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	$1.97 (at 1.60 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19-4092	Depositor
D D	0.174 , 0.202	Depositor
R, R_{free}	0.175 , 0.202	DCC
R_{free} test set	4601 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	17.9	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 54.5	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	5667	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PLP, CL, EDO, PEG, PGE, F6F, NA

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.32	0/1991	0.56	0/2713
2	В	0.43	0/3131	0.66	0/4229
All	All	0.39	0/5122	0.62	0/6942

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	А	1953	0	1917	19	0
2	В	3073	0	3014	21	0
3	А	21	0	9	1	0
3	В	21	0	9	0	0
4	А	4	0	6	1	0
4	В	12	0	18	8	0
5	А	1	0	0	0	0
5	В	5	0	0	0	0
6	В	10	0	14	6	0
7	В	15	0	6	0	0
8	В	7	0	10	0	0



0010	Continued from provide page									
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes				
9	В	2	0	0	0	0				
10	А	149	0	0	0	0				
10	В	394	0	0	9	0				
All	All	5667	0	5003	44	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 (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
2:B:114[B]:GLN:NE2	10:B:601:HOH:O	2.05	0.88
2:B:61:LYS:H	4:B:506:EDO:H11	1.48	0.78
2:B:211:GLU:HA	6:B:503:PGE:H12	1.69	0.75
2:B:60:THR:HA	4:B:506:EDO:H11	1.75	0.67
2:B:61:LYS:H	4:B:506:EDO:C1	2.11	0.64
2:B:61:LYS:N	4:B:506:EDO:H11	2.15	0.61
1:A:114:PHE:HA	4:A:302:EDO:H11	1.81	0.61
1:A:183:THR:HG21	3:A:301:F6F:H3	1.83	0.58
1:A:69:LEU:HD11	10:B:817:HOH:O	2.07	0.55
2:B:79:ASP:HB2	2:B:379:ARG:HB3	1.90	0.54
1:A:211:GLY:O	1:A:212:PHE:HB2	2.07	0.54
2:B:222[B]:ARG:NH2	10:B:610:HOH:O	2.41	0.53
2:B:65[B]:ILE:HD11	2:B:73:LEU:HD23	1.91	0.52
2:B:388:HIS:CD2	4:B:507:EDO:H21	2.44	0.52
2:B:114[C]:GLN:HG3	10:B:785:HOH:O	2.09	0.52
2:B:61:LYS:H	4:B:506:EDO:C2	2.24	0.50
6:B:503:PGE:H22	10:B:917:HOH:O	2.13	0.49
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.94	0.49
1:A:5:GLU:H	1:A:5:GLU:CD	2.16	0.48
1:A:133[B]:VAL:HG22	1:A:169:TYR:HD2	1.79	0.48
2:B:61:LYS:H	4:B:506:EDO:H22	1.79	0.47
6:B:503:PGE:H6	10:B:917:HOH:O	2.14	0.47
2:B:222[B]:ARG:NH1	10:B:606:HOH:O	2.37	0.47
1:A:264:ALA:HA	1:A:267:ARG:NH1	2.29	0.46
2:B:279:TYR:CG	2:B:280:PHE:N	2.84	0.46
1:A:182:VAL:HG11	2:B:175:ARG:HG2	1.97	0.45
1:A:197:ILE:O	1:A:201:LYS:HG3	2.17	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.44
2:B:388:HIS:CG	4:B:507:EDO:H21	2.53	0.44
1:A:14:ARG:NH2	1:A:16:GLU:OE2	2.50	0.44



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:O	1:A:40:LEU:HG	2.18	0.44
1:A:22:PHE:HA	1:A:49:GLU:O	2.17	0.43
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.53	0.43
2:B:260:HIS:HD2	2:B:266:GLU:OE1	2.01	0.43
1:A:21:PRO:HD2	1:A:47:ALA:O	2.19	0.43
2:B:16:TYR:O	2:B:281:GLY:HA2	2.19	0.43
1:A:87:LEU:O	1:A:91:LYS:HG3	2.19	0.42
1:A:160:ASP:O	1:A:164:ARG:HG3	2.19	0.42
6:B:503:PGE:H4	10:B:917:HOH:O	2.18	0.42
6:B:503:PGE:H6	6:B:503:PGE:H4	1.83	0.41
2:B:216:ILE:HG21	2:B:224:PRO:HD3	2.03	0.41
1:A:41:ILE:HD11	1:A:48:LEU:HD11	2.03	0.40
1:A:263:LYS:O	1:A:263:LYS:HD2	2.21	0.40
6:B:503:PGE:H2	10:B:890:HOH:O	2.21	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	Perce	ntiles
1	А	262/268~(98%)	255~(97%)	6~(2%)	1 (0%)	34	15
2	В	406/397~(102%)	399~(98%)	7(2%)	0	100	100
All	All	668/665~(100%)	654 (98%)	13 (2%)	1 (0%)	47	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	212	PHE



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	А	194/208~(93%)	194 (100%)	0	100 100
2	В	313/311 (101%)	313 (100%)	0	100 100
All	All	507/519~(98%)	507 (100%)	0	100 100

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

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	Tuno	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
MIOI	Type	Ullaili	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	EDO	А	302	-	3,3,3	0.46	0	2,2,2	0.41	0
4	EDO	В	506	-	3,3,3	0.40	0	2,2,2	0.69	0
4	EDO	В	507	-	$3,\!3,\!3$	0.41	0	2,2,2	0.48	0
6	PGE	В	503	-	$9,\!9,\!9$	0.33	0	8,8,8	0.58	0
7	PLP	В	504	2	$15,\!15,\!16$	1.45	3 (20%)	$20,\!22,\!23$	1.04	1 (5%)
8	PEG	В	505	-	$6,\!6,\!6$	0.27	0	$5,\!5,\!5$	0.30	0
4	EDO	В	501	-	3,3,3	0.43	0	2,2,2	0.44	0
3	F6F	А	301	-	21,21,21	0.33	0	29,30,30	0.33	0
3	F6F	В	502	-	21,21,21	0.32	0	29,30,30	0.33	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	EDO	А	302	-	-	1/1/1/1	-
4	EDO	В	506	-	-	1/1/1/1	-
4	EDO	В	507	-	-	0/1/1/1	-
6	PGE	В	503	-	-	3/7/7/7	-
7	PLP	В	504	2	-	0/6/6/8	0/1/1/1
8	PEG	В	505	-	-	2/4/4/4	-
4	EDO	В	501	-	-	0/1/1/1	-
3	F6F	А	301	-	-	4/17/17/17	0/1/1/1
3	F6F	В	502	-	-	6/17/17/17	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	В	504	PLP	P-O2P	-2.61	1.44	1.54
7	В	504	PLP	P-O3P	-2.50	1.45	1.54
7	В	504	PLP	C4A-C4	-2.41	1.46	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
7	В	504	PLP	O4P-C5A-C5	3.32	115.67	109.35

There are no chirality outliers.

All (17) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	В	502	F6F	C16-O17-P18-O21
6	В	503	PGE	O1-C1-C2-O2
8	В	505	PEG	C1-C2-O2-C3
4	А	302	EDO	O1-C1-C2-O2
3	В	502	F6F	O14-C12-N13-C15
3	В	502	F6F	C4-C12-N13-C15
3	А	301	F6F	C16-O17-P18-O20
6	В	503	PGE	C1-C2-O2-C3
8	В	505	PEG	C4-C3-O2-C2
3	А	301	F6F	C6-C1-O7-C8
4	В	506	EDO	O1-C1-C2-O2
3	В	502	F6F	C6-C1-O7-C8
3	А	301	F6F	C2-C1-O7-C8
3	В	502	F6F	C2-C1-O7-C8
6	В	503	PGE	O2-C3-C4-O3
3	А	301	F6F	C16-O17-P18-O19
3	В	502	F6F	C16-O17-P18-O19

There are no ring outliers.

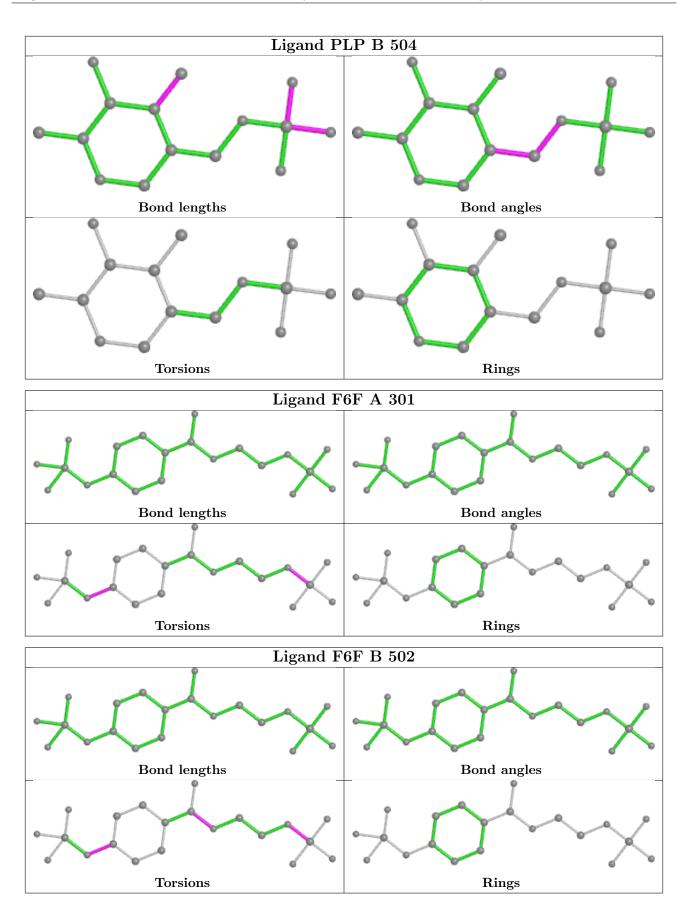
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	302	EDO	1	0
4	В	506	EDO	6	0
4	В	507	EDO	2	0
6	В	503	PGE	6	0
3	А	301	F6F	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 then 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 sufficient 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 (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, 95^{th} 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	А	265/268~(98%)	0.40	25 (9%) 8 7	16, 39, 63, 92	0
2	В	395/397~(99%)	-0.25	8 (2%) 65 64	11, 19, 34, 66	0
All	All	660/665~(99%)	0.01	33 (5%) 28 26	11, 24, 57, 92	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	185	ALA	6.7
1	А	192	PRO	5.6
1	А	247	SER	5.5
1	А	191	LEU	5.0
1	А	246	ALA	4.3
1	А	13	ASP	4.0
1	А	194	HIS	3.9
1	А	264	ALA	3.7
2	В	395	GLY	3.7
2	В	393	ALA	3.5
2	В	62	CYS	3.4
1	А	195	HIS	3.4
1	А	187	ASN	3.3
1	А	1	MET	3.2
2	В	390	ILE	2.8
1	А	224	VAL	2.7
1	А	250	GLN	2.6
1	А	14	ARG	2.5
1	А	186	GLU	2.4
2	В	385	PHE	2.4
1	А	252	LEU	2.3
1	А	183	THR	2.3
1	А	157	ASN	2.3
1	А	251	MET	2.3



Mol	Chain	Res	Type	RSRZ
1	А	253	ALA	2.3
1	А	203	TYR	2.3
1	А	256	ARG	2.2
1	А	12	ASN	2.2
1	А	248	PRO	2.2
2	В	392	LYS	2.2
2	В	83	GLY	2.2
2	В	85	ALA	2.1
1	А	257	SER	2.1

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 monosaccharides 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, 95^{th} 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.

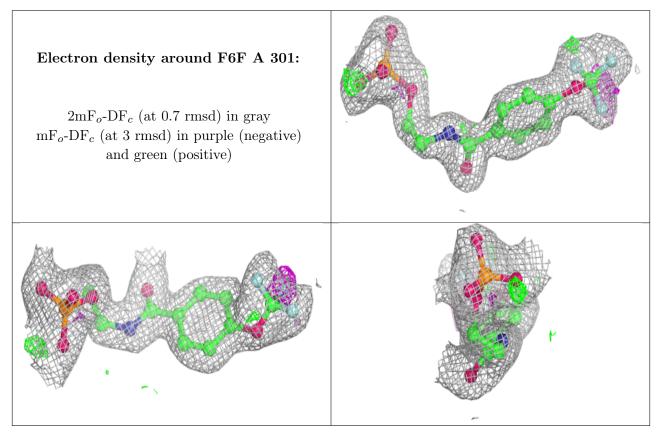
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	$\mathbf{Q}{<}0.9$
8	PEG	В	505	7/7	0.76	0.20	32,39,42,44	0
5	CL	В	513	1/1	0.81	0.08	70,70,70,70	0
6	PGE	В	503	10/10	0.83	0.14	$22,\!28,\!39,\!43$	0
4	EDO	А	302	4/4	0.84	0.15	33,36,42,43	0
5	CL	А	303	1/1	0.85	0.13	$68,\!68,\!68,\!68$	0
4	EDO	В	506	4/4	0.86	0.17	22,25,30,35	0
5	CL	В	512[B]	1/1	0.90	0.05	36, 36, 36, 36	1
5	CL	В	512[A]	1/1	0.90	0.05	44,44,44,44	1
5	CL	В	511	1/1	0.93	0.07	58, 58, 58, 58	0
4	EDO	В	501	4/4	0.93	0.07	39,41,42,48	0
5	CL	В	510	1/1	0.93	0.11	$65,\!65,\!65,\!65$	0
3	F6F	А	301	21/21	0.94	0.09	$31,\!35,\!42,\!45$	0
4	EDO	В	507	4/4	0.94	0.13	43,44,49,60	0
3	F6F	В	502	21/21	0.96	0.09	21,26,31,33	0



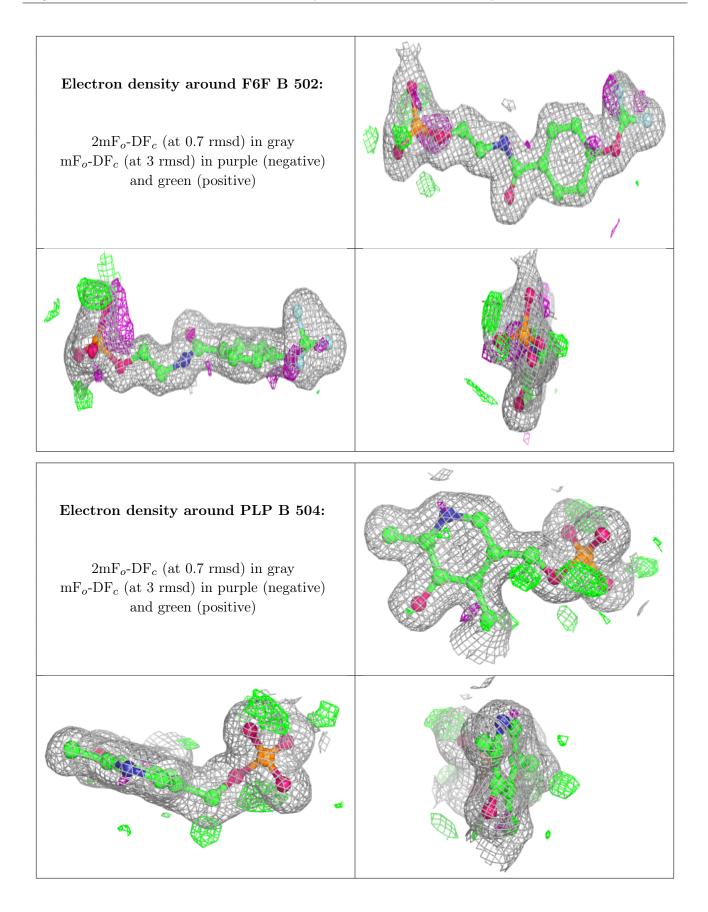
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Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	$B-factors(Å^2)$	Q < 0.9	
7	PLP	В	504	15/16	0.98	0.10	11,13,19,24	0	
9	NA	В	509	1/1	0.98	0.16	29,29,29,29	0	
9	NA	В	508	1/1	0.99	0.06	16, 16, 16, 16	0	

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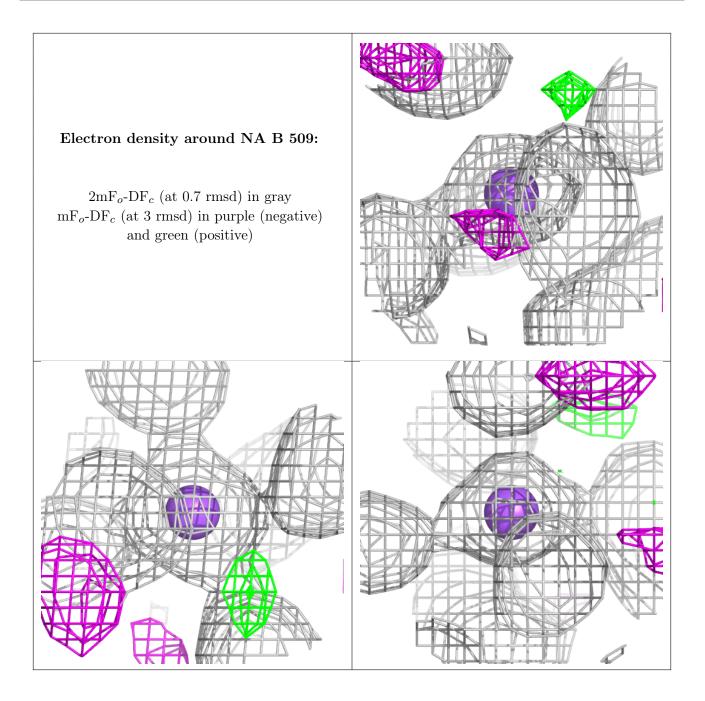
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



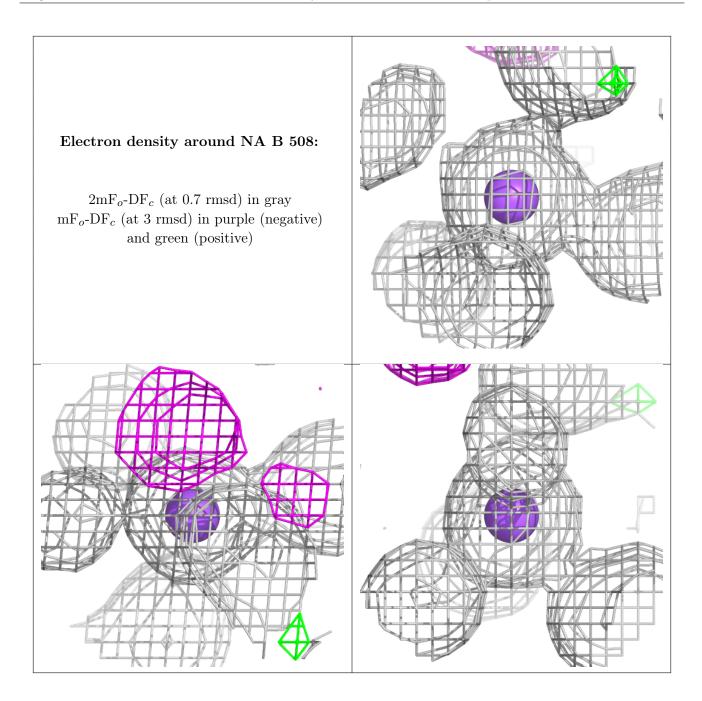












6.5 Other polymers (i)

There are no such residues in this entry.

