Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 07:07 pm GMT

PDB ID	:	6FRZ
Title	:	Phosphotriesterase PTE_A53_7
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Deposited on	:	2018-02-18
Resolution	:	1.65 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 (i)) were used in the production of this report:

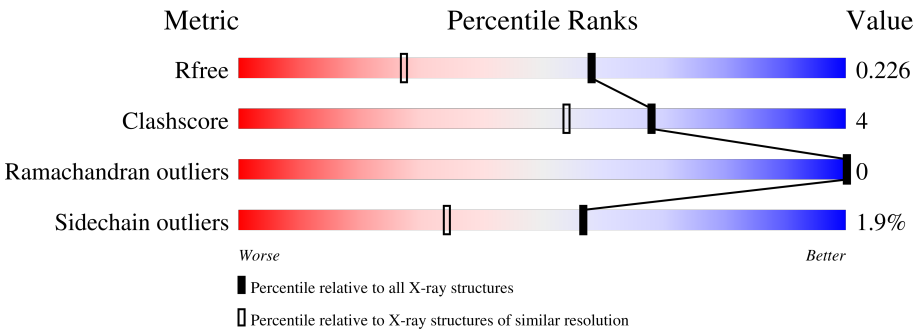
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.65 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}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	340	89% 7% •
1	B	340	94% 5% •

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
2	FMT	A	401	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PGE	A	408	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5486 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2477	1565	436	469	7	0	2	0
1	B	339	2558	1618	448	485	7	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ILE	-	expression tag	UNP P0A434
A	27	SER	-	expression tag	UNP P0A434
A	28	GLU	-	expression tag	UNP P0A434
A	29	PHE	-	expression tag	UNP P0A434
A	30	ILE	-	expression tag	UNP P0A434
A	31	THR	-	expression tag	UNP P0A434
A	32	ASN	GLY	conflict	UNP P0A434
A	33	SER	THR	conflict	UNP P0A434
A	77	ALA	LYS	conflict	UNP P0A434
A	80	VAL	ALA	conflict	UNP P0A434
A	106	ALA	ILE	conflict	UNP P0A434
A	132	GLU	PHE	conflict	UNP P0A434
A	173	GLN	THR	conflict	UNP P0A434
A	185	ARG	LYS	conflict	UNP P0A434
A	203	PHE	ALA	conflict	UNP P0A434
A	254	GLY	HIS	conflict	UNP P0A434
A	274	ASN	ILE	conflict	UNP P0A434
A	319	SER	ARG	conflict	UNP P0A434
B	26	ILE	-	expression tag	UNP P0A434
B	27	SER	-	expression tag	UNP P0A434
B	28	GLU	-	expression tag	UNP P0A434
B	29	PHE	-	expression tag	UNP P0A434
B	30	ILE	-	expression tag	UNP P0A434
B	31	THR	-	expression tag	UNP P0A434
B	32	ASN	GLY	conflict	UNP P0A434

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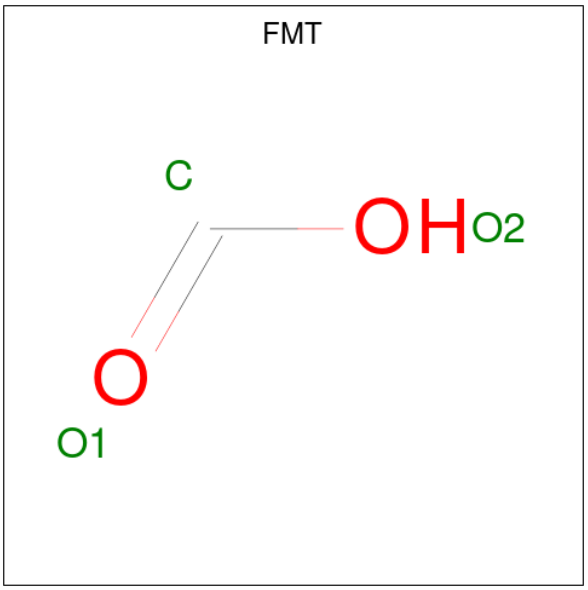
Chain	Residue	Modelled	Actual	Comment	Reference
B	33	SER	THR	conflict	UNP P0A434
B	77	ALA	LYS	conflict	UNP P0A434
B	80	VAL	ALA	conflict	UNP P0A434
B	106	ALA	ILE	conflict	UNP P0A434
B	132	GLU	PHE	conflict	UNP P0A434
B	173	GLN	THR	conflict	UNP P0A434
B	185	ARG	LYS	conflict	UNP P0A434
B	203	PHE	ALA	conflict	UNP P0A434
B	254	GLY	HIS	conflict	UNP P0A434
B	274	ASN	ILE	conflict	UNP P0A434
B	319	SER	ARG	conflict	UNP P0A434

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	3	1	2	0	0
			Total	C	O		
2	B	1	3	1	2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0

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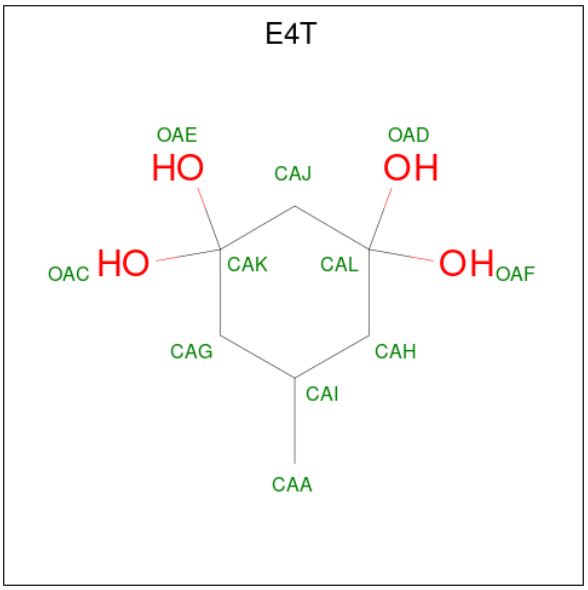
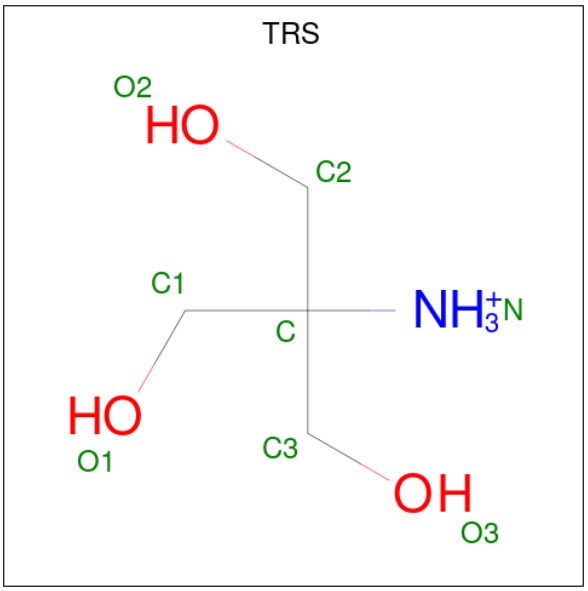
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	2	2	2	0	0

- Molecule 4 is 5-methylcyclohexane-1,1,3,3-tetrol (three-letter code: E4T) (formula: $C_7H_{14}O_4$).



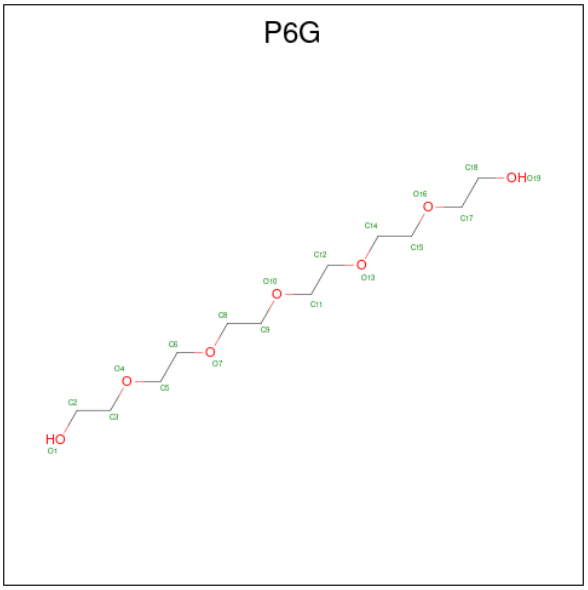
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	11	7	4	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



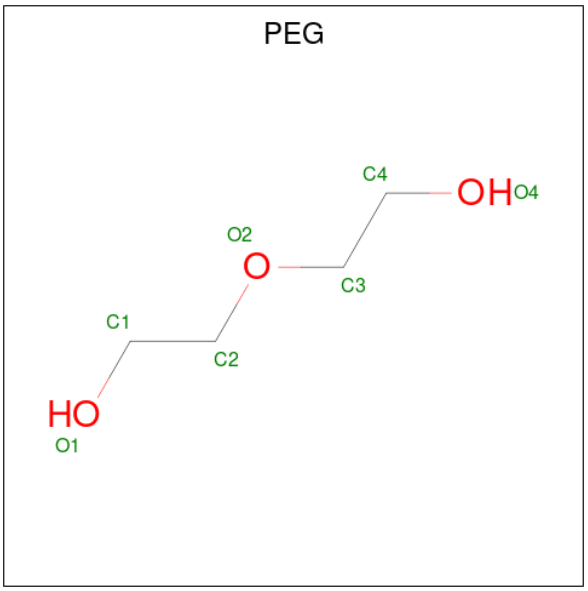
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	8	4	1	3	0	0

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



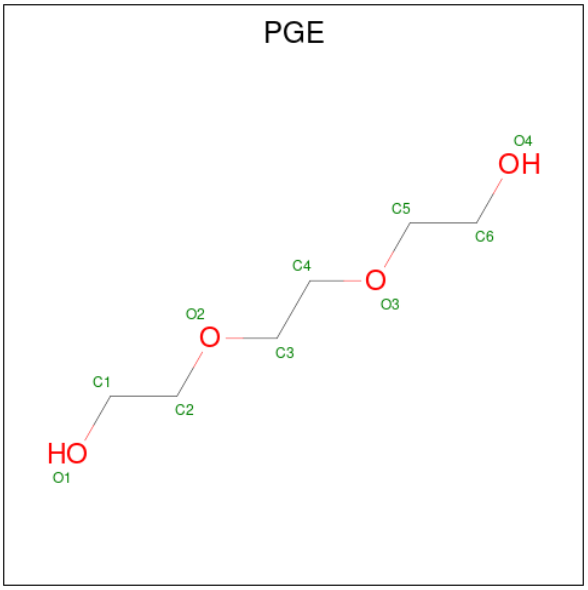
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	19	12	7	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	10	6	4	0	0

- Molecule 9 is water.

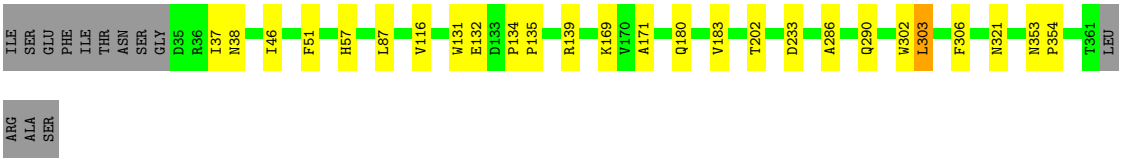
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	216	216	216	0	0
			Total	O		
9	B	170	170	170	0	0

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. 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. 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.

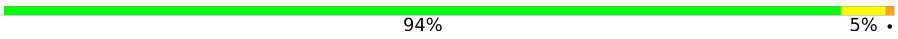
• Molecule 1: Parathion hydrolase

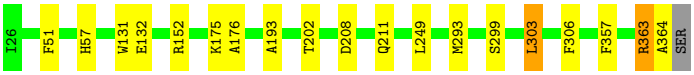
Chain A:



• Molecule 1: Parathion hydrolase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.35Å 81.12Å 70.58Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	24.19 – 1.65 25.24 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.19-1.65) 97.3 (25.24-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.68Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1692: ???)	Depositor
R, R_{free}	0.161 , 0.180 0.225 , 0.226	Depositor DCC
R_{free} test set	3443 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5486	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: P6G, PGE, E4T, ZN, FMT, TRS, PEG

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	0.35	0/2523	0.57	0/3430
1	B	0.33	0/2611	0.57	0/3550
All	All	0.34	0/5134	0.57	0/6980

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	THR	Peptide

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	2477	0	2467	30	0
1	B	2558	0	2549	8	0
2	A	3	0	1	8	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	11	0	0	0	0
5	A	8	0	12	2	0
6	A	19	0	26	0	0
7	A	7	0	10	0	0
8	A	10	0	14	11	0
9	A	216	0	0	2	0
9	B	170	0	0	0	0
All	All	5486	0	5079	39	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 (39) 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:169:LYS:NZ	2:A:401:FMT:C	1.76	1.46
1:A:169:LYS:HZ1	2:A:401:FMT:C	1.32	1.32
1:A:169:LYS:NZ	2:A:401:FMT:H	0.83	1.14
1:A:169:LYS:CE	2:A:401:FMT:H	1.94	0.96
1:A:169:LYS:HZ3	2:A:401:FMT:C	1.61	0.80
1:B:176:ALA:H	1:B:211:GLN:HE22	1.35	0.73
5:A:405:TRS:H21	9:A:565:HOH:O	1.89	0.73
1:A:169:LYS:CE	2:A:401:FMT:C	2.61	0.72
1:A:180:GLN:HG2	8:A:408:PGE:H22	1.74	0.70
1:A:169:LYS:HZ1	2:A:401:FMT:H	0.85	0.62
1:A:38:ASN:ND2	9:A:501:HOH:O	2.33	0.61
1:A:183:VAL:HG11	8:A:408:PGE:H1	1.82	0.61
1:A:183:VAL:CG1	8:A:408:PGE:H1	2.31	0.60
1:B:193:ALA:O	1:B:363:ARG:HG3	2.01	0.59
1:B:363:ARG:HD3	1:B:364:ALA:O	2.02	0.58
1:A:134:PRO:HD2	8:A:408:PGE:H6	1.85	0.58
1:A:171:ALA:H	8:A:408:PGE:H12	1.67	0.58
1:A:87:LEU:HD12	1:A:116:VAL:HG12	1.84	0.58
1:A:169:LYS:HZ3	2:A:401:FMT:H	0.76	0.57
1:A:183:VAL:HG21	8:A:408:PGE:H3	1.88	0.54
1:A:171:ALA:H	8:A:408:PGE:C1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LYS:HE3	1:B:176:ALA:O	2.08	0.53
1:A:180:GLN:NE2	8:A:408:PGE:H52	2.25	0.52
1:A:180:GLN:HE21	8:A:408:PGE:H52	1.73	0.52
1:A:183:VAL:CB	8:A:408:PGE:H1	2.40	0.52
1:A:183:VAL:HB	8:A:408:PGE:H1	1.91	0.51
1:A:135:PRO:O	1:A:139:ARG:HG3	2.15	0.46
1:A:233:ASP:OD2	5:A:405:TRS:H22	2.16	0.46
1:B:57:HIS:O	1:B:303:LEU:HA	2.17	0.45
1:A:46:ILE:HD12	1:A:46:ILE:HA	1.82	0.44
1:A:57:HIS:O	1:A:303:LEU:HA	2.18	0.44
1:B:202:THR:HB	1:B:208:ASP:HB2	2.00	0.44
1:A:37:ILE:HD11	1:A:46:ILE:CD1	2.48	0.42
1:B:131:TRP:CG	1:B:132:GLU:N	2.87	0.42
1:A:353:ASN:HB2	1:A:354:PRO:HD3	2.02	0.41
1:A:131:TRP:CG	1:A:132:GLU:N	2.88	0.41
1:A:286:ALA:O	1:A:290:GLN:HG2	2.20	0.41
1:A:302:TRP:CH2	1:A:321:ASN:HB3	2.55	0.41
1:B:249:LEU:HD12	1:B:357:PHE:CD1	2.56	0.41

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	327/340 (96%)	318 (97%)	9 (3%)	0	100	100
1	B	338/340 (99%)	330 (98%)	8 (2%)	0	100	100
All	All	665/680 (98%)	648 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	257/273 (94%)	254 (99%)	3 (1%)	71	53
1	B	267/273 (98%)	260 (97%)	7 (3%)	46	21
All	All	524/546 (96%)	514 (98%)	10 (2%)	57	34

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	303	LEU
1	A	306	PHE
1	B	51	PHE
1	B	152	ARG
1	B	293	MET
1	B	299	SER
1	B	303	LEU
1	B	306	PHE
1	B	363	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	TRS	A	405	-	7,7,7	0.39	0	9,9,9	0.58	0
2	FMT	A	401	3	2,2,2	1.43	0	1,1,1	1.08	0
6	P6G	A	406	-	18,18,18	0.56	0	17,17,17	0.48	0
7	PEG	A	407	-	6,6,6	0.51	0	5,5,5	0.48	0
8	PGE	A	408	-	9,9,9	0.47	0	8,8,8	2.11	1 (12%)
4	E4T	A	404	3	11,11,11	1.24	0	11,18,18	1.87	2 (18%)
2	FMT	B	401	3	2,2,2	1.27	0	1,1,1	0.42	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
5	TRS	A	405	-	-	0/9/9/9	-
6	P6G	A	406	-	-	3/16/16/16	-
8	PGE	A	408	-	-	3/7/7/7	-
7	PEG	A	407	-	-	0/4/4/4	-
4	E4T	A	404	3	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	408	PGE	C5-O3-C4	-5.36	90.04	113.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	404	E4T	OAF-CAL-CAJ	3.71	119.69	110.62
4	A	404	E4T	OAD-CAL-CAJ	-2.68	104.08	110.62

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	408	PGE	C4-C3-O2-C2
8	A	408	PGE	C1-C2-O2-C3
6	A	406	P6G	C15-C14-O13-C12
6	A	406	P6G	C9-C8-O7-C6
8	A	408	PGE	C6-C5-O3-C4
6	A	406	P6G	C18-C17-O16-C15

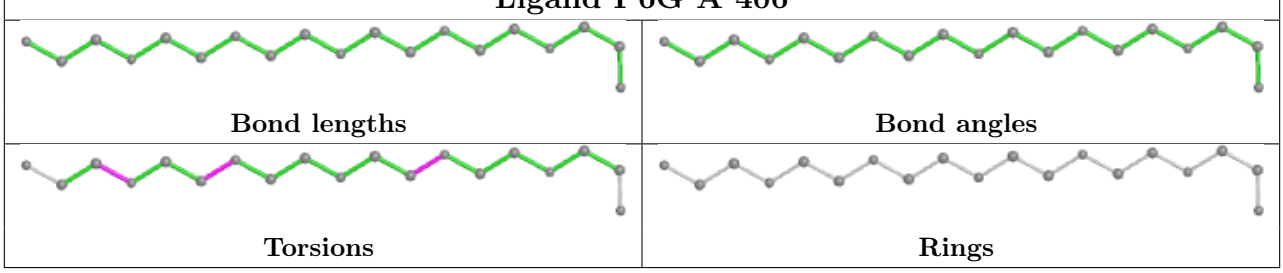
There are no ring outliers.

3 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	TRS	2	0
2	A	401	FMT	8	0
8	A	408	PGE	11	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 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 P6G A 406



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

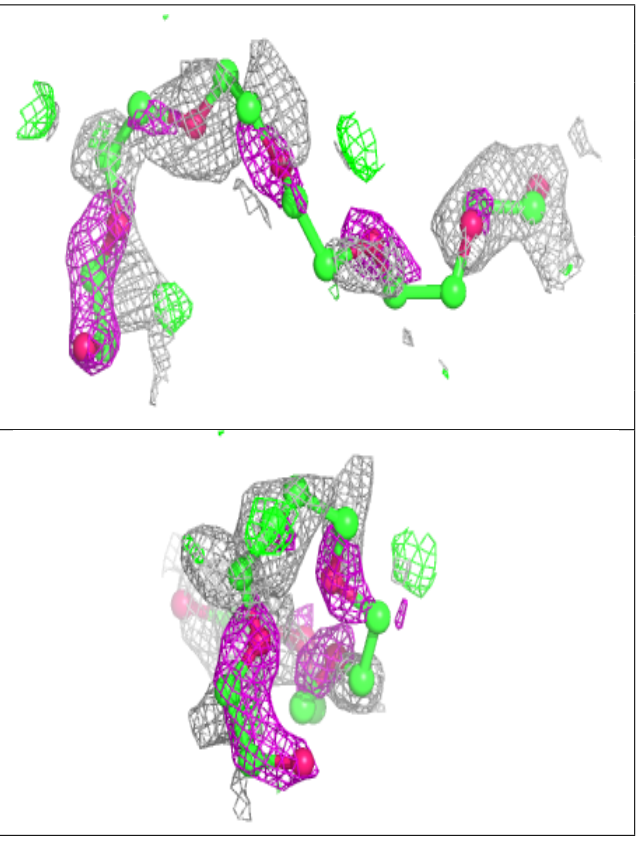
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 P6G A 406:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.