



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 10:49 AM EDT

PDB ID : 3T2D
Title : Fructose-1,6-bisphosphate aldolase/phosphatase from *Thermoproteus neutrophilus*, FBP-bound form
Authors : Du, J.; Say, R.; Lue, W.; Fuchs, G.; Einsle, O.
Deposited on : 2011-07-22
Resolution : 1.36 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

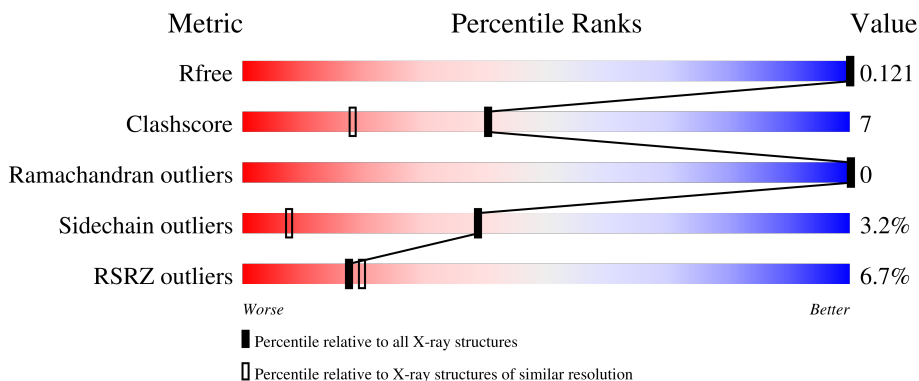
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	407	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3546 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 Fructose-1,6-bisphosphate aldolase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3160	2053	532	560	15	0	17	0

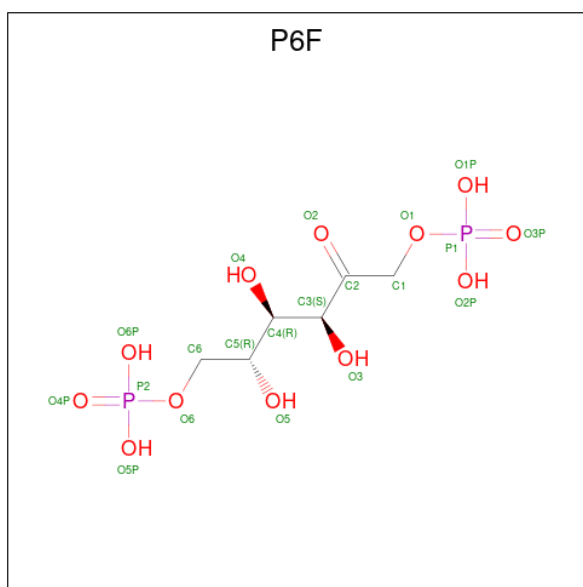
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	LEU	-	expression tag	UNP B1YAL1
A	401	GLU	-	expression tag	UNP B1YAL1
A	402	HIS	-	expression tag	UNP B1YAL1
A	403	HIS	-	expression tag	UNP B1YAL1
A	404	HIS	-	expression tag	UNP B1YAL1
A	405	HIS	-	expression tag	UNP B1YAL1
A	406	HIS	-	expression tag	UNP B1YAL1
A	407	HIS	-	expression tag	UNP B1YAL1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mg	0	0
			4	4		

- Molecule 3 is 1,6-di-O-phosphono-D-fructose (three-letter code: P6F) (formula: C₆H₁₄O₁₂P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	20	6	12	2	0	0

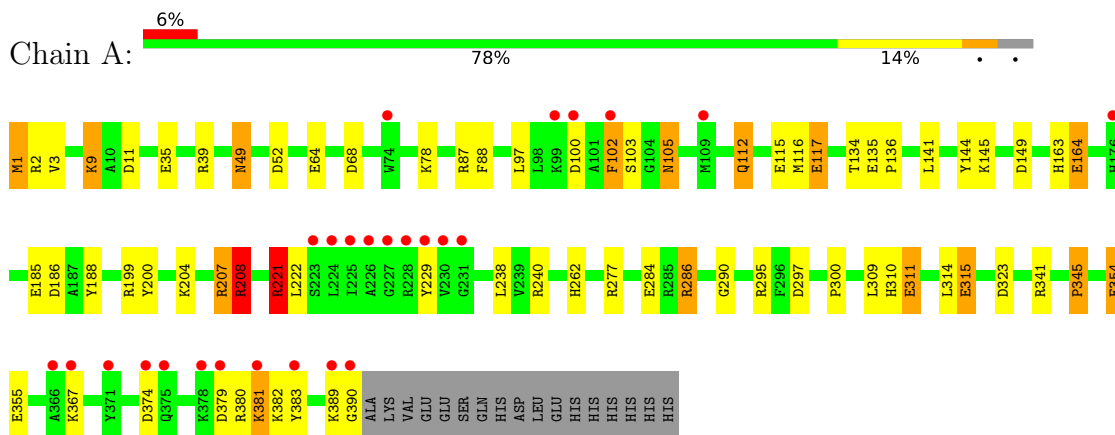
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	362	362	362	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 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: Fructose-1,6-bisphosphate aldolase/phosphatase



4 Data and refinement statistics i

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.29Å 112.29Å 151.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.78 – 1.36 54.78 – 1.36	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.78-1.36) 99.9 (54.78-1.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 1.36Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.104 , 0.126 0.100 , 0.121	Depositor DCC
R_{free} test set	5147 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for $-1/2^*h+1/2^*k-1/2^*l, 1/2^*h-1/2^*k-1/2^*l, -h-k$ 0.017 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3546	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: P6F, MG

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	1.56	39/3285 (1.2%)	1.33	36/4446 (0.8%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	GLU	CD-OE2	20.40	1.48	1.25
1	A	355	GLU	CD-OE2	16.12	1.43	1.25
1	A	354	GLU	CB-CG	13.34	1.77	1.52
1	A	354	GLU	CD-OE1	12.49	1.39	1.25
1	A	315	GLU	CB-CG	-11.62	1.30	1.52
1	A	207	ARG	CG-CD	-10.78	1.25	1.51
1	A	115	GLU	CB-CG	-10.10	1.32	1.52
1	A	117[A]	GLU	CD-OE2	-10.09	1.14	1.25
1	A	117[B]	GLU	CD-OE2	-10.09	1.14	1.25
1	A	207	ARG	CD-NE	-9.89	1.29	1.46
1	A	355	GLU	CG-CD	9.60	1.66	1.51
1	A	354	GLU	CG-CD	9.36	1.66	1.51
1	A	100	ASP	CB-CG	9.33	1.71	1.51
1	A	345	PRO	CA-CB	8.81	1.71	1.53
1	A	311	GLU	CD-OE2	8.73	1.35	1.25
1	A	112	GLN	CA-CB	-8.18	1.35	1.53
1	A	164	GLU	CD-OE1	8.07	1.34	1.25
1	A	35	GLU	CG-CD	7.27	1.62	1.51
1	A	311	GLU	CG-CD	-7.10	1.41	1.51
1	A	135	GLU	CD-OE2	-7.03	1.18	1.25
1	A	286	ARG	CD-NE	-6.97	1.34	1.46
1	A	355	GLU	CB-CG	6.10	1.63	1.52
1	A	208	ARG	CG-CD	-6.02	1.36	1.51
1	A	311	GLU	CD-OE1	5.88	1.32	1.25
1	A	295	ARG	CB-CG	-5.80	1.36	1.52
1	A	144	TYR	CE1-CZ	-5.76	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	GLU	CG-CD	5.55	1.60	1.51
1	A	207	ARG	NE-CZ	5.54	1.40	1.33
1	A	78	LYS	CD-CE	5.51	1.65	1.51
1	A	102	PHE	CE1-CZ	5.43	1.47	1.37
1	A	35	GLU	CD-OE1	5.38	1.31	1.25
1	A	135	GLU	CG-CD	5.33	1.59	1.51
1	A	383	TYR	CD2-CE2	-5.32	1.31	1.39
1	A	185	GLU	CB-CG	-5.29	1.42	1.52
1	A	64	GLU	CD-OE2	-5.19	1.20	1.25
1	A	208	ARG	CZ-NH1	-5.10	1.26	1.33
1	A	207	ARG	CB-CG	-5.08	1.38	1.52
1	A	149	ASP	CG-OD2	5.03	1.36	1.25
1	A	380	ARG	CZ-NH1	5.02	1.39	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH2	22.69	131.65	120.30
1	A	221	ARG	NE-CZ-NH1	-15.26	112.67	120.30
1	A	221	ARG	CD-NE-CZ	10.96	138.94	123.60
1	A	39	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	207	ARG	NE-CZ-NH2	9.55	125.08	120.30
1	A	97	LEU	CB-CG-CD1	8.23	124.99	111.00
1	A	208	ARG	CD-NE-CZ	8.12	134.97	123.60
1	A	208	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	345	PRO	N-CA-CB	-7.68	94.09	103.30
1	A	323	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	311	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	A	39	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	11	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	354	GLU	OE1-CD-OE2	6.62	131.25	123.30
1	A	240	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	204[A]	LYS	CD-CE-NZ	6.57	126.81	111.70
1	A	204[B]	LYS	CD-CE-NZ	6.57	126.81	111.70
1	A	207	ARG	NH1-CZ-NH2	-6.55	112.20	119.40
1	A	100	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	341	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	221	ARG	CG-CD-NE	6.06	124.53	111.80
1	A	208	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	188	TYR	CB-CG-CD1	6.00	124.60	121.00
1	A	379	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	1	MET	CG-SD-CE	5.80	109.48	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	380	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	186	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	188	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	315	GLU	CG-CD-OE2	-5.38	107.53	118.30
1	A	200	TYR	CZ-CE2-CD2	-5.35	114.98	119.80
1	A	52	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	277	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	199	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	355	GLU	CG-CD-OE1	-5.17	107.96	118.30
1	A	277	ARG	NE-CZ-NH2	-5.15	117.73	120.30

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	3160	0	3215	45	1
2	A	4	0	0	0	0
3	A	20	0	10	1	0
4	A	362	0	0	24	2
All	All	3546	0	3225	46	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 7.

All (46) 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:354:GLU:CB	1:A:354:GLU:CG	1.77	1.60
1:A:381:LYS:HD2	4:A:624:HOH:O	1.36	1.22
1:A:1:MET:CG	4:A:659:HOH:O	1.90	1.17
1:A:1:MET:HG3	4:A:659:HOH:O	1.40	1.16
1:A:1:MET:SD	4:A:659:HOH:O	2.03	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	4:A:659:HOH:O	1.97	1.09
1:A:381:LYS:CD	4:A:624:HOH:O	1.92	1.04
1:A:164:GLU:HG2	4:A:724:HOH:O	1.74	0.87
1:A:310:HIS:HD2	4:A:618:HOH:O	1.61	0.82
1:A:134[B]:THR:HG22	1:A:300:PRO:HB3	1.64	0.80
1:A:381:LYS:HD3	1:A:382:LYS:N	1.97	0.80
1:A:310:HIS:CD2	4:A:618:HOH:O	2.36	0.78
1:A:105:ASN:H	1:A:105:ASN:HD22	1.30	0.78
1:A:68[A]:ASP:OD2	4:A:535:HOH:O	2.05	0.73
3:A:412:P6F:O5P	4:A:660:HOH:O	2.14	0.65
1:A:3[B]:VAL:CG1	4:A:659:HOH:O	2.45	0.65
1:A:103:SER:HB2	4:A:660:HOH:O	1.96	0.64
1:A:116[B]:MET:HG2	1:A:238[B]:LEU:HD23	1.80	0.63
1:A:136:PRO:HG3	4:A:485:HOH:O	1.97	0.63
1:A:389:LYS:O	1:A:390:GLY:C	2.37	0.63
1:A:381:LYS:CD	1:A:382:LYS:N	2.61	0.63
1:A:381:LYS:HD3	1:A:382:LYS:H	1.66	0.60
1:A:311:GLU:HG2	4:A:749:HOH:O	2.02	0.59
1:A:163:HIS:ND1	4:A:725:HOH:O	2.31	0.58
1:A:262:HIS:HD2	4:A:641:HOH:O	1.86	0.57
1:A:207:ARG:HD2	4:A:469:HOH:O	2.06	0.55
1:A:3[B]:VAL:HG13	4:A:659:HOH:O	2.07	0.54
1:A:1:MET:CE	1:A:3[B]:VAL:HG12	2.40	0.52
1:A:1:MET:HE3	1:A:3[B]:VAL:HG12	1.93	0.51
1:A:49:ASN:ND2	1:A:290:GLY:H	2.10	0.50
1:A:141[B]:LEU:HD11	1:A:145:LYS:HE3	1.92	0.50
1:A:222:LEU:HD13	1:A:229:TYR:HB3	1.93	0.50
1:A:208:ARG:O	1:A:208:ARG:HG3	2.11	0.49
1:A:164:GLU:CG	4:A:724:HOH:O	2.48	0.48
1:A:9[B]:LYS:NZ	1:A:112:GLN:HE21	2.11	0.47
1:A:9[B]:LYS:HZ1	1:A:112:GLN:HE21	1.61	0.46
1:A:2:ARG:NH2	1:A:117[B]:GLU:OE1	2.32	0.46
1:A:381:LYS:CD	1:A:382:LYS:H	2.23	0.46
1:A:315:GLU:HB2	4:A:618:HOH:O	2.15	0.46
1:A:105:ASN:ND2	4:A:660:HOH:O	2.49	0.45
1:A:87:ARG:HD2	1:A:88:PHE:CE1	2.52	0.45
1:A:221:ARG:HH21	1:A:221:ARG:HB2	1.83	0.43
1:A:374:ASP:HB2	4:A:770:HOH:O	2.19	0.43
1:A:309[A]:LEU:HD23	1:A:314:LEU:HD23	2.00	0.41
1:A:354:GLU:CG	1:A:354:GLU:CA	2.84	0.41
1:A:102:PHE:HB3	4:A:688:HOH:O	2.20	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:102:PHE:CZ	4:A:699:HOH:O[4_455]	1.95	0.25
4:A:574:HOH:O	4:A:663:HOH:O[4_455]	2.03	0.17

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	405/407 (100%)	393 (97%)	12 (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	332/331 (100%)	321 (97%)	11 (3%)	38 7

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9[A]	LYS
1	A	9[B]	LYS
1	A	49	ASN
1	A	105	ASN
1	A	208	ARG

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Mol	Chain	Res	Type
1	A	221	ARG
1	A	284	GLU
1	A	286	ARG
1	A	345	PRO
1	A	367	LYS
1	A	381	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	70	HIS
1	A	105	ASN
1	A	112	GLN
1	A	163	HIS
1	A	176	HIS
1	A	262	HIS
1	A	310	HIS
1	A	347	GLN

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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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
3	P6F	A	412	2	18,19,19	6.99	4 (22%)	21,28,28	1.61	2 (9%)

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
3	P6F	A	412	2	-	1/24/24/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	412	P6F	O1-C1	29.20	1.63	1.43
3	A	412	P6F	O2-C2	2.68	1.26	1.21
3	A	412	P6F	C1-C2	-2.50	1.47	1.51
3	A	412	P6F	P1-O1	2.32	1.67	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	412	P6F	O1P-P1-O1	-5.73	91.48	106.73
3	A	412	P6F	O5P-P2-O6	-2.37	100.43	106.73

There are no chirality outliers.

All (1) torsion outliers are listed below:

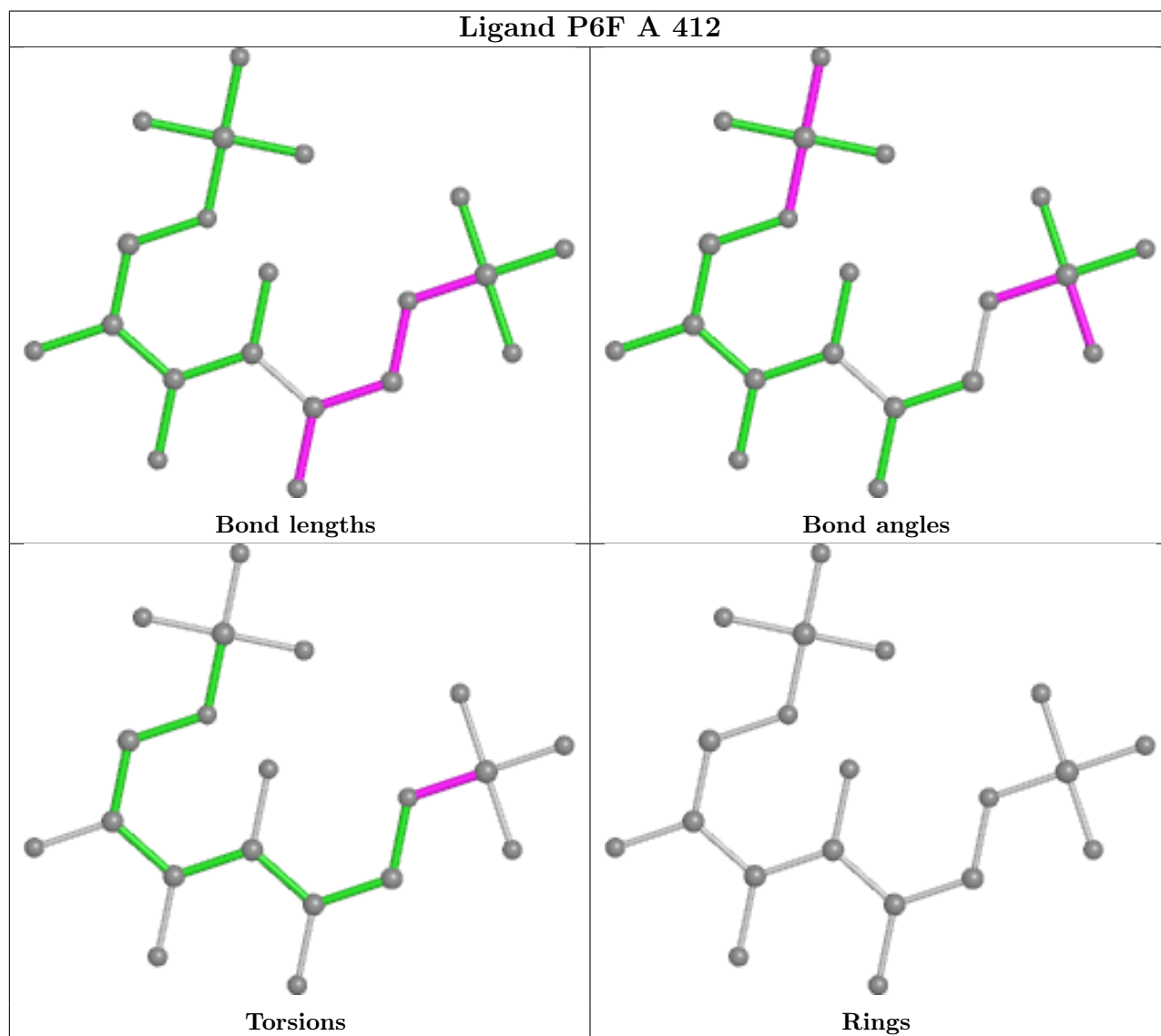
Mol	Chain	Res	Type	Atoms
3	A	412	P6F	C1-O1-P1-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	412	P6F	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

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	390/407 (95%)	0.07	26 (6%) 17 20	5, 12, 34, 47	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	10.8
1	A	224	LEU	9.5
1	A	390	GLY	8.3
1	A	226	ALA	8.2
1	A	229	TYR	6.8
1	A	227	GLY	6.7
1	A	381	LYS	5.2
1	A	383	TYR	4.5
1	A	389	LYS	4.0
1	A	378	LYS	3.6
1	A	228	ARG	3.3
1	A	100	ASP	3.3
1	A	375	GLN	3.2
1	A	74[A]	TRP	3.2
1	A	231	GLY	2.8
1	A	366	ALA	2.8
1	A	379	ASP	2.7
1	A	109	MET	2.7
1	A	99	LYS	2.6
1	A	102	PHE	2.6
1	A	374	ASP	2.4
1	A	230	VAL	2.4
1	A	371	TYR	2.3
1	A	176	HIS	2.3
1	A	223	SER	2.2
1	A	367	LYS	2.2

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](#)

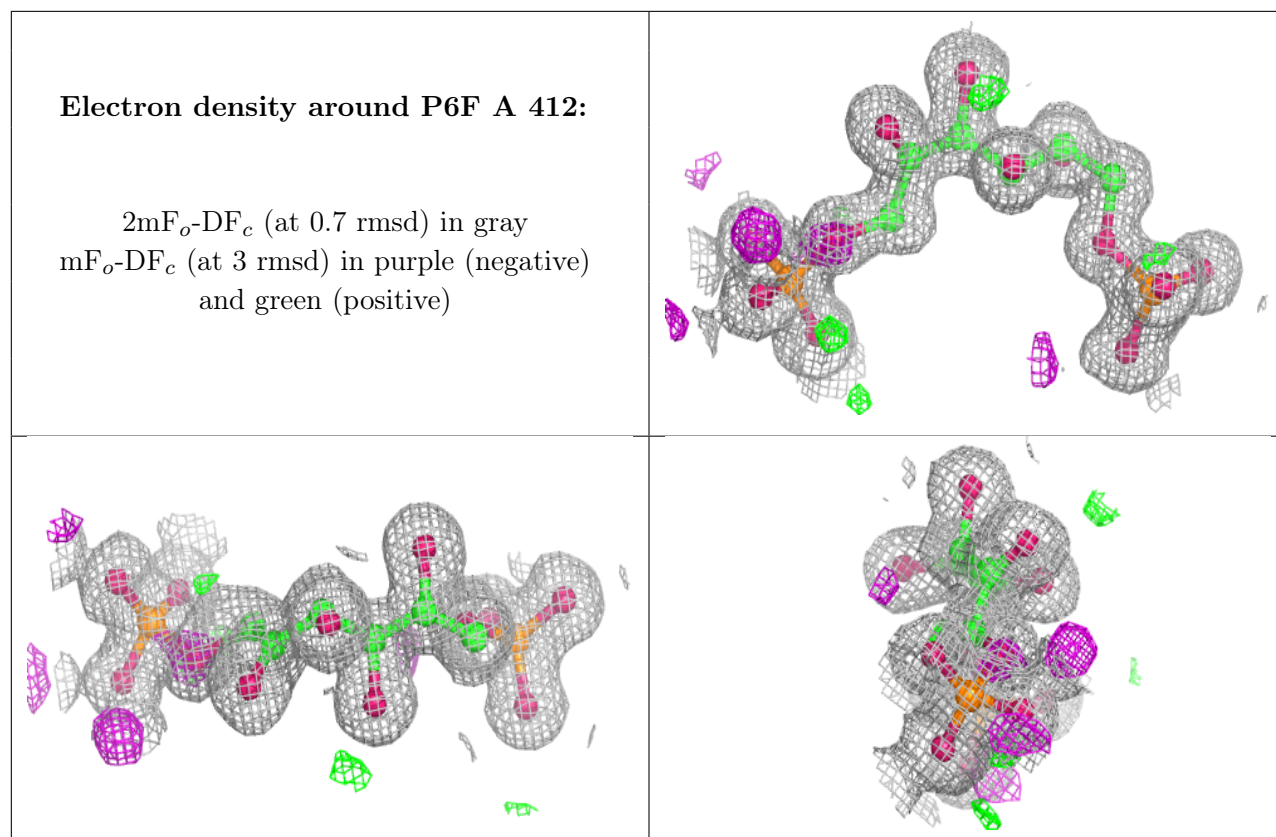
There are no monosaccharides in this entry.

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, 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(Å ²)	Q<0.9
2	MG	A	410	1/1	0.99	0.06	15,15,15,15	0
3	P6F	A	412	20/20	0.99	0.04	8,10,15,16	0
2	MG	A	408	1/1	1.00	0.05	7,7,7,7	0
2	MG	A	411	1/1	1.00	0.06	12,12,12,12	0
2	MG	A	409	1/1	1.00	0.04	8,8,8,8	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.