Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 09:43 AM EST

PDB ID	:	6AM7
Title	:	Engineered tryptophan synthase b-subunit from Pyrococcus furiosus, PfTrpB2B9
Authors	:	Buller, A.R.; van Roye, P.
Deposited on	:	2017-08-09
Resolution	:	1.47 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:

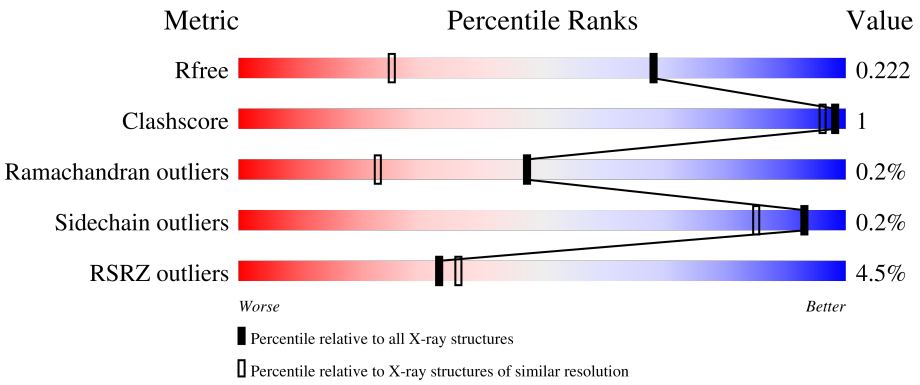
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.47 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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% 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	396	3% 95%
1	B	396	3% 94%
1	C	396	6% 94%
1	D	396	6% 95%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12528 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 beta chain 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	384	2906	1854	505	534	1	12	0	2	0
1	B	379	2911	1859	502	537	1	12	0	6	0
1	C	384	2931	1870	503	545	1	12	0	5	0
1	D	381	2899	1851	501	534	1	12	0	3	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	engineered mutation	UNP Q8U093
A	17	GLY	GLU	engineered mutation	UNP Q8U093
A	68	VAL	ILE	engineered mutation	UNP Q8U093
A	95	LEU	PHE	engineered mutation	UNP Q8U093
A	274	SER	PHE	engineered mutation	UNP Q8U093
A	292	SER	THR	engineered mutation	UNP Q8U093
A	321	ALA	THR	engineered mutation	UNP Q8U093
A	384	ALA	VAL	engineered mutation	UNP Q8U093
A	389	LEU	-	expression tag	UNP Q8U093
A	390	GLU	-	expression tag	UNP Q8U093
A	391	HIS	-	expression tag	UNP Q8U093
A	392	HIS	-	expression tag	UNP Q8U093
A	393	HIS	-	expression tag	UNP Q8U093
A	394	HIS	-	expression tag	UNP Q8U093
A	395	HIS	-	expression tag	UNP Q8U093
A	396	HIS	-	expression tag	UNP Q8U093
B	16	VAL	ILE	engineered mutation	UNP Q8U093
B	17	GLY	GLU	engineered mutation	UNP Q8U093
B	68	VAL	ILE	engineered mutation	UNP Q8U093
B	95	LEU	PHE	engineered mutation	UNP Q8U093
B	274	SER	PHE	engineered mutation	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
B	292	SER	THR	engineered mutation	UNP Q8U093
B	321	ALA	THR	engineered mutation	UNP Q8U093
B	384	ALA	VAL	engineered mutation	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
B	391	HIS	-	expression tag	UNP Q8U093
B	392	HIS	-	expression tag	UNP Q8U093
B	393	HIS	-	expression tag	UNP Q8U093
B	394	HIS	-	expression tag	UNP Q8U093
B	395	HIS	-	expression tag	UNP Q8U093
B	396	HIS	-	expression tag	UNP Q8U093
C	16	VAL	ILE	engineered mutation	UNP Q8U093
C	17	GLY	GLU	engineered mutation	UNP Q8U093
C	68	VAL	ILE	engineered mutation	UNP Q8U093
C	95	LEU	PHE	engineered mutation	UNP Q8U093
C	274	SER	PHE	engineered mutation	UNP Q8U093
C	292	SER	THR	engineered mutation	UNP Q8U093
C	321	ALA	THR	engineered mutation	UNP Q8U093
C	384	ALA	VAL	engineered mutation	UNP Q8U093
C	389	LEU	-	expression tag	UNP Q8U093
C	390	GLU	-	expression tag	UNP Q8U093
C	391	HIS	-	expression tag	UNP Q8U093
C	392	HIS	-	expression tag	UNP Q8U093
C	393	HIS	-	expression tag	UNP Q8U093
C	394	HIS	-	expression tag	UNP Q8U093
C	395	HIS	-	expression tag	UNP Q8U093
C	396	HIS	-	expression tag	UNP Q8U093
D	16	VAL	ILE	engineered mutation	UNP Q8U093
D	17	GLY	GLU	engineered mutation	UNP Q8U093
D	68	VAL	ILE	engineered mutation	UNP Q8U093
D	95	LEU	PHE	engineered mutation	UNP Q8U093
D	274	SER	PHE	engineered mutation	UNP Q8U093
D	292	SER	THR	engineered mutation	UNP Q8U093
D	321	ALA	THR	engineered mutation	UNP Q8U093
D	384	ALA	VAL	engineered mutation	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093
D	392	HIS	-	expression tag	UNP Q8U093
D	393	HIS	-	expression tag	UNP Q8U093
D	394	HIS	-	expression tag	UNP Q8U093
D	395	HIS	-	expression tag	UNP Q8U093

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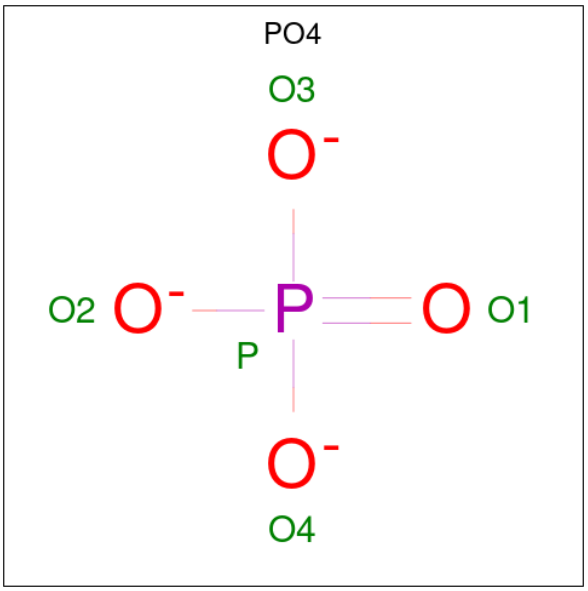
Chain	Residue	Modelled	Actual	Comment	Reference
D	396	HIS	-	expression tag	UNP Q8U093

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

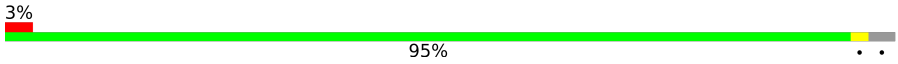
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	215	215	215	0	0
			Total	O		
4	B	229	229	229	0	0
			Total	O		
4	C	235	235	235	0	0
			Total	O		
4	D	175	175	175	0	0

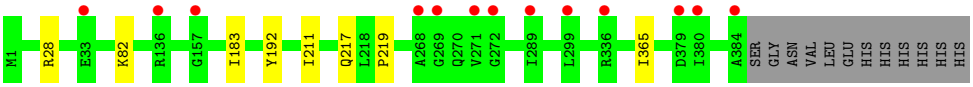
3 Residue-property plots (i)

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: Tryptophan synthase beta chain 1

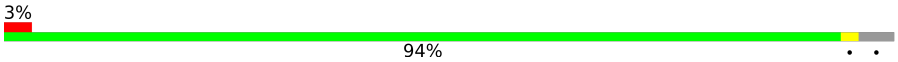
Chain A:

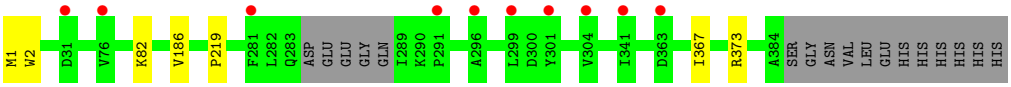




• Molecule 1: Tryptophan synthase beta chain 1

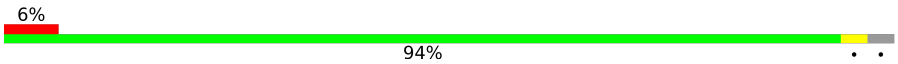
Chain B:

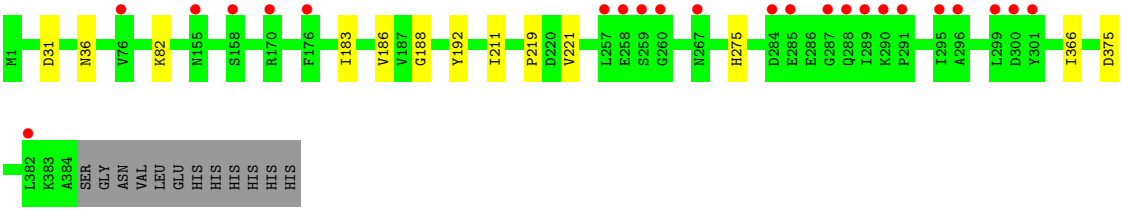




• Molecule 1: Tryptophan synthase beta chain 1

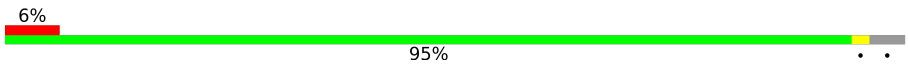
Chain C:

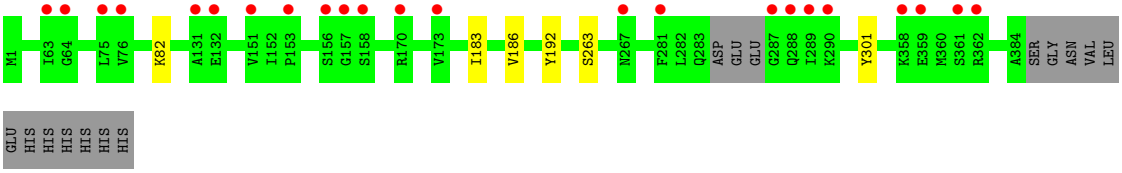




• Molecule 1: Tryptophan synthase beta chain 1

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.95Å 107.82Å 159.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.47 39.45 – 1.47	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-1.47) 98.4 (39.45-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.199 , 0.214 0.208 , 0.222	Depositor DCC
R_{free} test set	12028 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12528	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: PO4, NA, LLP

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	0.33	0/2946	0.56	0/3987
1	B	0.32	0/2962	0.56	0/4004
1	C	0.33	0/2974	0.57	0/4025
1	D	0.33	0/2941	0.55	0/3978
All	All	0.33	0/11823	0.56	0/15994

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	A	2906	0	2880	3	0
1	B	2911	0	2908	3	0
1	C	2931	0	2896	5	0
1	D	2899	0	2884	2	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	215	0	0	0	0
4	B	229	0	0	1	0
4	C	235	0	0	0	0
4	D	175	0	0	0	0
All	All	12528	0	11568	13	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 1.

All (13) 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:C:31:ASP:HA	1:C:36:ASN:HD21	1.73	0.53
1:B:1:MET:HG3	1:B:2:TRP:CD1	2.52	0.44
1:C:188:GLY:HA2	1:C:275:HIS:O	2.18	0.43
1:A:211:ILE:HG21	1:A:219:PRO:HD3	2.02	0.42
1:B:219:PRO:HG3	1:B:367:ILE:HD12	2.02	0.42
1:C:211:ILE:HG21	1:C:219:PRO:HD3	2.01	0.41
1:A:183:ILE:HD12	1:A:192:TYR:CD2	2.55	0.41
1:A:217:GLN:HE21	1:A:365:ILE:HD12	1.85	0.41
1:D:263[B]:SER:OG	1:D:301:TYR:O	2.39	0.41
1:B:373[B]:ARG:NH2	4:B:503:HOH:O	2.53	0.41
1:C:183:ILE:HD12	1:C:192:TYR:CD2	2.56	0.41
1:D:183:ILE:HD12	1:D:192:TYR:CD2	2.56	0.40
1:C:221:VAL:CG1	1:C:366:ILE:HG12	2.51	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	Percentiles	
1	A	383/396 (97%)	376 (98%)	7 (2%)	0	100	100
1	B	380/396 (96%)	374 (98%)	5 (1%)	1 (0%)	41	18
1	C	386/396 (98%)	379 (98%)	6 (2%)	1 (0%)	41	18
1	D	379/396 (96%)	371 (98%)	7 (2%)	1 (0%)	41	18
All	All	1528/1584 (96%)	1500 (98%)	25 (2%)	3 (0%)	47	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	186	VAL
1	B	186	VAL
1	C	186	VAL

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	286/312 (92%)	285 (100%)	1 (0%)	92	84
1	B	292/312 (94%)	292 (100%)	0	100	100
1	C	290/312 (93%)	289 (100%)	1 (0%)	92	84
1	D	288/312 (92%)	288 (100%)	0	100	100
All	All	1156/1248 (93%)	1154 (100%)	2 (0%)	93	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	C	375	ASP

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

Mol	Chain	Res	Type
1	C	36	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	LLP	D	82	1	23,24,25	2.63	5 (21%)	25,32,34	1.37	4 (16%)
1	LLP	A	82	1	23,24,25	2.66	5 (21%)	25,32,34	1.42	3 (12%)
1	LLP	B	82	1	23,24,25	2.59	5 (21%)	25,32,34	1.32	4 (16%)
1	LLP	C	82	1	23,24,25	2.56	5 (21%)	25,32,34	1.30	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	82	1	-	1/16/17/19	0/1/1/1
1	LLP	A	82	1	-	3/16/17/19	0/1/1/1
1	LLP	B	82	1	-	2/16/17/19	0/1/1/1
1	LLP	C	82	1	-	1/16/17/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	LLP	C3-C2	7.74	1.48	1.40
1	D	82	LLP	C3-C2	7.54	1.48	1.40
1	B	82	LLP	C3-C2	7.40	1.48	1.40
1	C	82	LLP	C3-C2	7.04	1.48	1.40
1	C	82	LLP	C4-C5	5.81	1.49	1.42
1	A	82	LLP	C4-C5	5.78	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	LLP	C4-C5	5.73	1.49	1.42
1	B	82	LLP	C4-C5	5.66	1.49	1.42
1	D	82	LLP	C4'-NZ	5.47	1.45	1.27
1	A	82	LLP	C4'-NZ	5.38	1.45	1.27
1	B	82	LLP	C4'-NZ	5.35	1.45	1.27
1	A	82	LLP	C4-C3	5.30	1.48	1.40
1	C	82	LLP	C4'-NZ	5.24	1.44	1.27
1	C	82	LLP	C4-C3	5.19	1.48	1.40
1	B	82	LLP	C4-C3	5.16	1.48	1.40
1	D	82	LLP	C4-C3	5.14	1.48	1.40
1	C	82	LLP	C4-C4'	2.64	1.51	1.46
1	D	82	LLP	C4-C4'	2.62	1.51	1.46
1	B	82	LLP	C4-C4'	2.58	1.51	1.46
1	A	82	LLP	C4-C4'	2.56	1.51	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	LLP	C4-C3-C2	-3.65	117.93	120.19
1	B	82	LLP	C4-C3-C2	-3.20	118.21	120.19
1	D	82	LLP	C4-C3-C2	-2.90	118.39	120.19
1	D	82	LLP	C3-C4-C5	-2.71	116.18	118.26
1	B	82	LLP	C4-C4'-NZ	-2.59	112.39	124.31
1	C	82	LLP	C4-C4'-NZ	-2.45	113.06	124.31
1	B	82	LLP	C6-N1-C2	2.39	123.59	119.17
1	C	82	LLP	C3-C4-C5	-2.36	116.44	118.26
1	D	82	LLP	C4-C4'-NZ	-2.34	113.58	124.31
1	C	82	LLP	C4-C3-C2	-2.32	118.75	120.19
1	A	82	LLP	C6-N1-C2	2.32	123.46	119.17
1	C	82	LLP	C6-N1-C2	2.24	123.32	119.17
1	A	82	LLP	C4-C4'-NZ	-2.22	114.13	124.31
1	D	82	LLP	C6-N1-C2	2.10	123.05	119.17
1	B	82	LLP	C3-C4-C5	-2.02	116.71	118.26

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	82	LLP	O-C-CA-CB
1	B	82	LLP	O-C-CA-CB
1	A	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	B	82	LLP	C4-C4'-NZ-CE
1	C	82	LLP	C4-C4'-NZ-CE
1	A	82	LLP	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	PO4	B	402	-	4,4,4	0.91	0	6,6,6	0.47	0
3	PO4	A	403	-	4,4,4	1.02	0	6,6,6	0.38	0
3	PO4	C	403	-	4,4,4	0.98	0	6,6,6	0.35	0
3	PO4	D	402	-	4,4,4	0.99	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	383/396 (96%)	0.33	13 (3%)	45	49	14, 24, 43, 60	0
1	B	378/396 (95%)	0.19	10 (2%)	56	60	14, 21, 34, 63	0
1	C	383/396 (96%)	0.23	23 (6%)	21	23	13, 21, 39, 85	0
1	D	380/396 (95%)	0.38	23 (6%)	21	22	16, 27, 54, 73	0
All	All	1524/1584 (96%)	0.28	69 (4%)	33	36	13, 23, 42, 85	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	ALA	4.6
1	C	76[A]	VAL	4.4
1	A	380	ILE	4.4
1	B	291	PRO	4.3
1	C	285	GLU	4.2
1	A	289	ILE	4.1
1	B	281	PHE	3.8
1	C	260	GLY	3.8
1	C	287	GLY	3.7
1	D	76[A]	VAL	3.7
1	D	131	ALA	3.7
1	C	382	LEU	3.6
1	D	281	PHE	3.5
1	C	258	GLU	3.4
1	D	287	GLY	3.4
1	C	299	LEU	3.3
1	D	170	ARG	3.2
1	D	158	SER	3.2
1	C	291	PRO	3.2
1	A	269	GLY	3.2
1	C	155	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	ARG	3.0
1	C	284	ASP	3.0
1	D	63	ILE	3.0
1	D	157	GLY	2.9
1	A	271	VAL	2.9
1	D	289	ILE	2.9
1	C	289	ILE	2.9
1	A	384	ALA	2.9
1	B	299	LEU	2.8
1	C	296	ALA	2.8
1	C	259	SER	2.7
1	D	362	ARG	2.7
1	D	153	PRO	2.7
1	B	363	ASP	2.6
1	C	158	SER	2.6
1	A	33	GLU	2.5
1	D	64	GLY	2.5
1	A	299	LEU	2.5
1	C	257	LEU	2.5
1	C	170	ARG	2.5
1	B	76[A]	VAL	2.5
1	C	290	LYS	2.4
1	C	288	GLN	2.4
1	C	267	ASN	2.4
1	D	290	LYS	2.4
1	A	272	GLY	2.4
1	A	157	GLY	2.3
1	B	31	ASP	2.3
1	B	341	ILE	2.3
1	D	156	SER	2.3
1	D	151	VAL	2.3
1	D	75	LEU	2.2
1	D	359	GLU	2.2
1	D	132	GLU	2.2
1	B	296	ALA	2.1
1	D	267	ASN	2.1
1	C	301	TYR	2.1
1	D	288	GLN	2.1
1	C	176	PHE	2.1
1	C	295	ILE	2.1
1	A	379	ASP	2.1
1	B	301	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	173	VAL	2.1
1	D	361	SER	2.1
1	A	336	ARG	2.0
1	D	358	LYS	2.0
1	B	304	VAL	2.0
1	C	300[A]	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	B	82	24/25	0.96	0.11	13,14,14,14	0
1	LLP	D	82	24/25	0.96	0.10	16,18,19,20	0
1	LLP	C	82	24/25	0.97	0.10	13,14,15,15	0
1	LLP	A	82	24/25	0.97	0.12	15,17,17,17	0

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	NA	A	402	1/1	0.82	0.14	35,35,35,35	0
2	NA	C	402	1/1	0.88	0.12	22,22,22,22	0
2	NA	C	404	1/1	0.89	0.15	35,35,35,35	0
3	PO4	C	403	5/5	0.93	0.14	33,34,34,34	0
3	PO4	B	402	5/5	0.94	0.09	26,26,27,27	0
2	NA	C	401	1/1	0.95	0.12	19,19,19,19	0
3	PO4	D	402	5/5	0.95	0.09	32,32,33,33	0
3	PO4	A	403	5/5	0.96	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	401	1/1	0.96	0.12	24,24,24,24	0
2	NA	B	401	1/1	0.97	0.12	18,18,18,18	0
2	NA	D	401	1/1	0.98	0.12	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.