



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:17 PM UTC

PDB ID : 6AMC / pdb_00006amc
Title : Engineered tryptophan synthase b-subunit from *Pyrococcus furiosus*, PfTrpB4D11
Authors : Buller, A.R.; Herger, M.
Deposited on : 2017-08-09
Resolution : 1.93 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

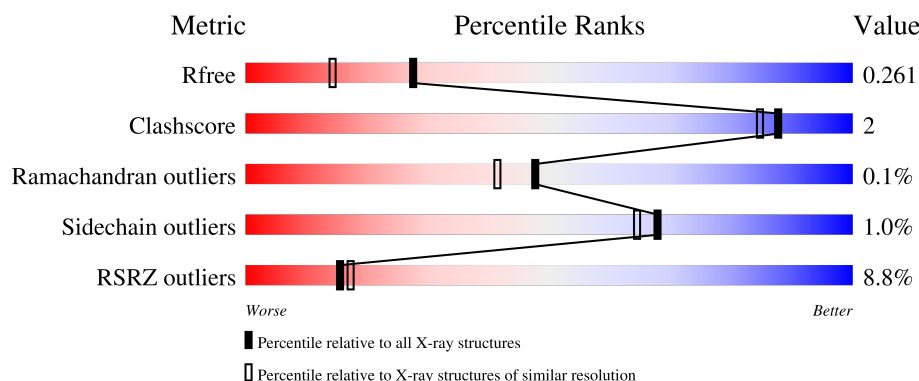
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

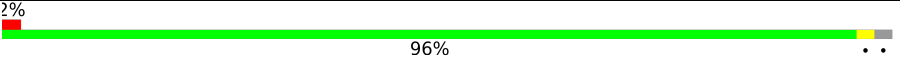
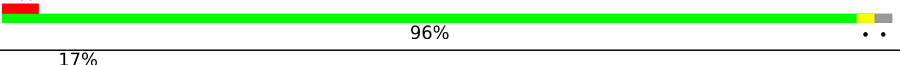
The reported resolution of this entry is 1.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	396	
1	B	396	
1	C	396	
1	D	396	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11776 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
1	A	387	Total	C	N	O	P	S	0	1	0
			2955	1880	511	551	1	12			
1	B	383	Total	C	N	O	P	S	0	0	0
			2847	1816	486	532	1	12			
1	C	387	Total	C	N	O	P	S	0	0	0
			2902	1849	497	543	1	12			
1	D	382	Total	C	N	O	P	S	0	0	0
			2805	1790	479	523	1	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLY	GLU	engineered mutation	UNP Q8U093
A	68	VAL	ILE	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	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	17	GLY	GLU	engineered mutation	UNP Q8U093
B	68	VAL	ILE	engineered mutation	UNP Q8U093
B	274	SER	PHE	engineered mutation	UNP Q8U093
B	292	SER	THR	engineered mutation	UNP Q8U093
B	321	ALA	THR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	17	GLY	GLU	engineered mutation	UNP Q8U093
C	68	VAL	ILE	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	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	17	GLY	GLU	engineered mutation	UNP Q8U093
D	68	VAL	ILE	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	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
D	396	HIS	-	expression tag	UNP Q8U093

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total 96	O 96	0	0
3	B	52	Total 52	O 52	0	0
3	C	76	Total 76	O 76	0	0
3	D	39	Total 39	O 39	0	0

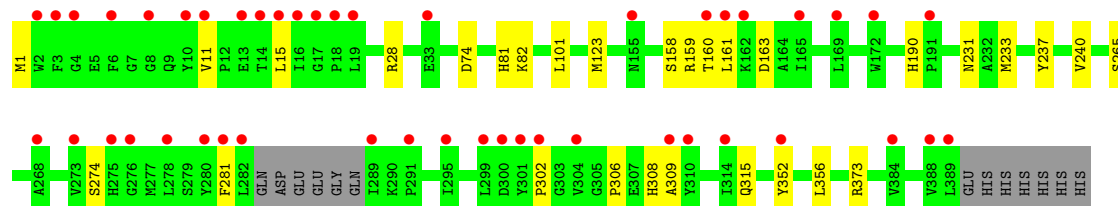
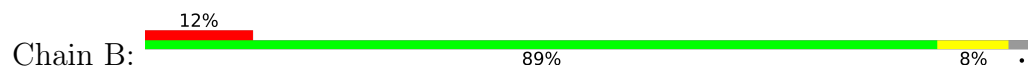
3 Residue-property plots [i](#)

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.

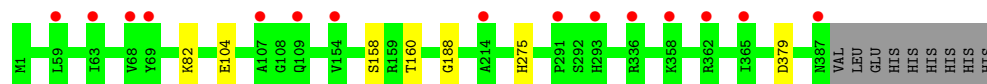
- Molecule 1: Tryptophan synthase beta chain 1



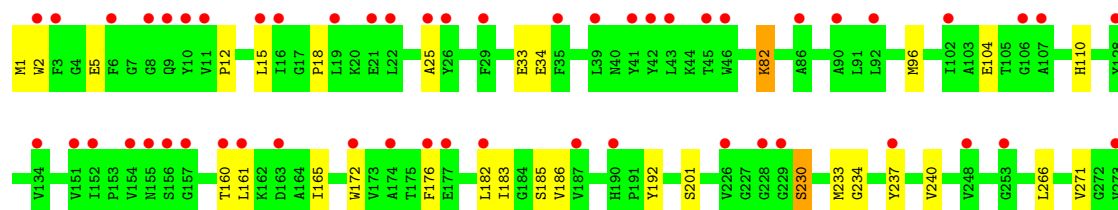
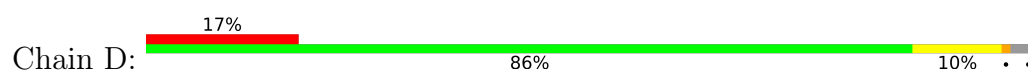
- Molecule 1: Tryptophan synthase beta chain 1

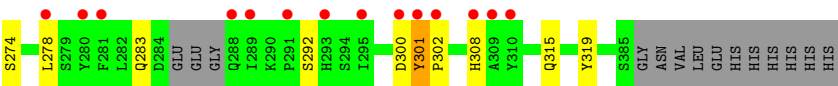


- Molecule 1: Tryptophan synthase beta chain 1



- Molecule 1: Tryptophan synthase beta chain 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 110.73Å 160.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.93 40.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-1.93) 99.5 (40.00-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.216 , 0.255 0.224 , 0.261	Depositor DCC
R_{free} test set	5711 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11776	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: 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	0.46	0/2993	0.82	0/4048
1	B	0.46	0/2881	0.83	0/3913
1	C	0.46	0/2937	0.85	0/3983
1	D	0.44	0/2839	0.86	2/3858 (0.1%)
All	All	0.46	0/11650	0.84	2/15802 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	SER	N-CA-C	5.84	117.32	111.07
1	D	301	TYR	N-CA-C	5.21	116.98	109.48

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	2955	0	2916	3	0
1	B	2847	0	2736	17	0
1	C	2902	0	2812	2	0
1	D	2805	0	2666	24	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	96	0	0	0	0
3	B	52	0	0	0	0
3	C	76	0	0	0	0
3	D	39	0	0	0	0
All	All	11776	0	11130	46	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 2.

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:D:301:TYR:CD1	1:D:302:PRO:HD2	2.29	0.68
1:D:292:SER:OG	1:D:300:ASP:O	2.14	0.65
1:D:12:PRO:HD2	1:D:15:LEU:HD12	1.80	0.64
1:D:160:THR:HG22	1:D:161:LEU:H	1.65	0.61
1:B:28:ARG:HH11	1:B:28:ARG:HG2	1.66	0.61
1:B:11:VAL:HB	1:B:15:LEU:HD12	1.83	0.61
1:B:160:THR:HG22	1:B:161:LEU:H	1.66	0.60
1:A:289:ILE:HG21	1:A:302:PRO:HB2	1.85	0.58
1:D:172:TRP:O	1:D:176:PHE:HB3	2.04	0.58
1:B:233:MET:HG2	1:B:308:HIS:NE2	2.19	0.57
1:B:159:ARG:N	1:B:163:ASP:OD2	2.41	0.53
1:D:25:ALA:CB	1:D:96:MET:HE3	2.39	0.53
1:D:183:ILE:HD12	1:D:192:TYR:CG	2.44	0.53
1:D:161:LEU:O	1:D:165:ILE:HG13	2.10	0.52
1:D:233:MET:HG2	1:D:308:HIS:NE2	2.25	0.51
1:D:160:THR:HG22	1:D:161:LEU:N	2.25	0.51
1:D:82:LLP:OP3	1:D:230:SER:OG	2.25	0.50
1:D:271:VAL:HG12	1:D:278:LEU:HD11	1.92	0.50
1:D:15:LEU:C	1:D:18:PRO:HD2	2.38	0.48
1:D:25:ALA:HB2	1:D:96:MET:HE3	1.94	0.48
1:B:265:SER:OG	1:B:302:PRO:O	2.21	0.48
1:B:160:THR:HG22	1:B:161:LEU:N	2.29	0.48
1:D:201:SER:HA	1:D:234:GLY:O	2.15	0.47
1:B:274:SER:HB3	1:B:281:PHE:CE2	2.49	0.47
1:D:183:ILE:HD12	1:D:192:TYR:CD2	2.50	0.47
1:A:188:GLY:HA2	1:A:275:HIS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:SER:HB3	1:B:163:ASP:OD2	2.15	0.47
1:B:306:PRO:O	1:B:309:ALA:HB3	2.15	0.46
1:D:1:MET:HG3	1:D:2:TRP:CD1	2.51	0.46
1:D:110:HIS:CE1	1:D:182:LEU:CD2	2.99	0.46
1:C:188:GLY:HA2	1:C:275:HIS:O	2.16	0.45
1:B:237:TYR:HA	1:B:240:VAL:HG23	1.98	0.45
1:B:81:HIS:CE1	1:B:231:ASN:HB3	2.51	0.45
1:B:101:LEU:HG	1:B:123:MET:HE2	1.99	0.44
1:B:74:ASP:HB2	1:B:373:ARG:HB3	2.00	0.43
1:A:55:TYR:HB2	1:A:69:TYR:CE2	2.54	0.43
1:D:82:LLP:O3	1:D:82:LLP:NZ	2.51	0.43
1:B:274:SER:HB3	1:B:281:PHE:CZ	2.54	0.42
1:D:237:TYR:HA	1:D:240:VAL:HG23	2.01	0.42
1:D:266:LEU:CD1	1:D:319:TYR:CD2	3.03	0.42
1:B:1:MET:HB2	1:B:190:HIS:CG	2.55	0.42
1:D:271:VAL:CG1	1:D:278:LEU:HD11	2.51	0.41
1:B:352:TYR:CE2	1:B:356:LEU:HD22	2.56	0.41
1:D:110:HIS:HE1	1:D:182:LEU:CD2	2.34	0.41
1:D:185:SER:HA	1:D:230:SER:HB3	2.04	0.40
1:C:158:SER:HB3	1:C:160:THR:HG22	2.02	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	385/396 (97%)	375 (97%)	10 (3%)	0	100	100
1	B	378/396 (96%)	373 (99%)	5 (1%)	0	100	100
1	C	384/396 (97%)	378 (98%)	6 (2%)	0	100	100
1	D	377/396 (95%)	369 (98%)	7 (2%)	1 (0%)	36	30
All	All	1524/1584 (96%)	1495 (98%)	28 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	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	294/313 (94%)	293 (100%)	1 (0%)	86	86
1	B	273/313 (87%)	272 (100%)	1 (0%)	84	84
1	C	281/313 (90%)	279 (99%)	2 (1%)	76	74
1	D	263/313 (84%)	256 (97%)	7 (3%)	39	26
All	All	1111/1252 (89%)	1100 (99%)	11 (1%)	68	64

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

Mol	Chain	Res	Type
1	A	104	GLU
1	B	315	GLN
1	C	104	GLU
1	C	379	ASP
1	D	5	GLU
1	D	33	GLU
1	D	34	GLU
1	D	104	GLU
1	D	274	SER
1	D	283	GLN
1	D	315	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	283	GLN
1	B	9	GLN

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Mol	Chain	Res	Type
1	B	85	ASN
1	B	89	GLN
1	B	387	ASN
1	C	40	ASN
1	C	89	GLN
1	C	109	GLN
1	C	110	HIS
1	C	270	GLN
1	C	283	GLN
1	C	332	HIS
1	C	369	ASN
1	D	36	ASN
1	D	110	HIS
1	D	217	GLN
1	D	275	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	2.49	5 (21%)	25,32,34	1.41	4 (16%)
1	LLP	C	82	1	23,24,25	2.20	4 (17%)	25,32,34	1.47	6 (24%)
1	LLP	A	82	1	23,24,25	2.27	5 (21%)	25,32,34	1.40	5 (20%)
1	LLP	B	82	1	23,24,25	2.50	5 (21%)	25,32,34	1.37	6 (24%)

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	-	4/16/17/19	0/1/1/1
1	LLP	C	82	1	-	2/16/17/19	0/1/1/1
1	LLP	A	82	1	-	4/16/17/19	0/1/1/1
1	LLP	B	82	1	-	5/16/17/19	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	LLP	C3-C2	7.29	1.48	1.41
1	B	82	LLP	C3-C2	7.28	1.48	1.41
1	A	82	LLP	C3-C2	6.44	1.47	1.41
1	C	82	LLP	C3-C2	5.87	1.47	1.41
1	B	82	LLP	C4'-NZ	5.37	1.45	1.27
1	D	82	LLP	C4'-NZ	5.36	1.45	1.27
1	B	82	LLP	C4-C5	5.20	1.49	1.42
1	A	82	LLP	C4'-NZ	5.18	1.44	1.27
1	D	82	LLP	C4-C5	5.08	1.49	1.42
1	C	82	LLP	C4'-NZ	5.00	1.43	1.27
1	D	82	LLP	C4-C3	4.74	1.48	1.41
1	B	82	LLP	C4-C3	4.72	1.48	1.41
1	C	82	LLP	C4-C5	4.61	1.48	1.42
1	C	82	LLP	C4-C3	4.37	1.48	1.41
1	A	82	LLP	C4-C5	4.36	1.48	1.42
1	A	82	LLP	C4-C3	4.26	1.48	1.41
1	D	82	LLP	C4-C4'	2.24	1.51	1.46
1	A	82	LLP	C4-C4'	2.16	1.51	1.46
1	B	82	LLP	C4-C4'	2.14	1.51	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	82	LLP	C4-C3-C2	-3.57	118.14	120.14
1	C	82	LLP	OP4-C5'-C5	3.35	115.64	109.36
1	D	82	LLP	C4-C4'-NZ	-2.84	110.93	124.04
1	A	82	LLP	C3-C4-C5	-2.79	116.03	118.28
1	A	82	LLP	C4-C4'-NZ	-2.75	111.36	124.04
1	C	82	LLP	C6-N1-C2	2.74	124.18	119.20
1	A	82	LLP	C4-C3-C2	-2.62	118.67	120.14
1	B	82	LLP	C4-C3-C2	-2.59	118.68	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	LLP	C3-C4-C5	-2.55	116.23	118.28
1	C	82	LLP	C4-C4'-NZ	-2.53	112.38	124.04
1	D	82	LLP	C3-C4-C5	-2.35	116.39	118.28
1	B	82	LLP	OP3-P-OP2	2.32	116.50	107.80
1	D	82	LLP	O3-C3-C2	2.24	122.23	117.58
1	B	82	LLP	C6-N1-C2	2.19	123.17	119.20
1	C	82	LLP	C2'-C2-N1	2.19	121.76	117.64
1	B	82	LLP	OP4-C5'-C5	2.14	113.38	109.36
1	B	82	LLP	C4-C4'-NZ	-2.12	114.28	124.04
1	A	82	LLP	C6-N1-C2	2.10	123.00	119.20
1	A	82	LLP	OP4-C5'-C5	2.07	113.24	109.36
1	C	82	LLP	C3-C2-N1	-2.05	118.38	120.96
1	C	82	LLP	C4-C3-C2	-2.03	119.00	120.14

There are no chirality outliers.

All (15) 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	C	82	LLP	O-C-CA-CB
1	D	82	LLP	O-C-CA-CB
1	B	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	C4-C4'-NZ-CE
1	A	82	LLP	C4-C4'-NZ-CE
1	C	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	C5'-OP4-P-OP1
1	D	82	LLP	CD-CE-NZ-C4'
1	B	82	LLP	CD-CE-NZ-C4'
1	A	82	LLP	CD-CE-NZ-C4'
1	A	82	LLP	C3-C4-C4'-NZ
1	B	82	LLP	C3-C4-C4'-NZ
1	D	82	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	82	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

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	386/396 (97%)	0.29	7 (1%) 67 74	19, 42, 58, 81	1 (0%)
1	B	382/396 (96%)	0.83	46 (12%) 9 10	33, 53, 83, 94	0
1	C	386/396 (97%)	0.54	15 (3%) 43 49	28, 44, 64, 73	0
1	D	381/396 (96%)	1.15	67 (17%) 4 4	35, 64, 95, 107	0
All	All	1535/1584 (96%)	0.70	135 (8%) 15 17	19, 49, 85, 107	1 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	PRO	4.3
1	B	161	LEU	4.0
1	B	300	ASP	4.0
1	D	107	ALA	4.0
1	B	388	VAL	3.8
1	C	387	ASN	3.7
1	D	289	ILE	3.7
1	B	389	LEU	3.7
1	B	13	GLU	3.7
1	D	302	PRO	3.7
1	B	301	TYR	3.6
1	B	276	GLY	3.6
1	D	161	LEU	3.5
1	D	10	TYR	3.4
1	D	229	GLY	3.4
1	D	41	TYR	3.4
1	B	11	VAL	3.4
1	C	107	ALA	3.4
1	B	8	GLY	3.3
1	D	228	GLY	3.3
1	A	107	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	273	VAL	3.3
1	D	46	TRP	3.3
1	A	289	ILE	3.2
1	D	29	PHE	3.2
1	C	69	TYR	3.2
1	B	2	TRP	3.1
1	B	273	VAL	3.1
1	C	68	VAL	3.1
1	B	278	LEU	3.1
1	B	18	PRO	3.1
1	D	15	LEU	3.0
1	B	33	GLU	3.0
1	D	151	VAL	3.0
1	B	275	HIS	3.0
1	B	6	PHE	3.0
1	D	291	PRO	3.0
1	D	278	LEU	2.9
1	B	352	TYR	2.9
1	A	300	ASP	2.9
1	B	172	TRP	2.9
1	B	295	ILE	2.9
1	D	152	ILE	2.9
1	D	43	LEU	2.9
1	D	35	PHE	2.9
1	D	163	ASP	2.9
1	D	300	ASP	2.9
1	D	19	LEU	2.9
1	D	295	ILE	2.9
1	B	282	LEU	2.8
1	C	59	LEU	2.8
1	C	63	ILE	2.8
1	D	16	ILE	2.8
1	D	22	LEU	2.8
1	D	92	LEU	2.8
1	B	14	THR	2.8
1	D	39	LEU	2.8
1	C	365	ILE	2.8
1	D	226	VAL	2.8
1	B	304	VAL	2.7
1	D	11	VAL	2.7
1	B	281	PHE	2.7
1	B	291	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	384	VAL	2.7
1	D	310	TYR	2.7
1	B	160	THR	2.7
1	B	289	ILE	2.7
1	D	187	VAL	2.7
1	B	17	GLY	2.6
1	D	154	VAL	2.6
1	D	253	GLY	2.6
1	B	314	ILE	2.6
1	B	4	GLY	2.6
1	A	301	TYR	2.6
1	A	302	PRO	2.5
1	B	280	TYR	2.5
1	D	172	TRP	2.5
1	D	288	GLN	2.5
1	D	42	TYR	2.5
1	D	157	GLY	2.5
1	D	301	TYR	2.5
1	C	109	GLN	2.5
1	D	174	ALA	2.5
1	B	19	LEU	2.4
1	D	21	GLU	2.4
1	D	177	GLU	2.4
1	B	165	ILE	2.4
1	D	90	ALA	2.4
1	D	134	VAL	2.4
1	D	6	PHE	2.4
1	D	25	ALA	2.4
1	D	2	TRP	2.4
1	D	190	HIS	2.4
1	C	358	LYS	2.4
1	B	3	PHE	2.4
1	D	102	ILE	2.4
1	C	291	PRO	2.4
1	B	155	ASN	2.4
1	D	156	SER	2.4
1	B	299	LEU	2.3
1	B	169	LEU	2.3
1	D	160	THR	2.3
1	D	308	HIS	2.3
1	D	280	TYR	2.3
1	A	285	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	16	ILE	2.2
1	B	191	PRO	2.2
1	C	214	ALA	2.2
1	D	309	ALA	2.2
1	D	155	ASN	2.2
1	D	8	GLY	2.2
1	D	86	ALA	2.2
1	D	176	PHE	2.2
1	D	237	TYR	2.2
1	B	162	LYS	2.2
1	B	15	LEU	2.2
1	D	106	GLY	2.2
1	C	336	ARG	2.2
1	D	128	TYR	2.1
1	D	182	LEU	2.1
1	B	309	ALA	2.1
1	D	281	PHE	2.1
1	B	10	TYR	2.1
1	D	45	THR	2.1
1	C	293	HIS	2.1
1	C	362	ARG	2.1
1	A	293	HIS	2.0
1	D	293	HIS	2.0
1	C	154	VAL	2.0
1	D	248	VAL	2.0
1	B	268	ALA	2.0
1	D	3	PHE	2.0
1	D	9	GLN	2.0
1	B	310	TYR	2.0
1	D	26	TYR	2.0

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

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	0.93	0.10	39,42,45,46	0
1	LLP	D	82	24/25	0.93	0.11	41,46,49,49	0
1	LLP	A	82	24/25	0.97	0.09	35,36,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	C	82	24/25	0.98	0.09	35,35,35,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	401	1/1	0.82	0.13	54,54,54,54	0
2	NA	C	401	1/1	0.90	0.11	48,48,48,48	0
2	NA	B	401	1/1	0.92	0.11	60,60,60,60	0
2	NA	D	401	1/1	0.94	0.15	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.