



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:04 AM UTC

PDB ID : 7RNQ / pdb_00007rnq
Title : Holo structure of engineered TrpB, 2B9-H275E, from *Pyrococcus furiosus* in the extended-open conformation
Authors : Higgins, P.M.; Buller, A.R.
Deposited on : 2021-07-29
Resolution : 2.10 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

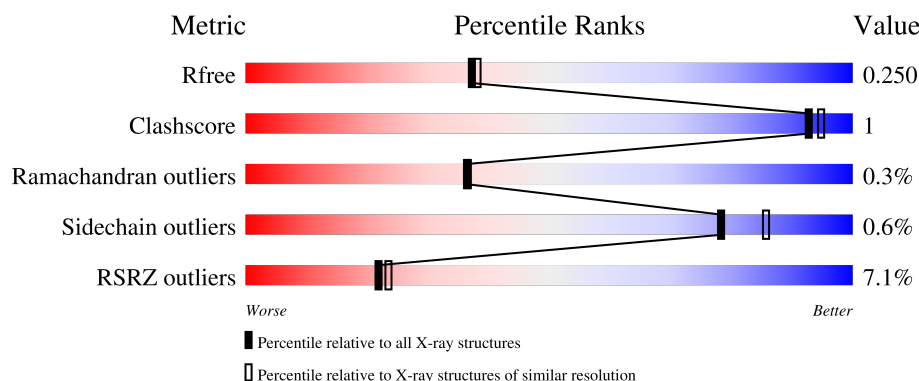
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	9% 95% • •
1	B	396	7% 93% 6% •
1	C	396	4% 93% 5% •
1	D	396	8% 91% 5% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11732 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	385	Total	C	N	O	P	S	0	1	0
			2832	1804	477	538	1	12			
1	B	389	Total	C	N	O	P	S	0	3	0
			2927	1866	503	545	1	12			
1	C	385	Total	C	N	O	P	S	0	1	0
			2858	1820	488	537	1	12			
1	D	379	Total	C	N	O	P	S	0	3	0
			2819	1802	478	526	1	12			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	conflict	UNP Q8U093
A	17	GLY	GLU	conflict	UNP Q8U093
A	68	VAL	ILE	conflict	UNP Q8U093
A	95	LEU	PHE	conflict	UNP Q8U093
A	274	SER	PHE	conflict	UNP Q8U093
A	275	GLU	HIS	engineered mutation	UNP Q8U093
A	292	SER	THR	conflict	UNP Q8U093
A	321	ALA	THR	conflict	UNP Q8U093
A	384	ALA	VAL	conflict	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	conflict	UNP Q8U093
B	17	GLY	GLU	conflict	UNP Q8U093
B	68	VAL	ILE	conflict	UNP Q8U093
B	95	LEU	PHE	conflict	UNP Q8U093

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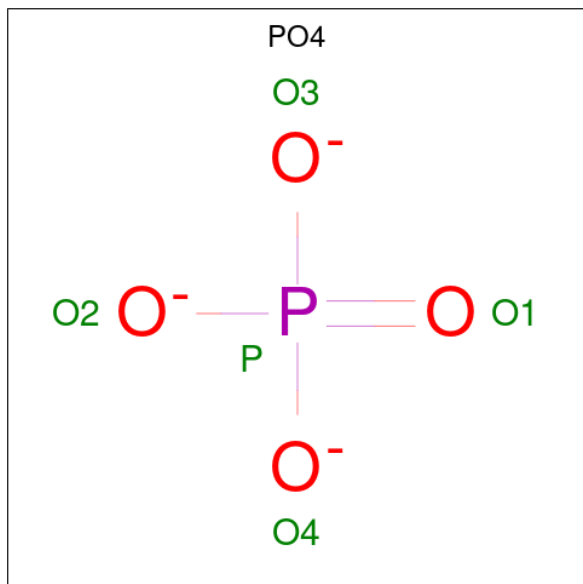
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	SER	PHE	conflict	UNP Q8U093
B	275	GLU	HIS	engineered mutation	UNP Q8U093
B	292	SER	THR	conflict	UNP Q8U093
B	321	ALA	THR	conflict	UNP Q8U093
B	384	ALA	VAL	conflict	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
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	conflict	UNP Q8U093
C	17	GLY	GLU	conflict	UNP Q8U093
C	68	VAL	ILE	conflict	UNP Q8U093
C	95	LEU	PHE	conflict	UNP Q8U093
C	274	SER	PHE	conflict	UNP Q8U093
C	275	GLU	HIS	engineered mutation	UNP Q8U093
C	292	SER	THR	conflict	UNP Q8U093
C	321	ALA	THR	conflict	UNP Q8U093
C	384	ALA	VAL	conflict	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	conflict	UNP Q8U093
D	17	GLY	GLU	conflict	UNP Q8U093
D	68	VAL	ILE	conflict	UNP Q8U093
D	95	LEU	PHE	conflict	UNP Q8U093
D	274	SER	PHE	conflict	UNP Q8U093
D	275	GLU	HIS	engineered mutation	UNP Q8U093
D	292	SER	THR	conflict	UNP Q8U093
D	321	ALA	THR	conflict	UNP Q8U093
D	384	ALA	VAL	conflict	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	expression tag	UNP Q8U093

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Chain	Residue	Modelled	Actual	Comment	Reference
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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

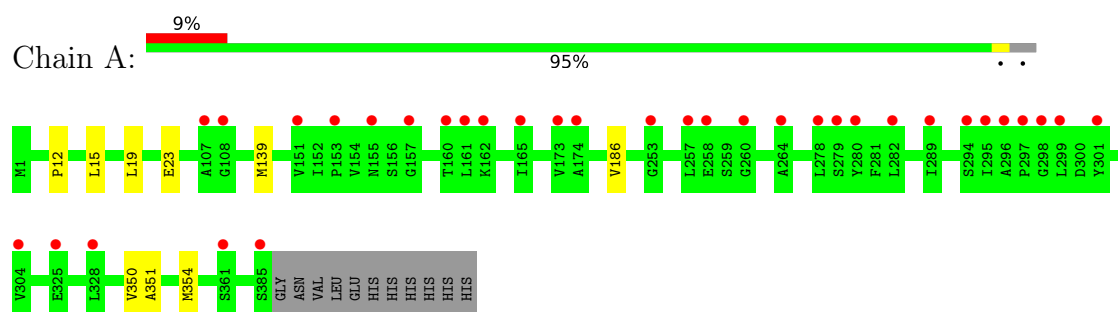
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	135	Total 135	O 135	0	0
4	C	53	Total 53	O 53	0	0
4	D	29	Total 29	O 29	0	0

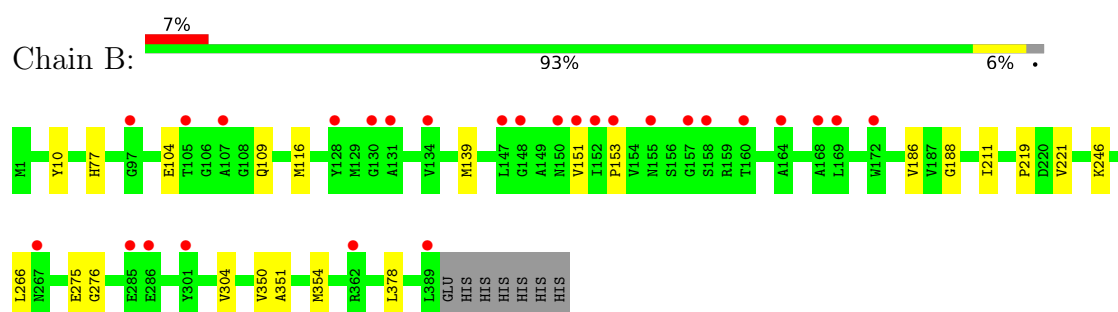
3 Residue-property plots [i](#)

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.

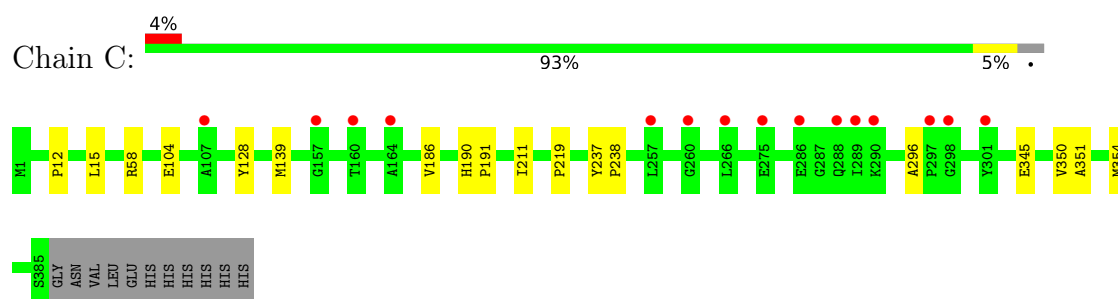
- Molecule 1: Tryptophan synthase beta chain 1



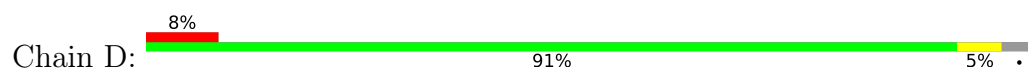
- Molecule 1: Tryptophan synthase beta chain 1

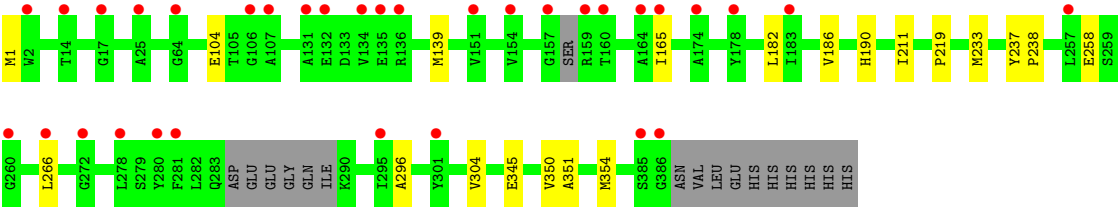


- Molecule 1: Tryptophan synthase beta chain 1



- 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	57.01Å 82.68Å 322.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.10) 99.5 (40.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.214 , 0.248 0.221 , 0.250	Depositor DCC
R_{free} test set	4501 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11732	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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: LLP, PO4, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/2868	1.48	0/3903
1	B	1.00	0/2967	1.44	0/4023
1	C	1.02	0/2894	1.50	0/3931
1	D	1.02	0/2859	1.50	0/3880
All	All	1.02	0/11588	1.48	0/15737

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	2832	0	2687	5	0
1	B	2927	0	2856	10	0
1	C	2858	0	2757	10	0
1	D	2819	0	2717	9	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	55	0	0	0	0
4	B	135	0	0	0	0
4	C	53	0	0	0	0
4	D	29	0	0	0	0
All	All	11732	0	11017	33	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 (33) 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:211:ILE:HG21	1:D:219:PRO:HD3	1.88	0.56
1:B:351:ALA:HA	1:B:354:MET:HE2	1.87	0.56
1:B:221:VAL:HG22	1:B:246:LYS:HE2	1.90	0.54
1:D:1:MET:HB3	1:D:190:HIS:CG	2.46	0.51
1:C:12:PRO:HD2	1:C:15:LEU:HD12	1.94	0.49
1:B:10:TYR:O	1:B:276:GLY:HA2	2.12	0.49
1:D:104:GLU:HG3	1:D:165:ILE:HG12	1.95	0.48
1:C:104:GLU:HA	1:C:128:TYR:O	2.14	0.47
1:D:266:LEU:HG	1:D:304:VAL:HG11	1.96	0.47
1:C:211:ILE:HG21	1:C:219:PRO:HD3	1.95	0.47
1:D:139:MET:HE3	1:D:139:MET:HA	1.97	0.47
1:B:77:HIS:CD2	1:B:116:MET:HE3	2.50	0.47
1:B:211:ILE:HG21	1:B:219:PRO:HD3	1.96	0.46
1:C:350:VAL:O	1:C:354:MET:HG3	2.16	0.45
1:B:188:GLY:HA2	1:B:275:GLU:O	2.16	0.45
1:B:151:VAL:O	1:B:153:PRO:HD3	2.17	0.44
1:A:12:PRO:HD2	1:A:15:LEU:HD12	1.99	0.44
1:A:351:ALA:HA	1:A:354:MET:HE2	1.99	0.43
1:C:190:HIS:CG	1:C:191:PRO:HA	2.53	0.43
1:B:266:LEU:HG	1:B:304:VAL:HG11	2.00	0.43
1:A:350:VAL:O	1:A:354:MET:HG3	2.19	0.42
1:A:19:LEU:O	1:A:23:GLU:HG3	2.20	0.42
1:D:237:TYR:HB3	1:D:238:PRO:HD3	2.01	0.42
1:C:296:ALA:HB1	1:C:345:GLU:HG3	2.02	0.41
1:D:296:ALA:HB1	1:D:345:GLU:HG3	2.02	0.41
1:D:350:VAL:O	1:D:354:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ALA:HA	1:C:354:MET:HE2	2.02	0.41
1:C:237:TYR:HB3	1:C:238:PRO:HD3	2.01	0.41
1:B:350:VAL:O	1:B:354:MET:HG3	2.20	0.41
1:A:139:MET:HE2	1:B:378:LEU:HB3	2.02	0.41
1:C:190:HIS:ND1	1:C:191:PRO:HA	2.36	0.41
1:D:351:ALA:HA	1:D:354:MET:HE2	2.02	0.40
1:C:139:MET:HA	1:C:139:MET:HE2	2.03	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%)	372 (97%)	10 (3%)	1 (0%)	36	36
1	B	389/396 (98%)	379 (97%)	9 (2%)	1 (0%)	36	36
1	C	383/396 (97%)	375 (98%)	7 (2%)	1 (0%)	36	36
1	D	375/396 (95%)	367 (98%)	7 (2%)	1 (0%)	36	36
All	All	1530/1584 (97%)	1493 (98%)	33 (2%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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	268/312 (86%)	268 (100%)	0	100	100
1	B	284/312 (91%)	281 (99%)	3 (1%)	65	74
1	C	275/312 (88%)	274 (100%)	1 (0%)	84	89
1	D	269/312 (86%)	266 (99%)	3 (1%)	65	74
All	All	1096/1248 (88%)	1089 (99%)	7 (1%)	78	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	GLU
1	B	109	GLN
1	B	139	MET
1	C	58	ARG
1	D	182	LEU
1	D	233	MET
1	D	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	B	155	ASN
1	B	270	GLN
1	C	85	ASN
1	C	89	GLN
1	C	109	GLN
1	C	267	ASN
1	D	38	GLN
1	D	89	GLN
1	D	267	ASN

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	A	82	1	23,24,25	0.47	0	25,32,34	0.48	0
1	LLP	B	82	1	23,24,25	0.47	0	25,32,34	0.64	0
1	LLP	C	82	1	23,24,25	0.46	0	25,32,34	0.53	0
1	LLP	D	82	1	23,24,25	0.48	0	25,32,34	0.54	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
1	LLP	A	82	1	-	5/16/17/19	0/1/1/1
1	LLP	B	82	1	-	3/16/17/19	0/1/1/1
1	LLP	C	82	1	-	3/16/17/19	0/1/1/1
1	LLP	D	82	1	-	3/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	82	LLP	C5'-OP4-P-OP1
1	A	82	LLP	C5'-OP4-P-OP3

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Mol	Chain	Res	Type	Atoms
1	B	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	O-C-CA-CB
1	D	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	O-C-CA-CB
1	D	82	LLP	CG-CD-CE-NZ
1	C	82	LLP	C4-C4'-NZ-CE
1	A	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	CG-CD-CE-NZ
1	C	82	LLP	CG-CD-CE-NZ
1	C	82	LLP	C5'-OP4-P-OP1
1	A	82	LLP	CG-CD-CE-NZ
1	A	82	LLP	C5'-OP4-P-OP2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	$\# Z > 2$
2	PO4	B	401	-	4,4,4	0.71	0	6,6,6	0.46	0
2	PO4	C	401	-	4,4,4	0.69	0	6,6,6	0.47	0
2	PO4	D	401	-	4,4,4	0.68	0	6,6,6	0.47	0
2	PO4	A	401	-	4,4,4	0.68	0	6,6,6	0.48	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

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	384/396 (96%)	0.71	34 (8%)	15	16	26, 54, 83, 96	1 (0%)
1	B	388/396 (97%)	0.35	27 (6%)	22	24	17, 37, 70, 102	3 (0%)
1	C	384/396 (96%)	0.56	15 (3%)	43	45	24, 51, 69, 78	1 (0%)
1	D	378/396 (95%)	0.80	33 (8%)	16	16	24, 58, 80, 95	3 (0%)
All	All	1534/1584 (96%)	0.60	109 (7%)	22	23	17, 51, 78, 102	8 (0%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301[A]	TYR	4.4
1	B	155	ASN	4.3
1	A	160	THR	4.0
1	A	108	GLY	3.7
1	D	174	ALA	3.6
1	B	389	LEU	3.5
1	B	285	GLU	3.4
1	B	107	ALA	3.3
1	B	168	ALA	3.3
1	B	160	THR	3.1
1	A	155	ASN	3.1
1	D	301[A]	TYR	3.1
1	A	301	TYR	3.1
1	A	107	ALA	3.1
1	C	301	TYR	3.0
1	D	107	ALA	3.0
1	A	174	ALA	3.0
1	B	158	SER	3.0
1	D	183	ILE	2.9
1	D	266	LEU	2.8
1	A	299	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	64	GLY	2.8
1	B	152	ILE	2.8
1	A	278	LEU	2.8
1	B	147	LEU	2.8
1	B	164	ALA	2.7
1	D	164	ALA	2.7
1	B	153	PRO	2.7
1	D	2	TRP	2.7
1	C	257	LEU	2.7
1	D	386	GLY	2.7
1	B	150	ASN	2.7
1	A	385	SER	2.6
1	A	295	ILE	2.6
1	D	281	PHE	2.6
1	B	134	VAL	2.6
1	C	260	GLY	2.5
1	C	298	GLY	2.5
1	D	257	LEU	2.5
1	A	151	VAL	2.5
1	A	173	VAL	2.5
1	D	106	GLY	2.5
1	B	151	VAL	2.5
1	D	14	THR	2.5
1	C	297	PRO	2.5
1	D	135	GLU	2.4
1	C	107	ALA	2.4
1	A	165	ILE	2.4
1	C	160	THR	2.4
1	B	157	GLY	2.4
1	A	258	GLU	2.4
1	A	289	ILE	2.4
1	D	260	GLY	2.4
1	A	294	SER	2.4
1	B	362	ARG	2.3
1	D	151	VAL	2.3
1	A	297	PRO	2.3
1	A	296	ALA	2.3
1	B	131	ALA	2.3
1	D	280	TYR	2.3
1	A	279	SER	2.3
1	D	134	VAL	2.3
1	C	288	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	253	GLY	2.3
1	A	257	LEU	2.3
1	B	97	GLY	2.3
1	B	128	TYR	2.3
1	C	157	GLY	2.3
1	C	266	LEU	2.3
1	B	172	TRP	2.3
1	B	105	THR	2.2
1	D	136	ARG	2.2
1	A	157	GLY	2.2
1	D	272	GLY	2.2
1	D	132	GLU	2.2
1	D	159	ARG	2.2
1	D	157	GLY	2.2
1	D	278	LEU	2.2
1	A	153	PRO	2.2
1	D	160	THR	2.2
1	D	154	VAL	2.2
1	A	280	TYR	2.2
1	C	289	ILE	2.1
1	A	264	ALA	2.1
1	B	267	ASN	2.1
1	D	165	ILE	2.1
1	D	295	ILE	2.1
1	D	25	ALA	2.1
1	D	385	SER	2.1
1	A	260	GLY	2.1
1	B	130	GLY	2.1
1	B	148	GLY	2.1
1	A	304	VAL	2.1
1	C	164	ALA	2.1
1	A	328	LEU	2.1
1	B	169	LEU	2.1
1	B	286	GLU	2.1
1	C	286	GLU	2.1
1	A	298	GLY	2.1
1	C	290	LYS	2.1
1	A	361	SER	2.1
1	C	275	GLU	2.0
1	D	131	ALA	2.1
1	A	161	LEU	2.0
1	A	282	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	325	GLU	2.0
1	A	162	LYS	2.0
1	D	17	GLY	2.0
1	D	178	TYR	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	D	82	24/25	0.92	0.10	39,44,47,48	0
1	LLP	C	82	24/25	0.94	0.10	34,40,42,43	0
1	LLP	A	82	24/25	0.95	0.08	33,43,47,50	0
1	LLP	B	82	24/25	0.95	0.09	26,29,32,32	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(Å ²)	Q<0.9
2	PO4	A	401	5/5	0.69	0.13	82,83,84,84	0
2	PO4	D	401	5/5	0.79	0.11	76,76,77,77	0
2	PO4	B	401	5/5	0.81	0.14	63,64,65,66	0
2	PO4	C	401	5/5	0.84	0.11	72,72,73,73	0
3	NA	D	402	1/1	0.90	0.09	52,52,52,52	0
3	NA	A	402	1/1	0.91	0.14	57,57,57,57	0
3	NA	C	402	1/1	0.95	0.06	47,47,47,47	0
3	NA	B	402	1/1	0.96	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.