



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 12:57 PM EST

PDB ID : 7RNQ  
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](mailto: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>.

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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 : 2.36  
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

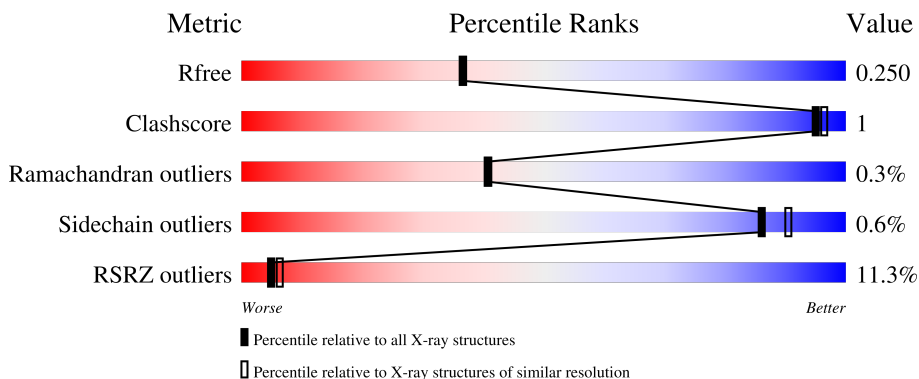
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 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	 12% 95%
1	B	396	 8% 94% 5%
1	C	396	 9% 93%
1	D	396	 14% 91%

## 2 Entry composition i

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
			Total	C	N	O	P	S			
1	A	385	2832	1804	477	538	1	12	0	1	0
1	B	389	2927	1866	503	545	1	12	0	3	0
1	C	385	2858	1820	488	537	1	12	0	1	0
1	D	379	2819	1802	478	526	1	12	0	3	0

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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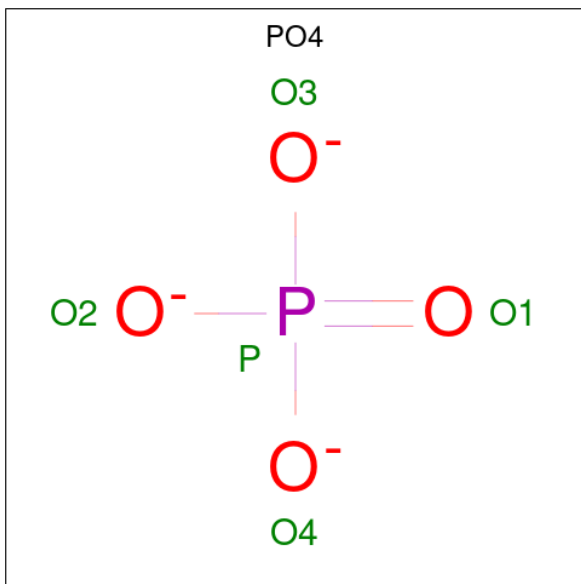
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	SER	PHE	conflict	UNP Q8U093
B	275	GLU	HIS	engineered mutation	UNP Q8U093
B	292	SER	THR	conflict	UNP Q8U093
B	321	ALA	THR	conflict	UNP Q8U093
B	384	ALA	VAL	conflict	UNP Q8U093
B	389	LEU	-	expression tag	UNP Q8U093
B	390	GLU	-	expression tag	UNP Q8U093
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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



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 (three-letter code: 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

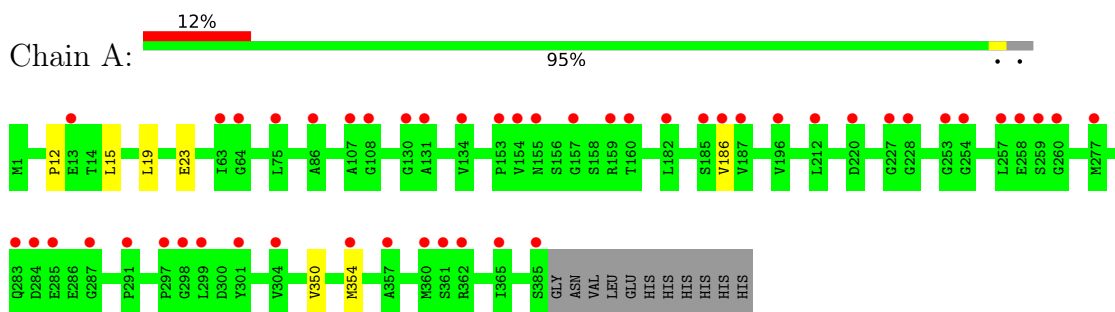
- Molecule 4 is water.

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

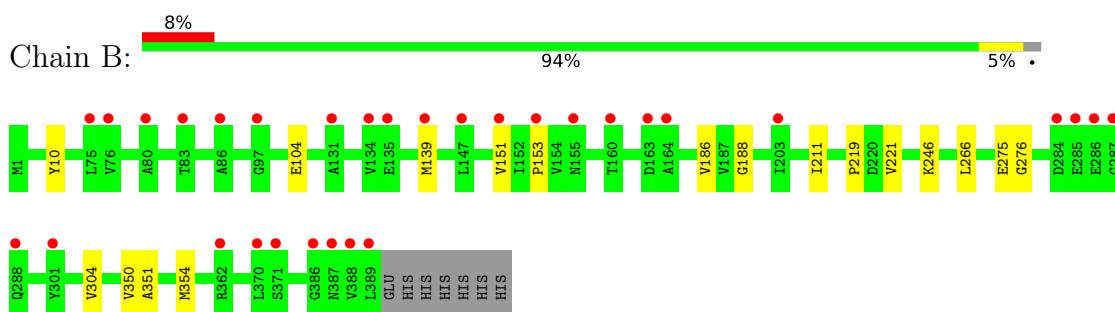
### 3 Residue-property plots [i](#)

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.

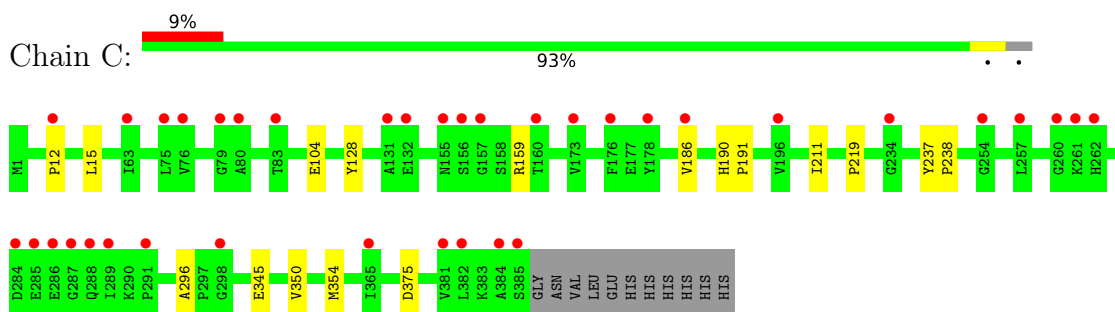
- Molecule 1: Tryptophan synthase beta chain 1



- Molecule 1: Tryptophan synthase beta chain 1

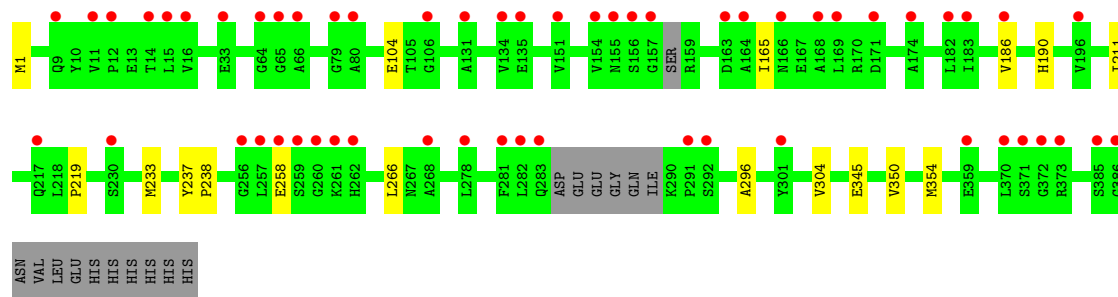


- Molecule 1: Tryptophan synthase beta chain 1



- 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, $\alpha$ , $\beta$ , $\gamma$	57.01Å 82.68Å 322.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.10) 99.5 (39.11-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.10Å)	Xtrriage
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 (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtrriage
Anisotropy	0.328	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, PO4, 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	0.67	0/2868	0.70	0/3903
1	B	0.65	0/2967	0.70	0/4023
1	C	0.67	0/2894	0.70	0/3931
1	D	0.67	0/2859	0.70	0/3880
All	All	0.66	0/11588	0.70	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	3	0
1	B	2927	0	2856	8	0
1	C	2858	0	2757	8	0
1	D	2819	0	2717	7	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	26	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 (26) 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: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:B:211:ILE:HG21	1:B:219:PRO:HD3	1.96	0.46
1:B:351:ALA:HA	1:B:354:MET:HE2	1.98	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: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
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:C:190:HIS:ND1	1:C:191:PRO:HA	2.36	0.41

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	383/396 (97%)	372 (97%)	10 (3%)	1 (0%)	41	41
1	B	389/396 (98%)	379 (97%)	9 (2%)	1 (0%)	41	41
1	C	383/396 (97%)	375 (98%)	7 (2%)	1 (0%)	41	41
1	D	375/396 (95%)	367 (98%)	7 (2%)	1 (0%)	41	41
All	All	1530/1584 (97%)	1493 (98%)	33 (2%)	4 (0%)	41	41

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 [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	268/312 (86%)	268 (100%)	0	100	100
1	B	284/312 (91%)	282 (99%)	2 (1%)	84	88
1	C	275/312 (88%)	273 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	269/312 (86%)	267 (99%)	2 (1%)	84	88
All	All	1096/1248 (88%)	1090 (100%)	6 (0%)	86	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	GLU
1	B	139	MET
1	C	159	ARG
1	C	375	ASP
1	D	233	MET
1	D	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	GLN
1	D	38	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](#)

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	0.46	0	25,32,34	0.48	0
1	LLP	B	82	1	23,24,25	0.45	0	25,32,34	0.63	0
1	LLP	C	82	1	23,24,25	0.45	0	25,32,34	0.52	0
1	LLP	D	82	1	23,24,25	0.47	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
1	B	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	O-C-CA-CB
1	C	82	LLP	C4-C4'-NZ-CE
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	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	D	401	-	4,4,4	0.64	0	6,6,6	0.44	0
2	PO4	B	401	-	4,4,4	0.67	0	6,6,6	0.43	0
2	PO4	C	401	-	4,4,4	0.65	0	6,6,6	0.43	0
2	PO4	A	401	-	4,4,4	0.63	0	6,6,6	0.44	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	384/396 (96%)	0.84	49 (12%) <b>3</b> <b>4</b>	27, 54, 83, 96	0
1	B	388/396 (97%)	0.56	31 (7%) <b>12</b> <b>16</b>	22, 37, 70, 102	0
1	C	384/396 (96%)	0.76	37 (9%) <b>8</b> <b>10</b>	33, 51, 69, 78	0
1	D	378/396 (95%)	0.90	56 (14%) <b>2</b> <b>3</b>	34, 58, 80, 95	0
All	All	1534/1584 (96%)	0.76	173 (11%) <b>5</b> <b>6</b>	22, 51, 78, 102	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	174	ALA	5.7
1	D	291	PRO	5.2
1	D	260	GLY	4.9
1	A	299	LEU	4.9
1	A	298	GLY	4.6
1	A	260	GLY	4.4
1	A	131	ALA	4.3
1	D	164	ALA	4.3
1	D	259	SER	4.3
1	D	301[A]	TYR	4.2
1	D	15	LEU	4.1
1	B	287	GLY	4.0
1	C	157	GLY	4.0
1	A	284	ASP	4.0
1	B	131	ALA	4.0
1	C	257	LEU	3.9
1	C	285	GLU	3.9
1	D	257	LEU	3.9
1	A	157	GLY	3.7
1	C	160	THR	3.7
1	C	288	GLN	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	259	SER	3.7
1	D	261	LYS	3.7
1	C	196	VAL	3.7
1	A	155	ASN	3.7
1	D	155	ASN	3.7
1	A	285	GLU	3.6
1	C	260	GLY	3.6
1	C	382	LEU	3.6
1	D	156	SER	3.5
1	B	285	GLU	3.4
1	B	387	ASN	3.4
1	C	289	ILE	3.4
1	B	388	VAL	3.4
1	A	287	GLY	3.4
1	C	186	VAL	3.4
1	C	286	GLU	3.3
1	A	283	GLN	3.3
1	D	157	GLY	3.3
1	A	360	MET	3.3
1	D	385	SER	3.3
1	C	63	ILE	3.3
1	A	154	VAL	3.3
1	D	135	GLU	3.3
1	C	156	SER	3.2
1	A	186	VAL	3.2
1	B	75	LEU	3.2
1	D	64	GLY	3.2
1	C	384	ALA	3.2
1	D	371	SER	3.2
1	A	357	ALA	3.1
1	D	80	ALA	3.1
1	D	14	THR	3.1
1	A	361	SER	3.1
1	A	160	THR	3.1
1	B	301[A]	TYR	3.1
1	D	256	GLY	3.1
1	A	196	VAL	3.1
1	C	254	GLY	3.0
1	A	63	ILE	3.0
1	C	155	ASN	3.0
1	C	176	PHE	3.0
1	D	12	PRO	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	134	VAL	2.9
1	C	287	GLY	2.9
1	D	281	PHE	2.9
1	A	108	GLY	2.9
1	B	370	LEU	2.9
1	D	268	ALA	2.9
1	D	282	LEU	2.9
1	A	153	PRO	2.9
1	C	132	GLU	2.9
1	D	183	ILE	2.8
1	C	178	TYR	2.8
1	B	389	LEU	2.8
1	D	386	GLY	2.8
1	B	155	ASN	2.8
1	D	283	GLN	2.8
1	D	166	ASN	2.8
1	A	75	LEU	2.8
1	D	186	VAL	2.7
1	D	131	ALA	2.7
1	A	365	ILE	2.7
1	D	262	HIS	2.7
1	D	79	GLY	2.7
1	A	257	LEU	2.7
1	D	168	ALA	2.7
1	D	370	LEU	2.7
1	C	131	ALA	2.6
1	B	386	GLY	2.6
1	A	253	GLY	2.6
1	B	135	GLU	2.6
1	D	106	GLY	2.6
1	C	261	LYS	2.6
1	C	284	ASP	2.5
1	A	301	TYR	2.5
1	A	258	GLU	2.5
1	A	277	MET	2.5
1	D	359	GLU	2.5
1	A	185	SER	2.5
1	A	227	GLY	2.5
1	C	291	PRO	2.5
1	B	362	ARG	2.5
1	B	76	VAL	2.5
1	B	153	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	64	GLY	2.5
1	D	196	VAL	2.4
1	D	171	ASP	2.4
1	A	304	VAL	2.4
1	D	278	LEU	2.4
1	C	365	ILE	2.4
1	B	160	THR	2.4
1	A	254	GLY	2.4
1	B	151	VAL	2.4
1	D	163	ASP	2.4
1	A	86	ALA	2.4
1	C	173	VAL	2.4
1	C	80	ALA	2.4
1	A	362	ARG	2.4
1	A	130	GLY	2.4
1	D	258	GLU	2.3
1	B	288	GLN	2.3
1	B	80	ALA	2.3
1	B	163	ASP	2.3
1	B	203	ILE	2.3
1	B	371	SER	2.3
1	C	385	SER	2.3
1	A	13	GLU	2.3
1	A	228	GLY	2.3
1	A	212	LEU	2.3
1	D	66	ALA	2.3
1	D	9	GLN	2.3
1	C	83	THR	2.2
1	C	262	HIS	2.2
1	A	159	ARG	2.2
1	B	286	GLU	2.2
1	B	97	GLY	2.2
1	D	11	VAL	2.2
1	C	12	PRO	2.2
1	D	134	VAL	2.2
1	A	220	ASP	2.2
1	D	373[A]	ARG	2.2
1	D	169	LEU	2.2
1	B	147	LEU	2.2
1	A	134	VAL	2.2
1	C	381	VAL	2.2
1	A	385	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	86	ALA	2.1
1	A	291	PRO	2.1
1	C	298	GLY	2.1
1	B	139	MET	2.1
1	D	217	GLN	2.1
1	D	372	GLY	2.1
1	C	75	LEU	2.1
1	D	292	SER	2.1
1	A	297	PRO	2.1
1	C	76	VAL	2.1
1	D	65	GLY	2.1
1	D	230	SER	2.0
1	B	83	THR	2.0
1	B	164	ALA	2.0
1	D	154	VAL	2.0
1	A	354	MET	2.0
1	A	182	LEU	2.0
1	D	33	GLU	2.0
1	D	151	VAL	2.0
1	A	107	ALA	2.0
1	D	182	LEU	2.0
1	A	187	VAL	2.0
1	B	284	ASP	2.0
1	C	79	GLY	2.0
1	C	234	GLY	2.0
1	D	16	VAL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	B	82	24/25	0.94	0.21	26,29,32,32	0
1	LLP	C	82	24/25	0.94	0.21	34,40,42,43	0
1	LLP	D	82	24/25	0.94	0.23	39,44,47,48	0
1	LLP	A	82	24/25	0.95	0.21	33,43,47,50	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NA	D	402	1/1	0.79	0.16	52,52,52,52	0
2	PO4	A	401	5/5	0.87	0.22	82,83,84,84	0
2	PO4	B	401	5/5	0.90	0.16	63,64,65,66	0
2	PO4	D	401	5/5	0.92	0.14	76,76,77,77	0
3	NA	A	402	1/1	0.95	0.31	57,57,57,57	0
2	PO4	C	401	5/5	0.96	0.10	72,72,73,73	0
3	NA	C	402	1/1	0.97	0.14	47,47,47,47	0
3	NA	B	402	1/1	0.97	0.13	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.