



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 01:22 PM EDT

PDB ID : 5DW3
Title : Tryptophan Synthase beta-subunit from *Pyrococcus furiosus* with product L-tryptophan non-covalently bound in the active site
Authors : Buller, A.R.; Arnold, F.H.
Deposited on : 2015-09-22
Resolution : 1.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

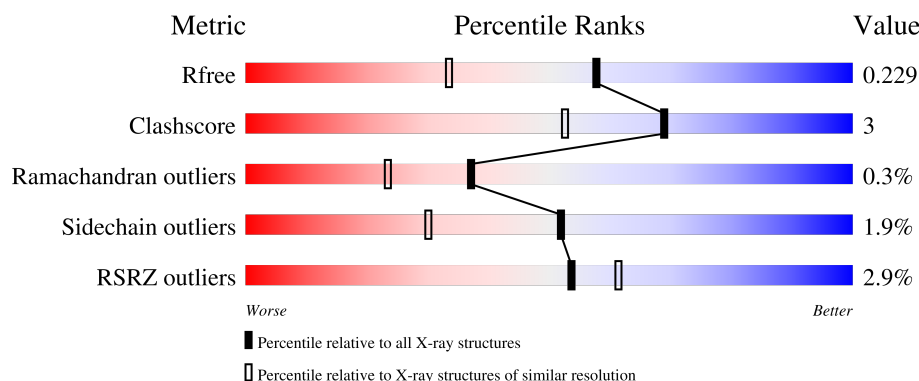
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


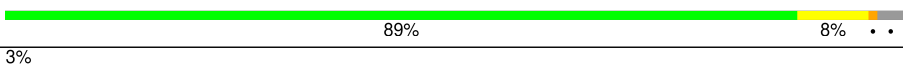
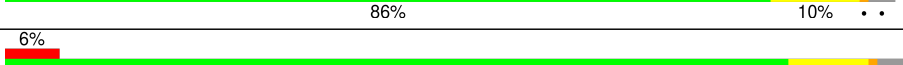

The reported resolution of this entry is 1.74 Å.

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}	164625	1043 (1.74-1.74)
Clashscore	180529	1119 (1.74-1.74)
Ramachandran outliers	177936	1112 (1.74-1.74)
Sidechain outliers	177891	1112 (1.74-1.74)
RSRZ outliers	164620	1043 (1.74-1.74)

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 5 unique types of molecules in this entry. The entry contains 12060 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	383	Total	C	N	O	P	S	0	1	0
			2930	1873	500	544	1	12			
1	B	386	Total	C	N	O	P	S	0	2	0
			2976	1898	515	550	1	12			
1	C	384	Total	C	N	O	P	S	0	1	0
			2914	1862	496	543	1	12			
1	D	384	Total	C	N	O	P	S	0	0	0
			2865	1830	489	533	1	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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

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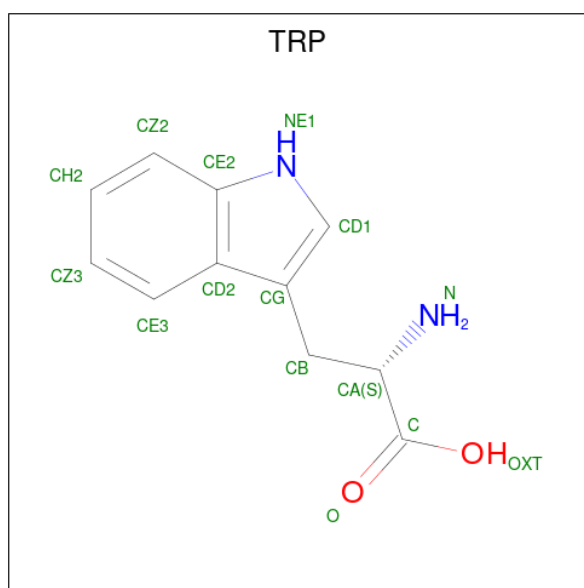
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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP Q8U093
C	395	HIS	-	expression tag	UNP Q8U093
C	396	HIS	-	expression tag	UNP Q8U093
D	389	LEU	-	expression tag	UNP Q8U093
D	390	GLU	-	expression tag	UNP Q8U093
D	391	HIS	-	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 (three-letter code: NA) (formula: Na).

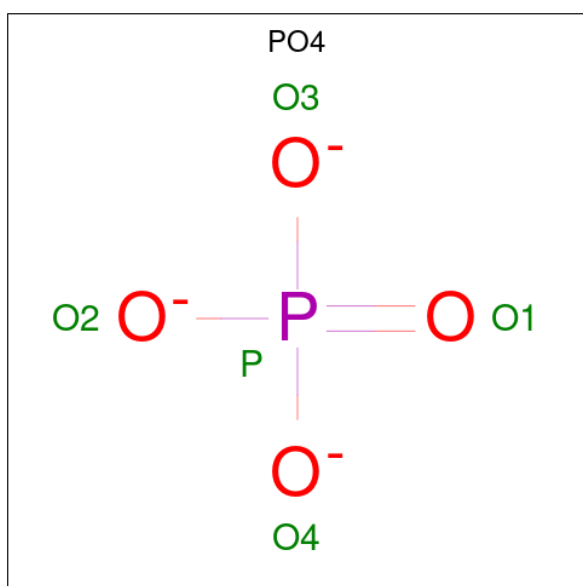
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	1
			15	11	2	2		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

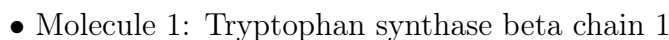


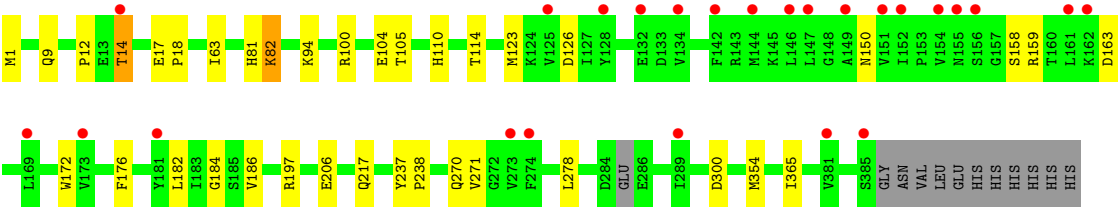
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	P	0	1
			5	4	1		
4	D	1	Total	O	P	0	1
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total	O	0	0
			103	103		
5	B	94	Total	O	0	2
			94	94		
5	C	51	Total	O	0	0
			51	51		
5	D	53	Total	O	0	0
			53	53		

- 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	83.74Å 108.93Å 160.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.74 40.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-1.74) 98.5 (40.00-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.185 , 0.224 0.193 , 0.229	Depositor DCC
R_{free} test set	7347 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12060	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.10% 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	0.97	0/2968	0.94	2/4014 (0.0%)
1	B	1.00	1/3014 (0.0%)	0.98	9/4072 (0.2%)
1	C	1.03	4/2953 (0.1%)	0.94	2/4002 (0.0%)
1	D	0.94	2/2898 (0.1%)	0.91	3/3928 (0.1%)
All	All	0.98	7/11833 (0.1%)	0.94	16/16016 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	GLU	CD-OE1	7.44	1.33	1.25
1	D	206	GLU	CD-OE1	6.86	1.33	1.25
1	C	5	GLU	CD-OE1	6.47	1.32	1.25
1	C	201	SER	CB-OG	-5.84	1.34	1.42
1	C	280	TYR	CB-CG	-5.79	1.43	1.51
1	C	104	GLU	CD-OE2	5.44	1.31	1.25
1	D	104	GLU	CD-OE1	5.20	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	336	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	143[A]	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	143[B]	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	373	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	197	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	D	197	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	B	354	MET	CG-SD-CE	5.85	109.57	100.20
1	C	100	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	58	ARG	NE-CZ-NH2	-5.53	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	D	197	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	D	100	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	76	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	C	198	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	197	ARG	NE-CZ-NH2	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2930	0	2896	21	0
1	B	2976	0	2956	18	0
1	C	2914	0	2839	23	0
1	D	2865	0	2772	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	15	0	9	1	0
3	B	15	0	9	0	0
3	C	15	0	9	2	0
3	D	15	0	9	1	0
4	C	5	0	0	1	0
4	D	5	0	0	1	0
5	A	103	0	0	2	0
5	B	94	0	0	4	0
5	C	51	0	0	0	0
5	D	53	0	0	1	0
All	All	12060	0	11499	78	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 3.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:NZ	1:A:318:GLU:OE1	2.18	0.77
1:C:105:THR:HA	4:C:403[B]:PO4:O2	1.87	0.73
1:C:109:GLN:HB2	3:C:402:TRP:O	1.93	0.69
1:B:73:GLU:O	1:B:76:VAL:HG12	1.95	0.65
1:D:94:LYS:HB2	1:D:123:MET:HE1	1.80	0.62
1:D:63:ILE:HD11	1:D:354:MET:HG2	1.82	0.62
1:C:177:GLU:H	1:C:177:GLU:CD	2.04	0.61
1:D:217:GLN:HE21	1:D:365:ILE:HD12	1.65	0.60
1:C:16:ILE:O	1:C:20:LYS:HG2	2.00	0.60
1:C:359:GLU:O	1:C:360:MET:HG3	2.04	0.58
1:C:165:ILE:HG21	1:C:275[A]:HIS:CD2	2.39	0.58
1:A:170:ARG:O	1:A:173:VAL:HG22	2.05	0.57
1:B:109[B]:GLN:HG2	5:B:509:HOH:O	2.04	0.57
1:B:143[B]:ARG:NH1	5:B:501:HOH:O	2.18	0.56
1:A:181:TYR:CZ	1:A:183:ILE:HG12	2.42	0.55
1:C:12:PRO:HB2	1:C:14:THR:HG22	1.88	0.55
1:B:77:HIS:NE2	1:B:116:MET:CE	2.70	0.54
1:B:133:ASP:OD1	1:B:136:ARG:NH2	2.39	0.54
1:A:177:GLU:H	1:A:177:GLU:CD	2.11	0.53
1:D:172:TRP:O	1:D:176:PHE:HB3	2.09	0.53
1:A:77:HIS:CD2	1:A:116:MET:CE	2.93	0.52
1:D:12:PRO:HG2	1:D:14:THR:HG23	1.92	0.52
1:A:181:TYR:CE2	1:A:183:ILE:HD11	2.44	0.52
1:A:94:LYS:HB2	1:A:123:MET:CE	2.40	0.51
1:C:325:GLU:O	1:C:329:LYS:HG3	2.10	0.51
1:A:177:GLU:HG2	5:A:594:HOH:O	2.10	0.51
1:A:300:ASP:OD1	1:A:300:ASP:C	2.47	0.51
1:D:82:LLP:HE2	5:D:521:HOH:O	2.11	0.50
1:C:66:ALA:HA	1:C:361:SER:O	2.12	0.49
1:C:110:HIS:CE1	1:C:184:GLY:HA2	2.47	0.49
1:B:271:VAL:CG1	1:B:278:LEU:HD11	2.43	0.48
1:D:271:VAL:HG12	1:D:278:LEU:HD11	1.96	0.48
1:A:284:ASP:OD1	1:A:286:GLU:N	2.46	0.47
1:C:174:ALA:O	1:C:177:GLU:OE2	2.31	0.47
1:D:114:THR:HG23	1:D:182:LEU:HD13	1.97	0.47
1:D:82:LLP:HE3	3:D:402[A]:TRP:HB2	1.95	0.46
1:D:126:ASP:OD1	1:D:150:ASN:HB2	2.15	0.46
1:A:28:ARG:HD3	1:A:29:PHE:CZ	2.50	0.46
1:A:1:MET:HA	1:A:190:HIS:ND1	2.31	0.46
1:C:82:LLP:O3	1:C:82:LLP:NZ	2.49	0.45
1:C:23:GLU:HG2	1:C:27:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:TYR:HB3	1:D:238:PRO:HD3	1.99	0.45
1:A:274:PHE:CD2	1:A:289:ILE:HD12	2.51	0.45
1:B:110:HIS:CE1	1:B:184:GLY:HA2	2.52	0.45
1:C:165:ILE:CG2	1:C:275[A]:HIS:CD2	2.99	0.45
1:A:109:GLN:HB2	3:A:402:TRP:OXT	2.17	0.45
1:C:2:TRP:HH2	1:C:10:TYR:HH	1.64	0.45
1:B:211:ILE:HG21	1:B:219:PRO:HD3	1.99	0.44
1:A:110:HIS:CE1	1:A:184:GLY:HA2	2.52	0.44
1:B:246:LYS:NZ	1:B:318:GLU:OE1	2.47	0.44
1:A:82:LLP:HE2	5:A:539:HOH:O	2.18	0.43
1:B:69:TYR:OH	1:B:215:GLU:OE2	2.29	0.43
1:C:165:ILE:HG21	1:C:275[A]:HIS:CG	2.52	0.43
1:B:82:LLP:HE2	5:B:515:HOH:O	2.19	0.43
1:B:143[B]:ARG:NE	5:B:501:HOH:O	2.48	0.43
1:C:284:ASP:N	1:C:288:GLN:O	2.41	0.43
1:A:158:SER:O	1:A:160:THR:HG23	2.19	0.43
1:D:1:MET:HE3	1:D:9:GLN:N	2.33	0.43
1:B:351:ALA:HA	1:B:354:MET:HE2	2.01	0.42
1:A:183:ILE:HD12	1:A:192:TYR:CD2	2.55	0.42
1:C:12:PRO:HD2	1:C:15:LEU:HD12	2.00	0.42
1:D:110:HIS:CE1	1:D:184:GLY:HA2	2.55	0.42
1:A:73:GLU:O	1:A:76:VAL:HG12	2.20	0.42
1:D:81:HIS:O	1:D:82:LLP:C	2.67	0.42
1:A:38:GLN:NE2	1:C:33:GLU:OE1	2.53	0.41
1:C:160:THR:OG1	1:C:161:LEU:N	2.50	0.41
1:B:170:ARG:O	1:B:173:VAL:HG22	2.20	0.41
1:B:77:HIS:NE2	1:B:116:MET:HE2	2.36	0.41
1:C:82:LLP:HD2	1:C:110:HIS:HA	2.03	0.41
1:D:82:LLP:O3	1:D:82:LLP:NZ	2.53	0.41
1:B:155:ASN:HA	1:B:159:ARG:HG2	2.02	0.41
1:D:17:GLU:N	1:D:18:PRO:HD2	2.36	0.41
1:B:82:LLP:O3	1:B:82:LLP:NZ	2.54	0.40
1:A:181:TYR:CE2	1:A:183:ILE:CG1	3.05	0.40
1:B:62:LYS:NZ	1:B:333:GLU:OE2	2.37	0.40
1:C:301:TYR:HB2	3:C:402:TRP:CZ3	2.57	0.40
1:D:105:THR:OG1	4:D:403[B]:PO4:O3	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	379/396 (96%)	368 (97%)	10 (3%)	1 (0%)	37	23
1	B	383/396 (97%)	375 (98%)	7 (2%)	1 (0%)	37	23
1	C	380/396 (96%)	370 (97%)	8 (2%)	2 (0%)	25	11
1	D	379/396 (96%)	369 (97%)	9 (2%)	1 (0%)	37	23
All	All	1521/1584 (96%)	1482 (97%)	34 (2%)	5 (0%)	37	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	GLU
1	C	186	VAL
1	D	186	VAL
1	A	186	VAL
1	B	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	292/315 (93%)	285 (98%)	7 (2%)	44	20
1	B	298/315 (95%)	296 (99%)	2 (1%)	81	74
1	C	286/315 (91%)	280 (98%)	6 (2%)	48	25
1	D	274/315 (87%)	268 (98%)	6 (2%)	47	23
All	All	1150/1260 (91%)	1129 (98%)	21 (2%)	52	32

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	14	THR
1	A	244	LYS
1	A	258	GLU
1	A	289	ILE
1	A	333	GLU
1	A	361	SER
1	B	30	LYS
1	B	288	GLN
1	C	5	GLU
1	C	28	ARG
1	C	177	GLU
1	C	270	GLN
1	C	300	ASP
1	C	385	SER
1	D	14	THR
1	D	158	SER
1	D	159	ARG
1	D	163	ASP
1	D	270	GLN
1	D	300	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	D	217	GLN

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	B	82	1	23,24,25	1.79	7 (30%)	25,32,34	1.85	6 (24%)
1	LLP	C	82	1	23,24,25	1.97	6 (26%)	25,32,34	1.82	9 (36%)
1	LLP	D	82	1	23,24,25	1.91	6 (26%)	25,32,34	1.51	5 (20%)
1	LLP	A	82	1	23,24,25	2.24	6 (26%)	25,32,34	1.90	9 (36%)

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	B	82	1	-	2/16/17/19	0/1/1/1
1	LLP	C	82	1	-	2/16/17/19	0/1/1/1
1	LLP	D	82	1	-	3/16/17/19	0/1/1/1
1	LLP	A	82	1	-	4/16/17/19	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	LLP	C3-C2	6.00	1.47	1.41
1	C	82	LLP	C3-C2	5.64	1.46	1.41
1	A	82	LLP	C4-C3	5.52	1.50	1.41
1	A	82	LLP	C4'-NZ	4.42	1.42	1.27
1	B	82	LLP	C4'-NZ	4.34	1.41	1.27
1	D	82	LLP	C4-C3	4.28	1.48	1.41
1	D	82	LLP	C4'-NZ	4.15	1.41	1.27
1	C	82	LLP	C4-C3	3.79	1.47	1.41
1	C	82	LLP	C4'-NZ	3.37	1.38	1.27
1	D	82	LLP	C4-C5	3.27	1.46	1.42
1	A	82	LLP	C4-C5	3.16	1.46	1.42
1	B	82	LLP	C3-C2	2.94	1.44	1.41
1	B	82	LLP	C4-C3	2.91	1.45	1.41
1	B	82	LLP	C4-C5	2.83	1.45	1.42
1	B	82	LLP	CB-CA	2.73	1.57	1.53
1	C	82	LLP	C4-C4'	2.62	1.52	1.46
1	D	82	LLP	C3-C2	2.54	1.43	1.41
1	D	82	LLP	C4-C4'	2.54	1.52	1.46
1	C	82	LLP	C6-C5	2.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	LLP	P-OP3	-2.29	1.46	1.54
1	B	82	LLP	CE-NZ	-2.29	1.41	1.46
1	A	82	LLP	O3-C3	-2.26	1.31	1.36
1	C	82	LLP	O3-C3	-2.17	1.31	1.36
1	A	82	LLP	P-OP1	2.06	1.56	1.50
1	D	82	LLP	O3-C3	-2.04	1.32	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	LLP	C6-N1-C2	4.24	126.88	119.20
1	B	82	LLP	C2'-C2-N1	3.81	124.83	117.64
1	C	82	LLP	C2'-C2-N1	3.54	124.31	117.64
1	A	82	LLP	C2'-C2-N1	3.44	124.12	117.64
1	A	82	LLP	C4-C4'-NZ	-3.44	108.19	124.04
1	B	82	LLP	C3-C2-N1	-3.41	116.66	120.96
1	D	82	LLP	C4-C4'-NZ	-3.30	108.82	124.04
1	B	82	LLP	C4-C3-C2	-3.24	118.32	120.14
1	C	82	LLP	C3-C2-N1	-3.12	117.03	120.96
1	A	82	LLP	C5'-C5-C6	3.09	124.40	119.36
1	A	82	LLP	OP3-P-OP1	2.91	122.17	110.83
1	A	82	LLP	C4-C3-C2	-2.80	118.57	120.14
1	C	82	LLP	C6-N1-C2	2.68	124.05	119.20
1	A	82	LLP	C3-C2-N1	-2.59	117.69	120.96
1	A	82	LLP	OP4-C5'-C5	2.58	114.19	109.36
1	D	82	LLP	OP3-P-OP4	-2.58	99.94	106.67
1	A	82	LLP	C6-N1-C2	2.58	123.87	119.20
1	C	82	LLP	C4-C4'-NZ	-2.50	112.49	124.04
1	C	82	LLP	OP4-C5'-C5	2.48	114.00	109.36
1	D	82	LLP	O3-C3-C2	2.40	122.56	117.58
1	B	82	LLP	OP4-C5'-C5	2.37	113.80	109.36
1	C	82	LLP	OP3-P-OP4	-2.36	100.51	106.67
1	C	82	LLP	OP3-P-OP2	2.35	116.62	107.80
1	A	82	LLP	C2'-C2-C3	-2.24	118.18	120.80
1	B	82	LLP	C4-C4'-NZ	-2.19	113.91	124.04
1	D	82	LLP	C6-N1-C2	2.14	123.07	119.20
1	D	82	LLP	C4-C3-C2	-2.09	118.97	120.14
1	C	82	LLP	CD-CG-CB	-2.09	105.76	113.62
1	C	82	LLP	C5-C4-C4'	-2.02	118.36	121.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	82	LLP	O-C-CA-CB
1	A	82	LLP	C4-C4'-NZ-CE
1	D	82	LLP	C4-C4'-NZ-CE
1	B	82	LLP	C4-C4'-NZ-CE
1	C	82	LLP	C4-C4'-NZ-CE
1	A	82	LLP	CD-CE-NZ-C4'
1	D	82	LLP	CD-CE-NZ-C4'
1	A	82	LLP	CG-CD-CE-NZ
1	D	82	LLP	C3-C4-C4'-NZ
1	A	82	LLP	C3-C4-C4'-NZ
1	B	82	LLP	C3-C4-C4'-NZ

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	82	LLP	2	0
1	C	82	LLP	2	0
1	D	82	LLP	4	0
1	A	82	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	TRP	B	402	-	14,16,16	1.69	3 (21%)	13,22,22	1.08	1 (7%)
4	PO4	D	403[B]	-	4,4,4	1.01	0	6,6,6	0.51	0
4	PO4	C	403[B]	3	4,4,4	1.27	0	6,6,6	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRP	D	402[A]	-	14,16,16	0.94	1 (7%)	13,22,22	1.30	2 (15%)
3	TRP	C	402	4	14,16,16	1.53	3 (21%)	13,22,22	1.38	2 (15%)
3	TRP	A	402	-	14,16,16	1.24	3 (21%)	13,22,22	0.92	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
3	TRP	D	402[A]	-	-	0/7/8/8	0/2/2/2
3	TRP	B	402	-	-	1/7/8/8	0/2/2/2
3	TRP	C	402	4	-	2/7/8/8	0/2/2/2
3	TRP	A	402	-	-	0/7/8/8	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	TRP	OXT-C	-3.82	1.18	1.30
3	B	402	TRP	CZ3-CE3	3.42	1.43	1.36
3	C	402	TRP	OXT-C	-3.36	1.19	1.30
3	B	402	TRP	CB-CG	-2.76	1.44	1.51
3	D	402[A]	TRP	OXT-C	-2.65	1.22	1.30
3	C	402	TRP	CB-CG	2.41	1.57	1.51
3	A	402	TRP	CZ3-CE3	2.28	1.41	1.36
3	A	402	TRP	OXT-C	-2.18	1.23	1.30
3	A	402	TRP	O-C	-2.16	1.15	1.22
3	C	402	TRP	CZ2-CE2	-2.15	1.38	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402[A]	TRP	OXT-C-O	-3.44	116.27	124.08
3	C	402	TRP	CH2-CZ2-CE2	-2.64	116.47	120.09
3	C	402	TRP	CZ3-CE3-CD2	-2.46	117.59	120.91
3	B	402	TRP	CZ3-CE3-CD2	-2.22	117.91	120.91
3	D	402[A]	TRP	CH2-CZ2-CE2	-2.07	117.25	120.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	TRP	CA-CB-CG-CD1
3	C	402	TRP	N-CA-CB-CG
3	B	402	TRP	OXT-C-CA-N

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	403[B]	PO4	1	0
4	C	403[B]	PO4	1	0
3	D	402[A]	TRP	1	0
3	C	402	TRP	2	0
3	A	402	TRP	1	0

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	382/396 (96%)	0.23	6 (1%) 70 76	20, 37, 57, 93	1 (0%)
1	B	385/396 (97%)	-0.03	1 (0%) 90 93	14, 34, 54, 69	2 (0%)
1	C	383/396 (96%)	0.41	13 (3%) 48 56	23, 42, 70, 89	2 (0%)
1	D	383/396 (96%)	0.52	25 (6%) 26 32	24, 43, 80, 118	0
All	All	1533/1584 (96%)	0.28	45 (2%) 54 61	14, 39, 68, 118	5 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	VAL	4.9
1	C	274	PHE	4.7
1	C	59	LEU	3.9
1	D	161	LEU	3.9
1	C	284	ASP	3.7
1	D	154	VAL	3.6
1	D	149	ALA	3.4
1	D	147	LEU	3.3
1	D	289	ILE	3.2
1	D	125	VAL	3.2
1	C	245	VAL	3.0
1	D	156	SER	2.9
1	C	69	TYR	2.9
1	C	289	ILE	2.9
1	D	128	TYR	2.8
1	D	162	LYS	2.7
1	D	146	LEU	2.7
1	D	14	THR	2.7
1	D	134	VAL	2.7
1	D	152	ILE	2.6
1	D	385	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	132	GLU	2.6
1	D	155	ASN	2.6
1	A	286	GLU	2.6
1	C	287	GLY	2.6
1	D	173	VAL	2.5
1	A	14	THR	2.5
1	A	274	PHE	2.4
1	D	274	PHE	2.4
1	D	151	VAL	2.4
1	B	63	ILE	2.4
1	D	381	VAL	2.4
1	C	68	ILE	2.3
1	C	286	GLU	2.3
1	D	169	LEU	2.3
1	A	300	ASP	2.2
1	C	221	VAL	2.2
1	A	288	GLN	2.2
1	C	214	ALA	2.2
1	C	212	LEU	2.2
1	D	273	VAL	2.1
1	D	142	PHE	2.1
1	D	181	TYR	2.1
1	D	144	MET	2.0
1	C	28	ARG	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	A	82	24/25	0.96	0.07	24,26,29,31	0
1	LLP	D	82	24/25	0.97	0.07	27,29,33,35	0
1	LLP	C	82	24/25	0.98	0.05	22,25,26,27	0
1	LLP	B	82	24/25	0.98	0.05	21,24,26,28	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
3	TRP	D	402[A]	15/15	0.81	0.30	39,41,44,46	15
4	PO4	D	403[B]	5/5	0.87	0.11	51,59,63,64	5
2	NA	C	401	1/1	0.89	0.10	37,37,37,37	0
3	TRP	C	402	15/15	0.89	0.12	29,32,33,33	15
4	PO4	C	403[B]	5/5	0.92	0.10	29,30,32,35	5
2	NA	B	401	1/1	0.93	0.07	35,35,35,35	0
3	TRP	A	402	15/15	0.93	0.08	32,34,36,37	0
2	NA	D	401	1/1	0.96	0.07	41,41,41,41	0
3	TRP	B	402	15/15	0.96	0.07	27,29,31,31	0
2	NA	A	401	1/1	0.97	0.05	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.