



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:57 PM UTC

PDB ID : 4JFA / pdb_00004jfa
Title : Crystal Structure of Plasmodium falciparum Tryptophanyl-tRNA synthetase
Authors : Khan, S.; Garg, A.; Manickam, Y.; Sharma, A.
Deposited on : 2013-02-28
Resolution : 2.60 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

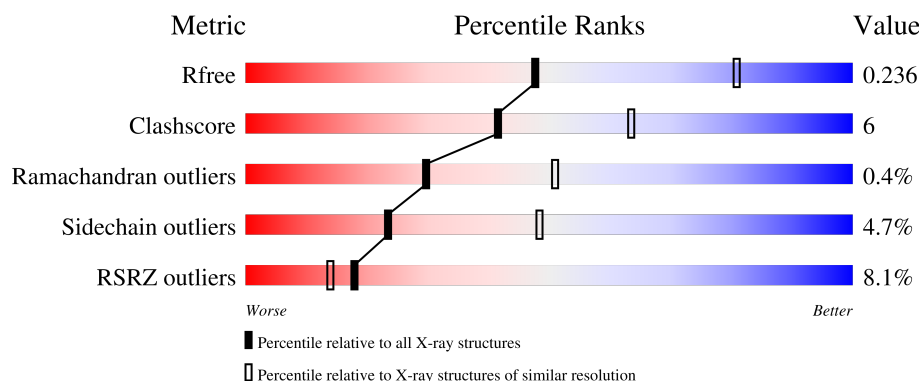
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	420	4% 71% 13% • 14%
1	B	420	4% 74% 13% • 12%
1	C	420	8% 67% 13% •• 17%
1	D	420	12% 67% 16% • 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11674 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-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2891	1870	479	531	11			
1	B	368	Total	C	N	O	S	0	2	0
			2958	1914	489	543	12			
1	C	348	Total	C	N	O	S	0	1	0
			2754	1783	455	505	11			
1	D	357	Total	C	N	O	S	0	0	0
			2758	1782	459	506	11			

There are 60 discrepancies between the modelled and reference sequences:

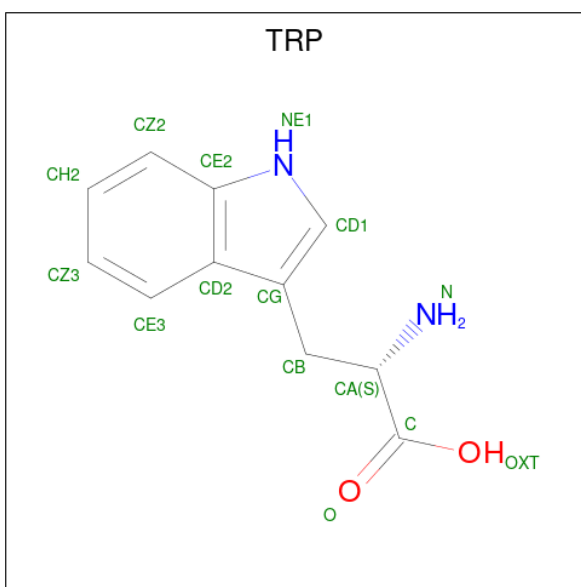
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	MET	-	expression tag	UNP Q8IDW3
A	227	ALA	-	expression tag	UNP Q8IDW3
A	633	GLU	-	expression tag	UNP Q8IDW3
A	634	ASN	-	expression tag	UNP Q8IDW3
A	635	LEU	-	expression tag	UNP Q8IDW3
A	636	TYR	-	expression tag	UNP Q8IDW3
A	637	PHE	-	expression tag	UNP Q8IDW3
A	638	GLN	-	expression tag	UNP Q8IDW3
A	639	GLY	-	expression tag	UNP Q8IDW3
A	640	HIS	-	expression tag	UNP Q8IDW3
A	641	HIS	-	expression tag	UNP Q8IDW3
A	642	HIS	-	expression tag	UNP Q8IDW3
A	643	HIS	-	expression tag	UNP Q8IDW3
A	644	HIS	-	expression tag	UNP Q8IDW3
A	645	HIS	-	expression tag	UNP Q8IDW3
B	226	MET	-	expression tag	UNP Q8IDW3
B	227	ALA	-	expression tag	UNP Q8IDW3
B	633	GLU	-	expression tag	UNP Q8IDW3
B	634	ASN	-	expression tag	UNP Q8IDW3
B	635	LEU	-	expression tag	UNP Q8IDW3
B	636	TYR	-	expression tag	UNP Q8IDW3

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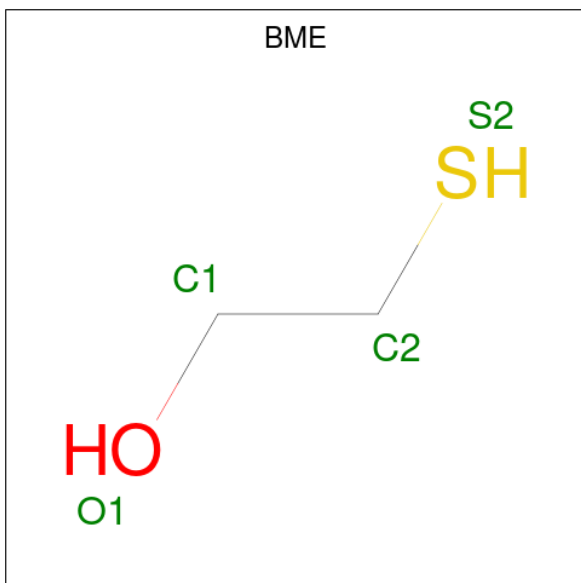
Chain	Residue	Modelled	Actual	Comment	Reference
B	637	PHE	-	expression tag	UNP Q8IDW3
B	638	GLN	-	expression tag	UNP Q8IDW3
B	639	GLY	-	expression tag	UNP Q8IDW3
B	640	HIS	-	expression tag	UNP Q8IDW3
B	641	HIS	-	expression tag	UNP Q8IDW3
B	642	HIS	-	expression tag	UNP Q8IDW3
B	643	HIS	-	expression tag	UNP Q8IDW3
B	644	HIS	-	expression tag	UNP Q8IDW3
B	645	HIS	-	expression tag	UNP Q8IDW3
C	226	MET	-	expression tag	UNP Q8IDW3
C	227	ALA	-	expression tag	UNP Q8IDW3
C	633	GLU	-	expression tag	UNP Q8IDW3
C	634	ASN	-	expression tag	UNP Q8IDW3
C	635	LEU	-	expression tag	UNP Q8IDW3
C	636	TYR	-	expression tag	UNP Q8IDW3
C	637	PHE	-	expression tag	UNP Q8IDW3
C	638	GLN	-	expression tag	UNP Q8IDW3
C	639	GLY	-	expression tag	UNP Q8IDW3
C	640	HIS	-	expression tag	UNP Q8IDW3
C	641	HIS	-	expression tag	UNP Q8IDW3
C	642	HIS	-	expression tag	UNP Q8IDW3
C	643	HIS	-	expression tag	UNP Q8IDW3
C	644	HIS	-	expression tag	UNP Q8IDW3
C	645	HIS	-	expression tag	UNP Q8IDW3
D	226	MET	-	expression tag	UNP Q8IDW3
D	227	ALA	-	expression tag	UNP Q8IDW3
D	633	GLU	-	expression tag	UNP Q8IDW3
D	634	ASN	-	expression tag	UNP Q8IDW3
D	635	LEU	-	expression tag	UNP Q8IDW3
D	636	TYR	-	expression tag	UNP Q8IDW3
D	637	PHE	-	expression tag	UNP Q8IDW3
D	638	GLN	-	expression tag	UNP Q8IDW3
D	639	GLY	-	expression tag	UNP Q8IDW3
D	640	HIS	-	expression tag	UNP Q8IDW3
D	641	HIS	-	expression tag	UNP Q8IDW3
D	642	HIS	-	expression tag	UNP Q8IDW3
D	643	HIS	-	expression tag	UNP Q8IDW3
D	644	HIS	-	expression tag	UNP Q8IDW3
D	645	HIS	-	expression tag	UNP Q8IDW3

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



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

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C_2H_6OS).



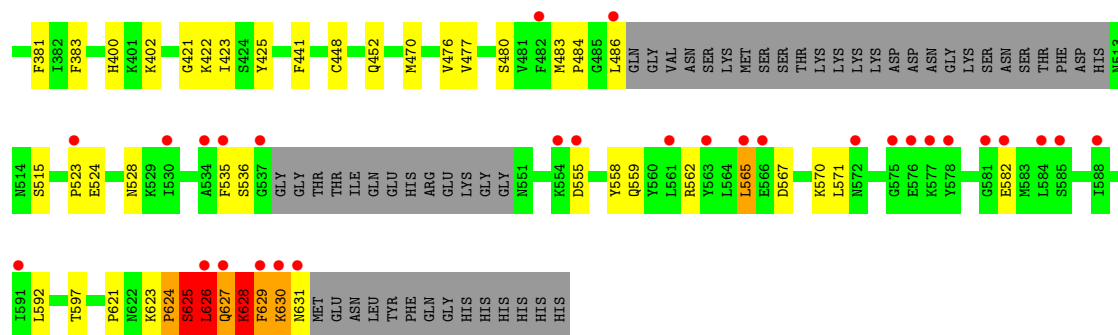
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0
3	D	1	Total C O S 4 2 1 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

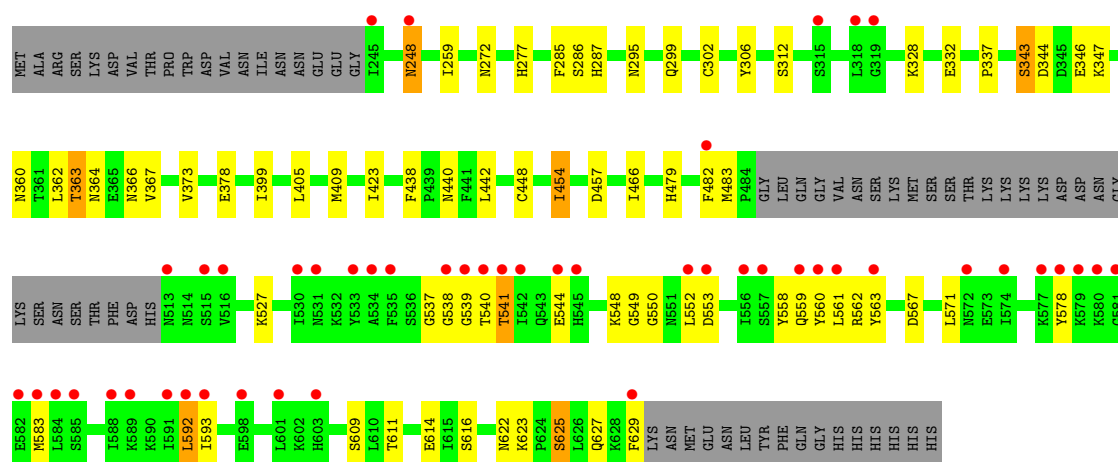
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total O 74 74	0	0
5	B	79	Total O 79 79	0	0
5	C	43	Total O 43 43	0	0
5	D	43	Total O 43 43	0	0



● Molecule 1: Tryptophan-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.18Å 213.25Å 101.95Å 90.00° 97.15° 90.00°	Depositor
Resolution (Å)	47.83 – 2.60 47.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.83-2.60) 94.2 (47.83-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.191 , 0.229 0.198 , 0.236	Depositor DCC
R_{free} test set	1274 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11674	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: K, BME

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	0.39	0/2964	0.79	3/4013 (0.1%)
1	B	0.49	1/3039 (0.0%)	0.80	1/4112 (0.0%)
1	C	0.50	1/2827 (0.0%)	0.89	14/3835 (0.4%)
1	D	0.39	0/2831	0.80	3/3845 (0.1%)
All	All	0.45	2/11661 (0.0%)	0.82	21/15805 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	625	SER	CA-C	-6.04	1.44	1.52
1	B	303	PHE	C-O	-5.73	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	LYS	N-CA-C	-9.86	95.41	110.10
1	C	624	PRO	N-CA-C	-8.62	103.43	114.03
1	D	541	THR	N-CA-C	-8.41	94.56	108.34
1	C	626	LEU	N-CA-C	-8.20	102.29	111.07
1	C	627	GLN	N-CA-C	-7.70	101.87	111.11
1	C	629	PHE	N-CA-C	7.20	119.21	111.36
1	C	625	SER	N-CA-C	-6.75	96.41	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	515	SER	N-CA-C	-5.99	106.22	112.93
1	D	548	LYS	N-CA-C	5.98	117.49	110.97
1	C	536	SER	N-CA-C	5.83	120.44	112.68
1	C	625	SER	CA-C-N	-5.70	113.03	120.44
1	C	625	SER	C-N-CA	-5.70	113.03	120.44
1	A	540	THR	CB-CA-C	-5.62	110.12	116.63
1	D	440	ASN	N-CA-C	5.55	117.33	111.28
1	B	629	PHE	N-CA-CB	-5.46	102.09	110.01
1	C	629	PHE	CA-C-N	-5.18	113.51	120.82
1	C	629	PHE	C-N-CA	-5.18	113.51	120.82
1	A	438	PHE	CA-C-N	5.18	124.97	119.28
1	A	438	PHE	C-N-CA	5.18	124.97	119.28
1	C	628	LYS	CA-C-N	-5.04	113.14	120.29
1	C	628	LYS	C-N-CA	-5.04	113.14	120.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	626	LEU	Peptide

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	2891	0	2781	38	0
1	B	2958	0	2835	28	0
1	C	2754	0	2602	41	0
1	D	2758	0	2507	36	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	1	0
3	A	4	0	5	1	0
3	B	4	0	5	0	0
3	D	4	0	5	1	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
5	A	74	0	0	0	0
5	B	79	0	0	0	0
5	C	43	0	0	1	0
5	D	43	0	0	0	0
All	All	11674	0	10776	142	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 6.

All (142) 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:541:THR:CB	1:D:544:GLU:CB	2.37	1.01
1:A:530:ILE:HG22	1:A:589:LYS:HG3	1.66	0.76
1:B:546:ARG:O	1:B:546:ARG:NH1	2.20	0.74
1:C:626:LEU:O	1:C:627:GLN:C	2.30	0.74
1:A:248:ASN:OD1	1:A:258:LYS:CE	2.36	0.73
1:C:625:SER:O	1:C:626:LEU:C	2.30	0.69
1:A:590:LYS:O	1:A:593:ILE:HG22	1.93	0.68
1:A:266:ARG:NH2	1:A:295:ASN:OD1	2.23	0.68
1:B:623:LYS:O	1:B:627:GLN:HG3	1.94	0.68
1:C:623:LYS:C	1:C:625:SER:H	2.02	0.67
1:A:248:ASN:OD1	1:A:258:LYS:NZ	2.29	0.65
1:C:629:PHE:O	1:C:630:LYS:C	2.36	0.64
1:A:526:ILE:O	1:A:530:ILE:HG12	1.98	0.64
1:D:454:ILE:HG22	1:D:479:HIS:HB3	1.79	0.64
1:A:588:ILE:HA	1:A:591:ILE:HD12	1.80	0.64
1:B:530:ILE:HG22	1:B:589:LYS:HD2	1.82	0.61
1:A:454:ILE:HG12	3:A:702:BME:H11	1.82	0.61
1:D:538:GLY:HA3	1:D:550:GLY:HA2	1.82	0.60
1:D:362:LEU:O	1:D:366:ASN:ND2	2.34	0.60
1:B:567:ASP:HB3	1:B:570:LYS:HD3	1.84	0.59
1:C:570:LYS:H	1:C:570:LYS:HD2	1.68	0.59
1:C:582:GLU:N	1:C:582:GLU:OE1	2.35	0.58
1:C:523:PRO:HG3	1:C:597:THR:HG23	1.86	0.57
1:C:312:SER:HB3	1:C:347:LYS:HD2	1.87	0.56
1:B:539:GLY:HA2	1:B:545:HIS:HB2	1.88	0.56
1:B:629:PHE:CD1	1:B:629:PHE:N	2.71	0.55
1:C:486:LEU:HD22	1:C:535:PHE:HB2	1.89	0.55
1:B:339:VAL:HG13	1:B:383:PHE:HE1	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ASN:HB2	1:B:529:LYS:HE2	1.89	0.55
1:C:562:ARG:NH1	5:C:840:HOH:O	2.39	0.55
1:C:339:VAL:HG13	1:C:383:PHE:HE1	1.72	0.54
1:B:454:ILE:HD13	1:B:454:ILE:H	1.72	0.54
1:D:360:ASN:HA	1:D:363:THR:HG23	1.90	0.53
1:A:263:HIS:NE2	1:A:291:ASP:OD1	2.40	0.53
1:C:524:GLU:O	1:C:528:ASN:ND2	2.39	0.53
1:D:346:GLU:OE1	2:D:701:TRP:N	2.42	0.53
1:A:284:PHE:HD2	1:A:478:VAL:HG12	1.74	0.51
1:D:611:THR:HG23	1:D:614:GLU:H	1.75	0.51
1:A:536:SER:O	1:A:538:GLY:N	2.41	0.51
1:D:399:ILE:HG23	1:D:466:ILE:HD13	1.93	0.51
1:B:288:ARG:HB2	1:B:477:VAL:HG22	1.92	0.51
1:B:457:ASP:OD2	1:B:461:ARG:NH1	2.39	0.50
1:D:378:GLU:O	1:D:625:SER:HB2	2.11	0.50
1:A:521:ASP:OD2	1:A:529:LYS:NZ	2.42	0.50
1:C:293:LEU:HB2	1:C:476:VAL:HG21	1.93	0.49
1:C:624:PRO:O	1:C:625:SER:O	2.29	0.49
1:A:344:ASP:N	1:A:344:ASP:OD1	2.45	0.49
1:A:331:GLN:NE2	1:A:380:THR:OG1	2.35	0.48
1:B:441:PHE:N	1:B:441:PHE:CD1	2.82	0.48
1:D:343:SER:HB2	1:D:346:GLU:HB3	1.95	0.48
1:A:578:TYR:HA	1:A:583:MET:HB3	1.95	0.48
1:D:328:LYS:NZ	1:D:332:GLU:OE2	2.35	0.48
1:C:284:PHE:CE2	1:C:480:SER:HB3	2.48	0.48
1:C:555:ASP:OD2	1:C:558:TYR:N	2.37	0.48
1:D:344:ASP:N	1:D:344:ASP:OD1	2.45	0.48
1:D:578:TYR:HA	1:D:583:MET:HB2	1.95	0.48
1:C:402:LYS:HE2	1:C:470:MET:HG2	1.96	0.47
1:D:248:ASN:OD1	1:D:248:ASN:N	2.48	0.47
1:A:530:ILE:CG2	1:A:589:LYS:HG3	2.41	0.47
1:B:284:PHE:CE2	1:B:480:SER:HB3	2.49	0.47
1:C:441:PHE:O	1:C:630:LYS:O	2.31	0.47
1:A:293:LEU:HB2	1:A:476:VAL:HG21	1.97	0.47
1:D:622:ASN:O	1:D:627:GLN:NE2	2.48	0.47
1:B:534:ALA:HB3	1:B:589:LYS:HE2	1.96	0.47
1:A:527:LYS:HG3	1:A:593:ILE:HG12	1.95	0.47
1:C:570:LYS:HD2	1:C:570:LYS:N	2.28	0.47
1:A:536:SER:O	1:A:578:TYR:OH	2.33	0.46
1:B:251:ILE:HG23	1:B:256:CYS:O	2.15	0.46
1:D:560:TYR:HB2	1:D:592:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:PRO:C	1:C:625:SER:O	2.57	0.46
1:A:486:LEU:N	1:A:515:SER:O	2.44	0.46
1:D:552:LEU:HD13	1:D:558:TYR:CE2	2.50	0.46
1:A:325:TYR:CE1	1:A:373:VAL:HG22	2.51	0.46
1:C:349:LEU:HD22	1:C:421:GLY:HA3	1.98	0.46
1:D:623:LYS:O	1:D:627:GLN:HG3	2.17	0.45
1:A:538:GLY:HA2	1:A:550:GLY:HA2	1.98	0.45
1:C:623:LYS:C	1:C:625:SER:N	2.68	0.45
1:C:344:ASP:N	1:C:344:ASP:OD1	2.48	0.45
1:D:259:ILE:HD11	1:D:287:HIS:HB3	1.98	0.45
1:D:438:PHE:HB2	1:D:442:LEU:HD12	1.98	0.45
1:A:513:ASN:HA	1:A:514:ASN:HA	1.70	0.44
1:B:346:GLU:HB2	1:B:425:TYR:CE2	2.53	0.44
1:C:281:ARG:NH2	1:C:565:LEU:O	2.51	0.44
1:D:561:LEU:HG	1:D:592:LEU:CD1	2.47	0.44
1:C:343:SER:HB2	1:C:346:GLU:HB3	1.99	0.44
1:A:574:ILE:HG23	1:A:583:MET:SD	2.58	0.44
1:C:346:GLU:HB2	1:C:425:TYR:CE2	2.53	0.44
1:A:463:SER:OG	1:A:475:PRO:HG2	2.17	0.44
1:A:248:ASN:OD1	1:A:258:LYS:HE3	2.16	0.44
1:A:360:ASN:HA	1:A:363:THR:HG23	1.99	0.44
1:A:409:MET:HE1	1:A:416:HIS:CE1	2.53	0.43
1:B:634:ASN:O	1:B:638:GLN:HG3	2.18	0.43
1:C:350:PHE:CD1	1:C:422:LYS:HE3	2.54	0.43
1:D:295:ASN:O	1:D:299:GLN:HG2	2.19	0.43
1:A:419:ASN:HB2	1:C:400:HIS:O	2.18	0.43
1:D:527:LYS:HA	1:D:593:ILE:HD13	1.99	0.43
1:B:284:PHE:HD2	1:B:478:VAL:HG12	1.83	0.43
1:D:559:GLN:HA	1:D:562:ARG:HG3	2.00	0.43
1:D:552:LEU:HD12	1:D:553:ASP:N	2.34	0.43
1:C:275:ALA:O	1:C:280:ARG:NH1	2.52	0.43
1:C:347:LYS:HD3	1:C:347:LYS:HA	1.81	0.43
1:C:626:LEU:O	1:C:628:LYS:N	2.51	0.43
1:D:286:SER:OG	1:D:479:HIS:HB2	2.19	0.43
1:B:275:ALA:O	1:B:280:ARG:NH1	2.49	0.43
1:B:281:ARG:HB3	1:B:562:ARG:NH2	2.34	0.42
1:C:565:LEU:HD12	1:C:565:LEU:HA	1.84	0.42
1:A:593:ILE:O	1:A:597:THR:OG1	2.23	0.42
1:C:567:ASP:HB3	1:C:570:LYS:HD3	2.00	0.42
1:A:284:PHE:CZ	1:A:480:SER:HB3	2.55	0.42
1:C:381:PHE:CE1	1:C:621:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ILE:HG12	1:D:285:PHE:O	2.20	0.42
1:B:585:SER:O	1:B:589:LYS:HG2	2.20	0.42
1:B:629:PHE:H	1:B:629:PHE:HD1	1.59	0.42
1:C:306:TYR:HB3	1:C:448:CYS:SG	2.59	0.42
1:C:452:GLN:NE2	1:C:477:VAL:HG13	2.35	0.42
1:A:366:ASN:N	1:A:366:ASN:HD22	2.17	0.42
1:A:433:CYS:HB3	1:A:475:PRO:HG3	2.01	0.42
1:B:293:LEU:HB2	1:B:476:VAL:HG21	2.02	0.41
1:B:318:LEU:HD11	1:B:596:LEU:HD21	2.01	0.41
1:C:559:GLN:O	1:C:562:ARG:HB2	2.20	0.41
1:D:306:TYR:HB3	1:D:448:CYS:SG	2.60	0.41
1:A:281:ARG:NH2	1:A:565:LEU:O	2.53	0.41
1:A:486:LEU:HB2	1:A:515:SER:HA	2.01	0.41
1:D:457:ASP:OD2	3:D:702:BME:H12	2.19	0.41
1:B:377:PRO:O	1:B:623:LYS:HE2	2.20	0.41
1:A:613:GLU:CD	1:A:613:GLU:H	2.29	0.41
1:C:342:LEU:HD22	1:C:363:THR:HG23	2.03	0.41
1:D:364:ASN:O	1:D:367:VAL:HG12	2.20	0.41
1:D:454:ILE:HD11	1:D:482:PHE:CE2	2.56	0.41
1:C:281:ARG:NH1	1:C:565:LEU:O	2.53	0.41
1:D:277:HIS:HE1	1:D:563:TYR:O	2.03	0.41
1:D:312:SER:HB3	1:D:347:LYS:HD2	2.03	0.41
1:D:337:PRO:HD3	1:D:629:PHE:CZ	2.56	0.41
1:D:539:GLY:HA2	1:D:540:THR:HA	1.52	0.41
1:A:487:GLN:HG3	1:A:533:TYR:O	2.22	0.40
1:C:629:PHE:O	1:C:631:ASN:N	2.54	0.40
1:A:522:THR:O	1:A:526:ILE:HG13	2.22	0.40
1:B:325:TYR:CE1	1:B:373:VAL:HG22	2.56	0.40
1:B:409:MET:HE1	1:B:416:HIS:CE1	2.56	0.40
1:C:483:MET:HG3	1:C:484:PRO:HD2	2.04	0.40
1:B:526:ILE:O	1:B:530:ILE:HG12	2.21	0.40
1:D:405:LEU:HG	1:D:409:MET:HE2	2.03	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	358/420 (85%)	349 (98%)	7 (2%)	2 (1%)	21	42
1	B	366/420 (87%)	360 (98%)	5 (1%)	1 (0%)	36	58
1	C	343/420 (82%)	335 (98%)	7 (2%)	1 (0%)	36	58
1	D	353/420 (84%)	338 (96%)	13 (4%)	2 (1%)	21	42
All	All	1420/1680 (84%)	1382 (97%)	32 (2%)	6 (0%)	30	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	GLY
1	A	539	GLY
1	C	625	SER
1	B	549	GLY
1	D	537	GLY
1	D	549	GLY

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	313/388 (81%)	297 (95%)	16 (5%)	21	45
1	B	318/388 (82%)	303 (95%)	15 (5%)	23	48
1	C	292/388 (75%)	282 (97%)	10 (3%)	32	60
1	D	274/388 (71%)	259 (94%)	15 (6%)	19	41
All	All	1197/1552 (77%)	1141 (95%)	56 (5%)	23	48

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	VAL
1	A	342	LEU
1	A	357	GLU
1	A	363	THR
1	A	366	ASN
1	A	373	VAL
1	A	454	ILE
1	A	487	GLN
1	A	516	VAL
1	A	517	ILE
1	A	527	LYS
1	A	556	ILE
1	A	571	LEU
1	A	589	LYS
1	A	593	ILE
1	A	613	GLU
1	B	262	ASN
1	B	272	ASN
1	B	299	GLN
1	B	301	LYS
1	B	339	VAL
1	B	373	VAL
1	B	400	HIS
1	B	423	ILE
1	B	454	ILE
1	B	516	VAL
1	B	556	ILE
1	B	571	LEU
1	B	592	LEU
1	B	635	LEU
1	B	638	GLN
1	C	250	LEU
1	C	272	ASN
1	C	332	GLU
1	C	339	VAL
1	C	373	VAL
1	C	423	ILE
1	C	565	LEU
1	C	571	LEU
1	C	592	LEU
1	C	628	LYS
1	D	248	ASN
1	D	272	ASN

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Mol	Chain	Res	Type
1	D	302	CYS
1	D	343	SER
1	D	363	THR
1	D	373	VAL
1	D	423	ILE
1	D	454	ILE
1	D	483	MET
1	D	567	ASP
1	D	571	LEU
1	D	592	LEU
1	D	609	SER
1	D	616	SER
1	D	625	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	335	ASN
1	B	262	ASN
1	B	551	ASN
1	C	248	ASN
1	C	300	HIS
1	C	436	GLN
1	C	473	HIS
1	D	277	HIS
1	D	300	HIS
1	D	513	ASN
1	D	604	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	TRP	B	701	-	15,16,16	0.73	1 (6%)	18,22,22	0.75	1 (5%)
2	TRP	A	701	-	15,16,16	0.74	1 (6%)	18,22,22	0.74	1 (5%)
2	TRP	D	701	-	15,16,16	0.71	1 (6%)	18,22,22	0.79	1 (5%)
3	BME	A	702	1	3,3,3	0.98	0	2,2,2	1.35	0
2	TRP	C	701	-	15,16,16	0.73	1 (6%)	18,22,22	0.74	1 (5%)
3	BME	B	702	1	3,3,3	0.19	0	2,2,2	0.32	0
3	BME	D	702	1	3,3,3	0.22	0	2,2,2	1.09	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
2	TRP	B	701	-	-	0/8/8/8	0/2/2/2
2	TRP	A	701	-	-	2/8/8/8	0/2/2/2
2	TRP	D	701	-	-	1/8/8/8	0/2/2/2
3	BME	A	702	1	-	1/1/1/1	-
2	TRP	C	701	-	-	0/8/8/8	0/2/2/2
3	BME	B	702	1	-	1/1/1/1	-
3	BME	D	702	1	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	TRP	OXT-C	-2.20	1.23	1.30
2	C	701	TRP	OXT-C	-2.20	1.23	1.30
2	D	701	TRP	OXT-C	-2.19	1.23	1.30
2	B	701	TRP	OXT-C	-2.18	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	TRP	OXT-C-O	-2.75	117.83	124.08
2	B	701	TRP	OXT-C-O	-2.73	117.90	124.08
2	C	701	TRP	OXT-C-O	-2.70	117.95	124.08
2	A	701	TRP	OXT-C-O	-2.67	118.02	124.08

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	BME	O1-C1-C2-S2
3	B	702	BME	O1-C1-C2-S2
2	A	701	TRP	OXT-C-CA-N
2	D	701	TRP	OXT-C-CA-N
2	A	701	TRP	O-C-CA-N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	TRP	1	0
3	A	702	BME	1	0
3	D	702	BME	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	362/420 (86%)	0.07	17 (4%)	36	30	19, 41, 100, 143	0
1	B	368/420 (87%)	0.14	17 (4%)	37	32	19, 43, 105, 136	2 (0%)
1	C	348/420 (82%)	0.41	33 (9%)	14	10	19, 53, 101, 122	1 (0%)
1	D	357/420 (85%)	0.72	49 (13%)	6	5	21, 61, 127, 149	0
All	All	1435/1680 (85%)	0.33	116 (8%)	18	14	19, 49, 110, 149	3 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	582	GLU	5.5
1	A	489	VAL	5.3
1	D	585	SER	4.8
1	D	542	ILE	4.4
1	B	540	THR	4.3
1	B	513	ASN	4.3
1	C	486	LEU	4.2
1	A	513	ASN	4.0
1	B	541	THR	3.9
1	C	629	PHE	3.8
1	D	588	ILE	3.8
1	C	537	GLY	3.8
1	D	540	THR	3.6
1	C	581	GLY	3.6
1	C	248	ASN	3.5
1	B	245	ILE	3.5
1	D	248	ASN	3.5
1	C	627	GLN	3.5
1	D	556	ILE	3.4
1	C	631	ASN	3.4
1	A	540	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	531	ASN	3.3
1	D	552	LEU	3.3
1	D	581	GLY	3.3
1	D	530	ILE	3.3
1	D	541	THR	3.3
1	B	537	GLY	3.2
1	C	575	GLY	3.2
1	D	544	GLU	3.2
1	C	630	LYS	3.1
1	C	584	LEU	3.1
1	D	561	LEU	3.1
1	D	591	ILE	3.1
1	D	535	PHE	3.1
1	C	626	LEU	3.0
1	B	539	GLY	3.0
1	B	535	PHE	3.0
1	A	543	GLN	3.0
1	D	589	LYS	3.0
1	C	582	GLU	2.9
1	C	585	SER	2.9
1	D	557	SER	2.9
1	A	629	PHE	2.9
1	D	584	LEU	2.9
1	B	629	PHE	2.9
1	B	585	SER	2.9
1	D	560	TYR	2.9
1	D	578	TYR	2.9
1	C	577	LYS	2.9
1	C	482	PHE	2.8
1	B	588	ILE	2.8
1	D	583	MET	2.8
1	D	534	ALA	2.8
1	C	534	ALA	2.7
1	A	541	THR	2.7
1	B	584	LEU	2.7
1	C	530	ILE	2.7
1	D	563	TYR	2.6
1	B	542	ILE	2.6
1	D	574	ILE	2.6
1	D	601	LEU	2.6
1	B	544	GLU	2.6
1	D	559	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	544	GLU	2.6
1	B	538	GLY	2.6
1	D	629	PHE	2.6
1	D	318	LEU	2.5
1	B	581	GLY	2.5
1	D	482	PHE	2.5
1	D	553	ASP	2.5
1	D	577	LYS	2.5
1	D	319	GLY	2.5
1	A	535	PHE	2.4
1	D	539	GLY	2.4
1	C	535	PHE	2.4
1	C	588	ILE	2.4
1	A	537	GLY	2.4
1	C	561	LEU	2.3
1	D	603	HIS	2.3
1	D	515	SER	2.3
1	C	523	PRO	2.3
1	A	588	ILE	2.3
1	D	245	ILE	2.3
1	C	572	ASN	2.3
1	C	315	SER	2.3
1	B	587	GLU	2.3
1	D	580	LYS	2.3
1	D	315	SER	2.3
1	C	246	ASN	2.3
1	D	592	LEU	2.3
1	C	566	GLU	2.2
1	D	598	GLU	2.2
1	A	596	LEU	2.2
1	B	486	LEU	2.2
1	C	247	TYR	2.2
1	D	538	GLY	2.2
1	D	593	ILE	2.2
1	C	578	TYR	2.2
1	C	554	LYS	2.2
1	C	563	TYR	2.1
1	C	565	LEU	2.1
1	A	538	GLY	2.1
1	A	516	VAL	2.1
1	C	555	ASP	2.1
1	A	539	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	545	HIS	2.1
1	D	516	VAL	2.1
1	A	545	HIS	2.0
1	A	542	ILE	2.0
1	C	591	ILE	2.0
1	C	576	GLU	2.0
1	D	579	LYS	2.0
1	A	593	ILE	2.0
1	D	513	ASN	2.0
1	D	572	ASN	2.0
1	D	533	TYR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
3	BME	D	702	4/4	0.84	0.17	63,70,72,89	0
3	BME	A	702	4/4	0.85	0.21	51,62,64,93	0
3	BME	B	702	4/4	0.87	0.17	50,53,67,83	0
4	K	C	702	1/1	0.92	0.14	61,61,61,61	0
4	K	D	703	1/1	0.92	0.07	63,63,63,63	0
2	TRP	D	701	15/15	0.93	0.09	29,40,51,57	0
2	TRP	C	701	15/15	0.95	0.08	24,36,49,58	0
2	TRP	A	701	15/15	0.97	0.06	15,22,36,37	0
2	TRP	B	701	15/15	0.98	0.06	17,24,42,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.