



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 10:57 AM EDT

PDB ID : 4JFA
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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

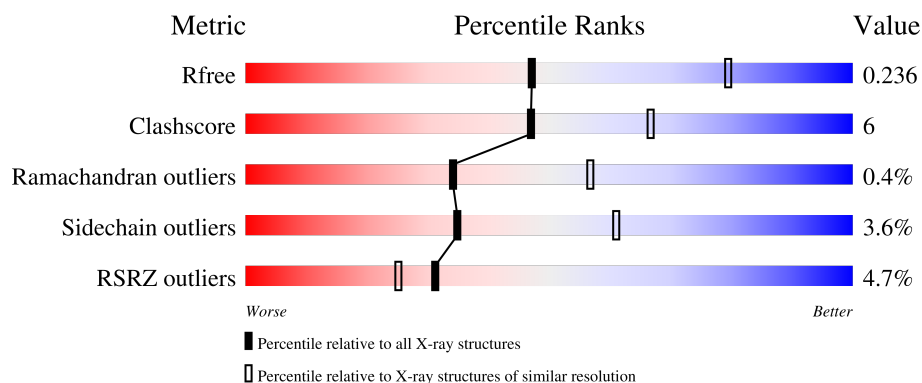
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


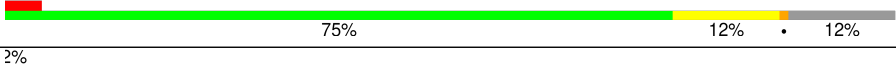
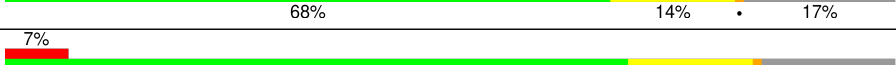

The reported resolution of this entry is 2.60 Å.

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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	
1	B	420	
1	C	420	
1	D	420	

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:

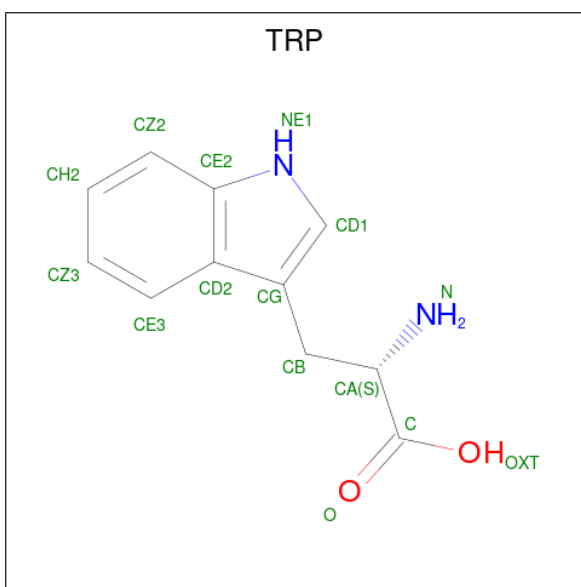
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	MET	-	EXPRESSION TAG	UNP Q8IDW3
A	227	ALA	-	EXPRESSION TAG	UNP Q8IDW3
A	633	GLU	-	EXPRESSION TAG	UNP Q8IDW3
A	634	ASN	-	EXPRESSION TAG	UNP Q8IDW3
A	635	LEU	-	EXPRESSION TAG	UNP Q8IDW3
A	636	TYR	-	EXPRESSION TAG	UNP Q8IDW3
A	637	PHE	-	EXPRESSION TAG	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

Continued on next page...

Continued from previous page...

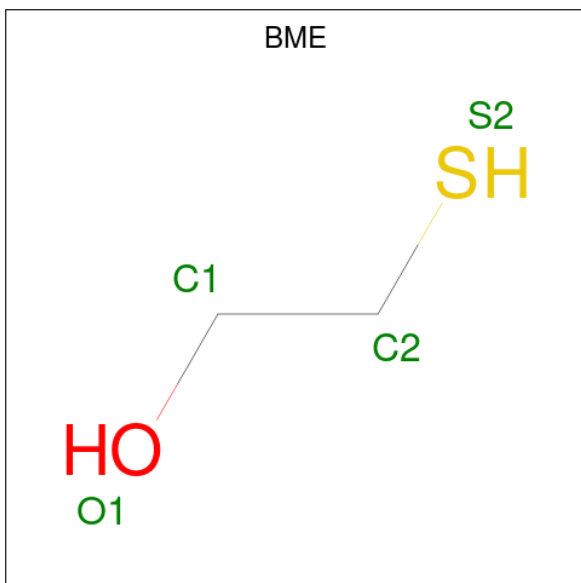
Chain	Residue	Modelled	Actual	Comment	Reference
B	637	PHE	-	EXPRESSION TAG	UNP Q8IDW3
B	638	GLN	-	EXPRESSION TAG	UNP Q8IDW3
B	639	GLY	-	EXPRESSION TAG	UNP Q8IDW3
B	640	HIS	-	EXPRESSION TAG	UNP Q8IDW3
B	641	HIS	-	EXPRESSION TAG	UNP Q8IDW3
B	642	HIS	-	EXPRESSION TAG	UNP Q8IDW3
B	643	HIS	-	EXPRESSION TAG	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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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

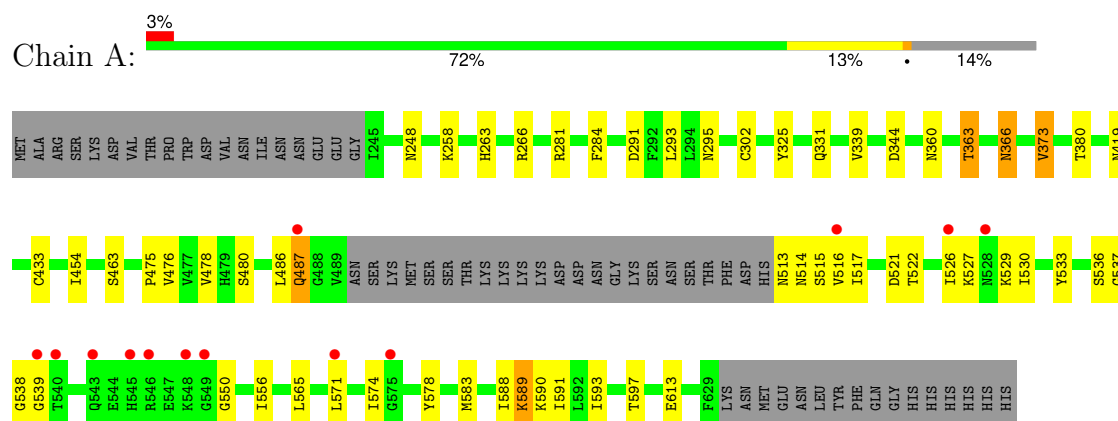
- Molecule 5 is water.

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

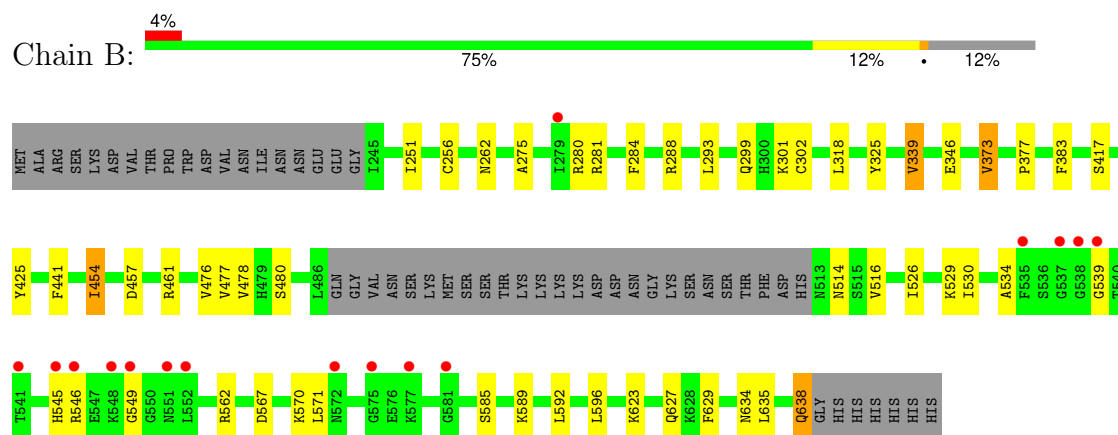
3 Residue-property plots [i](#)

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.

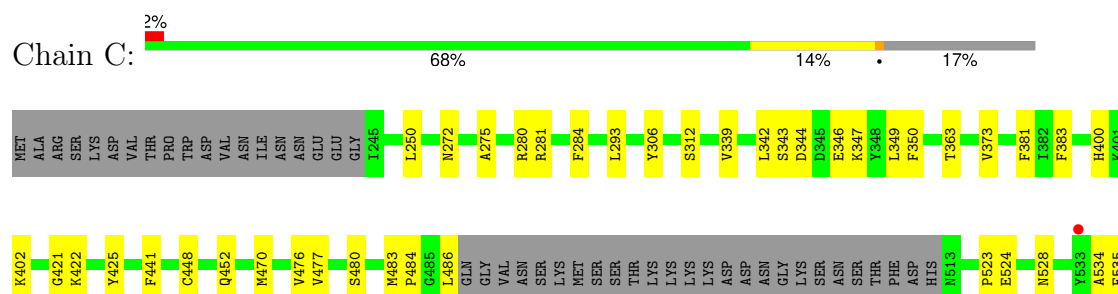
• Molecule 1: Tryptophan-tRNA ligase



• Molecule 1: Tryptophan-tRNA ligase

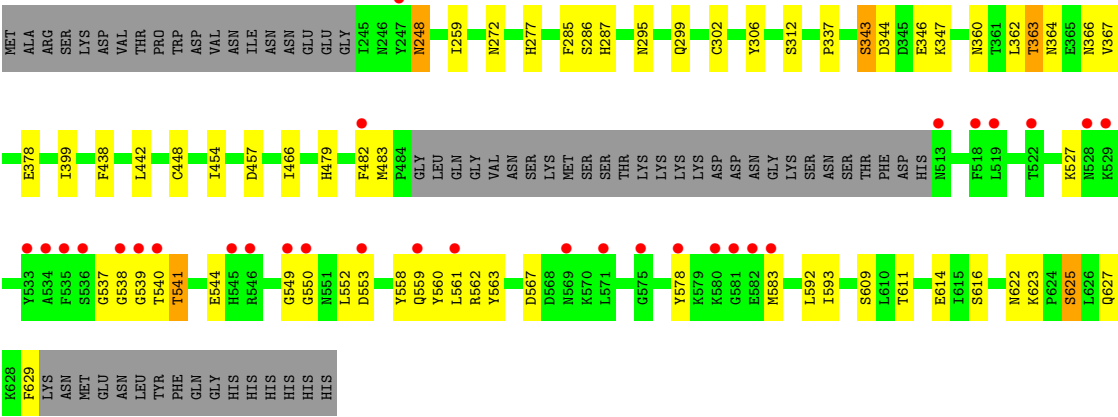


• Molecule 1: Tryptophan-tRNA ligase





● 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 (2.04%)	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 , 53.8	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

5.1 Standard geometry

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	0.31	0/2964	0.45	0/4013
1	B	0.39	0/3039	0.47	0/4112
1	C	0.36	0/2827	0.51	2/3835 (0.1%)
1	D	0.31	0/2831	0.46	1/3845 (0.0%)
All	All	0.35	0/11661	0.47	3/15805 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	541	THR	N-CA-C	-6.09	94.56	111.00
1	C	630	LYS	N-CA-C	-5.78	95.41	111.00
1	C	625	SER	N-CA-C	-5.40	96.41	111.00

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	36	0
1	B	2958	0	2835	27	0
1	C	2754	0	2602	42	0
1	D	2758	0	2507	34	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
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	138	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 (138) 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:A:248:ASN:OD1	1:A:258:LYS:CE	2.36	0.73
1:C:626:LEU:O	1:C:627:GLN: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:A:248:ASN:OD1	1:A:258:LYS:NZ	2.29	0.65
1:C:625:SER:O	1:C:626:LEU:C	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:629:PHE:O	1:C:630:LYS:C	2.36	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:623:LYS:C	1:C:625:SER:H	2.02	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
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: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:C:284:PHE:CE2	1:C:480:SER:HB3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ASP:OD2	1:A:529:LYS:NZ	2.42	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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:623:LYS:C	1:C:625:SER:N	2.68	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
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:C:624:PRO:C	1:C:625:SER:O	2.57	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:C:342:LEU:HD22	1:C:363:THR:HG23	2.03	0.41
1:C:534:ALA:O	1:C:589:LYS:NZ	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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	358/420 (85%)	349 (98%)	7 (2%)	2 (1%)	25	47
1	B	366/420 (87%)	360 (98%)	5 (1%)	1 (0%)	41	64
1	C	343/420 (82%)	335 (98%)	7 (2%)	1 (0%)	41	64
1	D	353/420 (84%)	338 (96%)	13 (4%)	2 (1%)	25	47
All	All	1420/1680 (84%)	1382 (97%)	32 (2%)	6 (0%)	34	57

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%)	301 (96%)	12 (4%)	33	59
1	B	318/388 (82%)	305 (96%)	13 (4%)	30	56
1	C	292/388 (75%)	284 (97%)	8 (3%)	44	71
1	D	274/388 (71%)	264 (96%)	10 (4%)	35	61
All	All	1197/1552 (77%)	1154 (96%)	43 (4%)	35	61

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	339	VAL
1	A	363	THR
1	A	366	ASN
1	A	373	VAL
1	A	487	GLN
1	A	516	VAL
1	A	517	ILE
1	A	556	ILE
1	A	571	LEU
1	A	589	LYS
1	A	613	GLU
1	B	262	ASN
1	B	299	GLN
1	B	301	LYS
1	B	302	CYS
1	B	339	VAL
1	B	373	VAL
1	B	417	SER
1	B	454	ILE
1	B	516	VAL
1	B	571	LEU
1	B	592	LEU
1	B	635	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	638	GLN
1	C	250	LEU
1	C	272	ASN
1	C	373	VAL
1	C	570	LYS
1	C	571	LEU
1	C	592	LEU
1	C	599	LEU
1	C	628	LYS
1	D	248	ASN
1	D	272	ASN
1	D	302	CYS
1	D	343	SER
1	D	363	THR
1	D	483	MET
1	D	567	ASP
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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	248	ASN
1	D	277	HIS

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 monosaccharides 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	C	701	-	14,16,16	0.87	1 (7%)	13,22,22	1.13	1 (7%)
3	BME	D	702	1	3,3,3	0.22	0	2,2,2	1.09	0
3	BME	A	702	1	3,3,3	0.98	0	2,2,2	1.35	0
2	TRP	D	701	-	14,16,16	0.85	1 (7%)	13,22,22	1.18	2 (15%)
2	TRP	A	701	-	14,16,16	0.86	1 (7%)	13,22,22	1.13	1 (7%)
3	BME	B	702	1	3,3,3	0.19	0	2,2,2	0.32	0
2	TRP	B	701	-	14,16,16	0.84	1 (7%)	13,22,22	1.15	1 (7%)

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	C	701	-	-	0/7/8/8	0/2/2/2
3	BME	D	702	1	-	0/1/1/1	-
3	BME	A	702	1	-	1/1/1/1	-
2	TRP	D	701	-	-	1/7/8/8	0/2/2/2
2	TRP	A	701	-	-	2/7/8/8	0/2/2/2
3	BME	B	702	1	-	1/1/1/1	-
2	TRP	B	701	-	-	0/7/8/8	0/2/2/2

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 (5) 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
2	D	701	TRP	CH2-CZ2-CE2	-2.07	117.25	120.09

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
3	D	702	BME	1	0
3	A	702	BME	1	0
2	D	701	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	362/420 (86%)	-0.00	13 (3%) 42 35	19, 41, 100, 143	0
1	B	368/420 (87%)	0.10	16 (4%) 35 28	19, 43, 105, 136	0
1	C	348/420 (82%)	0.01	8 (2%) 60 54	21, 53, 101, 122	0
1	D	357/420 (85%)	0.26	30 (8%) 11 7	21, 61, 127, 149	0
All	All	1435/1680 (85%)	0.09	67 (4%) 31 25	19, 49, 110, 149	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	537	GLY	5.3
1	D	539	GLY	5.1
1	A	549	GLY	4.6
1	D	578	TYR	4.5
1	D	582	GLU	4.4
1	B	548	LYS	4.3
1	A	540	THR	4.2
1	D	536	SER	4.2
1	D	545	HIS	4.1
1	A	548	LYS	4.1
1	B	549	GLY	4.1
1	B	581	GLY	4.1
1	D	581	GLY	3.8
1	D	538	GLY	3.8
1	C	582	GLU	3.7
1	D	571	LEU	3.4
1	B	545	HIS	3.4
1	C	578	TYR	3.3
1	C	533	TYR	3.3
1	A	528	ASN	3.2
1	D	550	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	549	GLY	3.2
1	D	535	PHE	3.2
1	C	575	GLY	3.1
1	D	553	ASP	3.0
1	D	533	TYR	3.0
1	B	551	ASN	2.9
1	B	539	GLY	2.9
1	A	571	LEU	2.9
1	A	539	GLY	2.8
1	A	545	HIS	2.8
1	C	567	ASP	2.8
1	D	583	MET	2.7
1	D	482	PHE	2.7
1	D	575	GLY	2.7
1	D	247	TYR	2.7
1	D	522	THR	2.7
1	D	513	ASN	2.7
1	D	561	LEU	2.6
1	D	528	ASN	2.5
1	D	534	ALA	2.5
1	A	487	GLN	2.4
1	D	529	LYS	2.4
1	A	575	GLY	2.4
1	D	580	LYS	2.4
1	A	543	GLN	2.4
1	D	518	PHE	2.3
1	B	552	LEU	2.3
1	B	572	ASN	2.3
1	B	575	GLY	2.3
1	C	561	LEU	2.2
1	D	546	ARG	2.2
1	B	538	GLY	2.2
1	A	516	VAL	2.2
1	A	526	ILE	2.1
1	D	569	ASN	2.1
1	C	581	GLY	2.1
1	D	540	THR	2.1
1	D	559	GLN	2.1
1	B	577	LYS	2.1
1	B	546	ARG	2.1
1	B	541	THR	2.1
1	B	279	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	519	LEU	2.0
1	C	583	MET	2.0
1	B	535	PHE	2.0
1	A	546	ARG	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 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(\AA^2)	Q<0.9
3	BME	B	702	4/4	0.87	0.24	50,53,67,83	0
3	BME	D	702	4/4	0.87	0.18	63,70,72,89	0
3	BME	A	702	4/4	0.90	0.21	51,62,64,93	0
4	K	C	702	1/1	0.92	0.19	61,61,61,61	0
4	K	D	703	1/1	0.95	0.12	63,63,63,63	0
2	TRP	C	701	15/15	0.96	0.16	24,36,49,58	0
2	TRP	D	701	15/15	0.97	0.17	29,40,51,57	0
2	TRP	B	701	15/15	0.98	0.20	17,24,42,45	0
2	TRP	A	701	15/15	0.98	0.16	15,22,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.