



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:14 AM UTC

PDB ID : 7T7T / pdb_00007t7t
Title : Structure of TSK/BRU1 bound to histone H3.1
Authors : Davarinejad, H.; Couture, J.F.
Deposited on : 2021-12-15
Resolution : 3.17 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

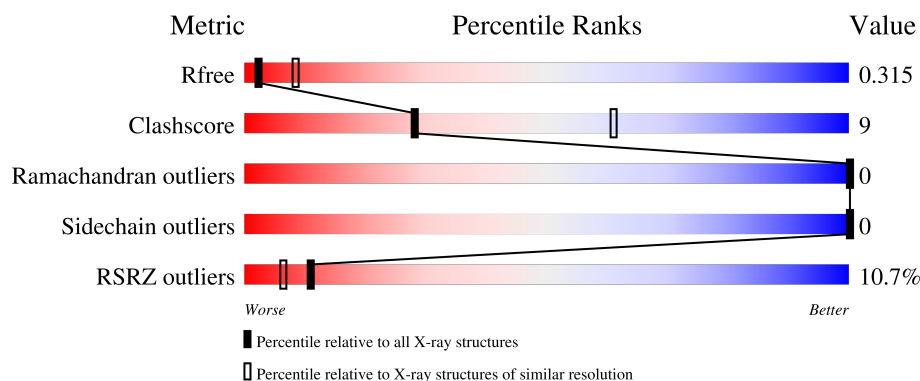
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	531	8% 70% 18% 12%
1	B	531	9% 66% 15% 19%
2	W	45	13% 47% 16% 38%
2	X	45	49% 7% 44%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7176 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 Protein TONSOKU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	Se	0	0	0
			3586	2252	634	676	8	16			
1	B	432	Total	C	N	O	S	Se	0	0	0
			3246	2028	566	628	8	16			

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MSE	-	initiating methionine	UNP A0A2H5Q1B8
A	-39	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-38	SER	-	expression tag	UNP A0A2H5Q1B8
A	-37	SER	-	expression tag	UNP A0A2H5Q1B8
A	-36	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-35	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-34	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-33	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-32	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-31	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-30	SER	-	expression tag	UNP A0A2H5Q1B8
A	-29	SER	-	expression tag	UNP A0A2H5Q1B8
A	-28	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-27	LEU	-	expression tag	UNP A0A2H5Q1B8
A	-26	VAL	-	expression tag	UNP A0A2H5Q1B8
A	-25	PRO	-	expression tag	UNP A0A2H5Q1B8
A	-24	ARG	-	expression tag	UNP A0A2H5Q1B8
A	-23	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-22	SER	-	expression tag	UNP A0A2H5Q1B8
A	-21	HIS	-	expression tag	UNP A0A2H5Q1B8
A	-20	MSE	-	expression tag	UNP A0A2H5Q1B8
A	-19	ALA	-	expression tag	UNP A0A2H5Q1B8
A	-18	SER	-	expression tag	UNP A0A2H5Q1B8
A	-17	MSE	-	expression tag	UNP A0A2H5Q1B8
A	-16	THR	-	expression tag	UNP A0A2H5Q1B8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-14	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-13	GLN	-	expression tag	UNP A0A2H5Q1B8
A	-12	GLN	-	expression tag	UNP A0A2H5Q1B8
A	-11	MSE	-	expression tag	UNP A0A2H5Q1B8
A	-10	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-9	ARG	-	expression tag	UNP A0A2H5Q1B8
A	-8	GLY	-	expression tag	UNP A0A2H5Q1B8
A	-7	SER	-	expression tag	UNP A0A2H5Q1B8
A	-6	GLU	-	expression tag	UNP A0A2H5Q1B8
A	-5	ASN	-	expression tag	UNP A0A2H5Q1B8
A	-4	LEU	-	expression tag	UNP A0A2H5Q1B8
A	-3	TYR	-	expression tag	UNP A0A2H5Q1B8
A	-2	PHE	-	expression tag	UNP A0A2H5Q1B8
A	-1	GLN	-	expression tag	UNP A0A2H5Q1B8
A	0	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-40	MSE	-	initiating methionine	UNP A0A2H5Q1B8
B	-39	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-38	SER	-	expression tag	UNP A0A2H5Q1B8
B	-37	SER	-	expression tag	UNP A0A2H5Q1B8
B	-36	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-35	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-34	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-33	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-32	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-31	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-30	SER	-	expression tag	UNP A0A2H5Q1B8
B	-29	SER	-	expression tag	UNP A0A2H5Q1B8
B	-28	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-27	LEU	-	expression tag	UNP A0A2H5Q1B8
B	-26	VAL	-	expression tag	UNP A0A2H5Q1B8
B	-25	PRO	-	expression tag	UNP A0A2H5Q1B8
B	-24	ARG	-	expression tag	UNP A0A2H5Q1B8
B	-23	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-22	SER	-	expression tag	UNP A0A2H5Q1B8
B	-21	HIS	-	expression tag	UNP A0A2H5Q1B8
B	-20	MSE	-	expression tag	UNP A0A2H5Q1B8
B	-19	ALA	-	expression tag	UNP A0A2H5Q1B8
B	-18	SER	-	expression tag	UNP A0A2H5Q1B8
B	-17	MSE	-	expression tag	UNP A0A2H5Q1B8
B	-16	THR	-	expression tag	UNP A0A2H5Q1B8
B	-15	GLY	-	expression tag	UNP A0A2H5Q1B8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-13	GLN	-	expression tag	UNP A0A2H5Q1B8
B	-12	GLN	-	expression tag	UNP A0A2H5Q1B8
B	-11	MSE	-	expression tag	UNP A0A2H5Q1B8
B	-10	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-9	ARG	-	expression tag	UNP A0A2H5Q1B8
B	-8	GLY	-	expression tag	UNP A0A2H5Q1B8
B	-7	SER	-	expression tag	UNP A0A2H5Q1B8
B	-6	GLU	-	expression tag	UNP A0A2H5Q1B8
B	-5	ASN	-	expression tag	UNP A0A2H5Q1B8
B	-4	LEU	-	expression tag	UNP A0A2H5Q1B8
B	-3	TYR	-	expression tag	UNP A0A2H5Q1B8
B	-2	PHE	-	expression tag	UNP A0A2H5Q1B8
B	-1	GLN	-	expression tag	UNP A0A2H5Q1B8
B	0	GLY	-	expression tag	UNP A0A2H5Q1B8

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	25	Total	C	N	O	0	0	0
			159	97	32	30			
2	W	28	Total	C	N	O	0	0	0
			184	113	37	34			

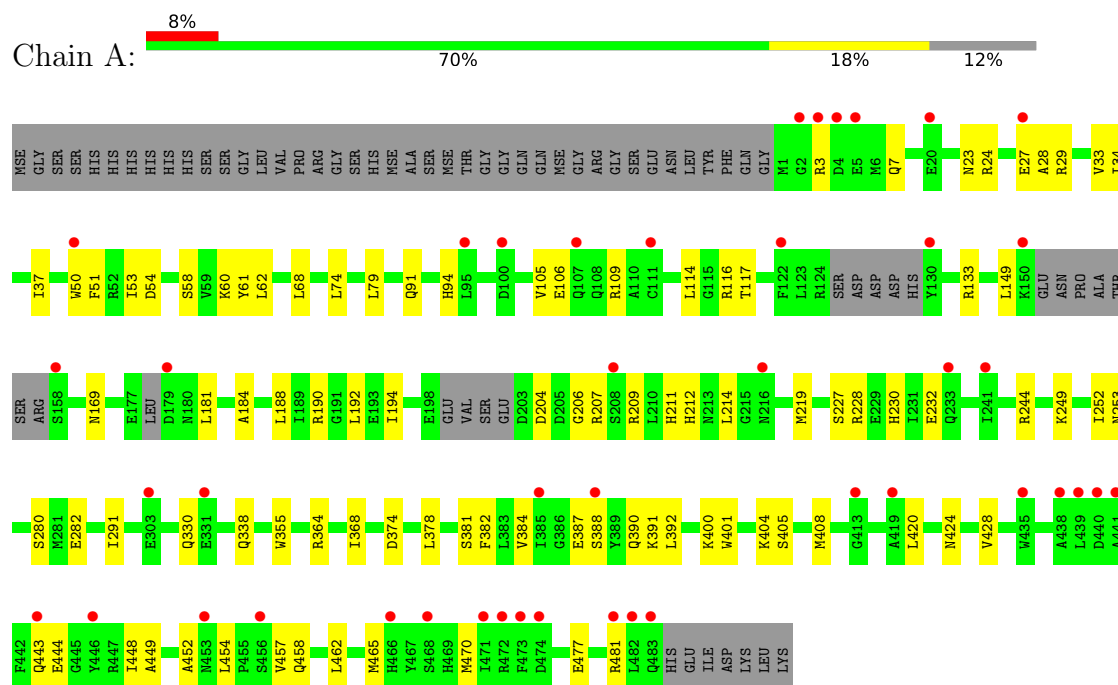
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	O	0	0
			1	1		

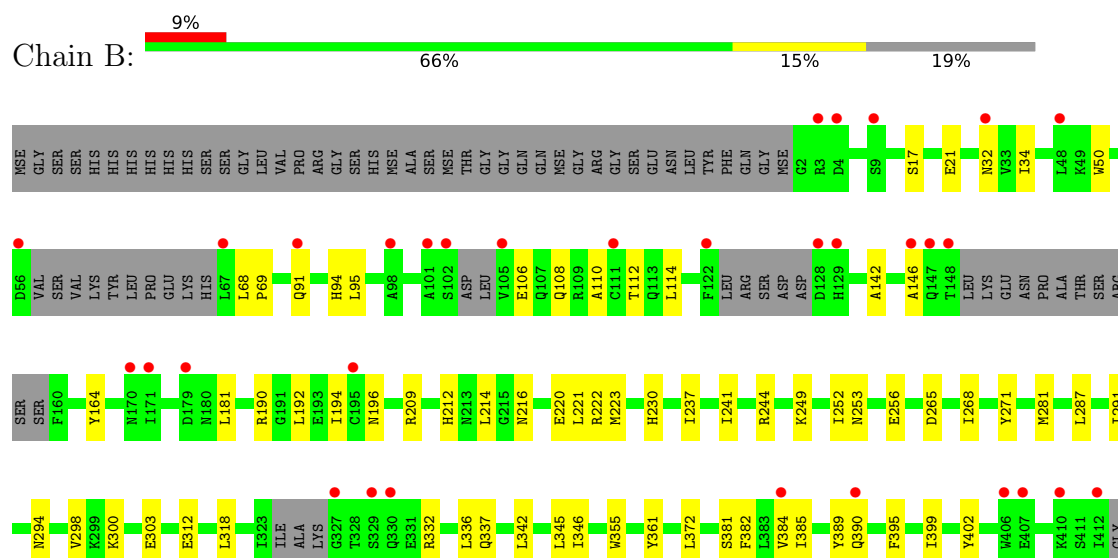
3 Residue-property plots

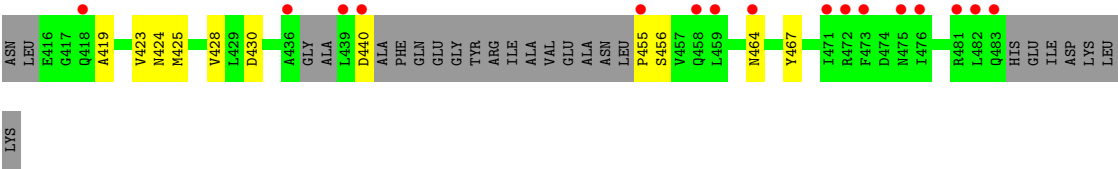
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein TONSOKU



• Molecule 1: Protein TONSOKU

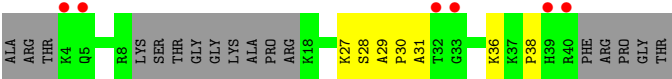




● Molecule 2: Histone H3.1



● Molecule 2: Histone H3.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.89Å 92.33Å 209.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.53 – 3.17 38.53 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.53-3.17) 97.4 (38.53-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.279 , 0.318 0.277 , 0.315	Depositor DCC
R_{free} test set	2000 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	7176	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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](#)

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	0.18	0/3621	0.45	1/4847 (0.0%)
1	B	0.18	0/3273	0.46	0/4386
2	W	0.24	0/184	0.61	0/246
2	X	0.20	0/158	0.58	0/211
All	All	0.18	0/7236	0.46	1/9690 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	GLN	N-CA-C	-5.59	106.46	113.28

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	3586	0	3398	71	0
1	B	3246	0	2931	53	0
2	W	184	0	185	9	0
2	X	159	0	157	4	0
3	B	1	0	0	0	0
All	All	7176	0	6671	123	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 9.

All (123) 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:420:LEU:O	1:A:424:ASN:ND2	2.21	0.73
1:A:209:ARG:HG2	2:W:27:LYS:HB3	1.71	0.73
1:B:440:ASP:OD2	1:B:464:ASN:ND2	2.27	0.68
1:A:477:GLU:O	1:A:481:ARG:HG2	1.94	0.67
1:B:332:ARG:O	1:B:336:LEU:HD12	1.95	0.67
1:B:108:GLN:O	1:B:112:THR:HG23	1.94	0.67
1:A:212:HIS:CE1	1:A:253:ASN:HD22	2.13	0.67
1:A:91:GLN:HB3	1:A:114:LEU:HD22	1.78	0.66
1:A:378:LEU:HD22	1:A:408:MSE:HE3	1.77	0.65
1:A:91:GLN:NE2	1:A:117:THR:OG1	2.29	0.65
1:A:444:GLU:O	1:A:448:ILE:HD12	1.97	0.65
1:B:192:LEU:O	1:B:196:ASN:ND2	2.31	0.64
1:B:68:LEU:HB3	1:B:69:PRO:HD3	1.79	0.63
1:A:462:LEU:HA	1:A:465:MSE:HE3	1.80	0.62
1:A:94:HIS:HE1	1:A:106:GLU:HG3	1.64	0.62
1:B:190:ARG:O	1:B:194:ILE:HG13	1.99	0.62
1:A:204:ASP:HB3	1:A:207:ARG:HG3	1.82	0.61
1:A:190:ARG:O	1:A:194:ILE:HG13	2.00	0.61
1:B:249:LYS:HA	1:B:252:ILE:HG22	1.83	0.61
1:A:209:ARG:NH1	2:W:30:PRO:HD2	2.16	0.60
1:B:34:ILE:HD11	1:B:50:TRP:CE3	2.37	0.59
1:B:346:ILE:HG23	1:B:361:TYR:HB2	1.84	0.59
1:A:79:LEU:HD13	1:A:116:ARG:HH21	1.67	0.59
1:B:390:GLN:HG2	1:B:428:VAL:HG22	1.85	0.59
1:B:318:LEU:HD13	1:B:337:GLN:HB3	1.84	0.58
1:A:50:TRP:HA	1:A:53:ILE:HG12	1.86	0.57
1:A:338:GLN:HE21	1:A:364:ARG:NH1	2.02	0.57
1:A:387:GLU:HA	1:A:390:GLN:HG2	1.86	0.57
1:A:454:LEU:O	1:A:458:GLN:HG3	2.05	0.56
1:A:209:ARG:HH11	2:W:29:ALA:HA	1.71	0.56
1:B:17:SER:O	1:B:21:GLU:HG2	2.06	0.56
1:A:169:ASN:HD21	1:A:209:ARG:HB2	1.70	0.55
1:A:51:PHE:HB3	1:A:74:LEU:HD13	1.87	0.54
1:A:382:PHE:HB3	1:A:405:SER:HB3	1.89	0.54
1:B:216:ASN:HD21	2:X:26:ARG:NH1	2.05	0.54
1:A:214:LEU:HB3	1:A:230:HIS:ND1	2.23	0.54
1:B:252:ILE:HD12	1:B:291:ILE:HG12	1.88	0.54
1:B:294:ASN:O	1:B:298:VAL:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLY:HA2	1:A:209:ARG:HH21	1.71	0.54
1:A:228:ARG:O	1:A:232:GLU:HB2	2.08	0.53
1:B:91:GLN:HB3	1:B:114:LEU:HD22	1.89	0.53
1:A:382:PHE:CE2	1:A:404:LYS:HD3	2.43	0.52
1:B:430:ASP:OD2	1:B:467:TYR:HE2	1.92	0.52
1:A:24:ARG:HG2	1:A:61:TYR:CD1	2.44	0.52
1:B:146:ALA:HB1	1:B:164:TYR:HA	1.92	0.52
1:A:381:SER:HA	1:A:384:VAL:HG22	1.91	0.52
1:B:312:GLU:OE2	1:B:361:TYR:OH	2.28	0.51
1:A:424:ASN:O	1:A:428:VAL:HG23	2.09	0.51
1:B:212:HIS:CE1	1:B:253:ASN:HD22	2.29	0.51
1:A:228:ARG:NE	1:A:232:GLU:OE2	2.33	0.51
1:B:342:LEU:O	1:B:346:ILE:HG12	2.11	0.50
1:B:212:HIS:CG	2:X:27:LYS:HD3	2.45	0.50
1:B:237:ILE:O	1:B:241:ILE:HG13	2.12	0.50
1:A:3:ARG:O	1:A:7:GLN:HB2	2.11	0.50
1:A:252:ILE:HD12	1:A:291:ILE:HG12	1.93	0.50
1:A:116:ARG:HH11	2:W:30:PRO:HA	1.77	0.49
1:A:29:ARG:HG2	2:W:36:LYS:HB3	1.94	0.49
1:A:169:ASN:HD21	1:A:209:ARG:CB	2.26	0.49
1:B:402:TYR:HB3	1:B:425:MSE:HB2	1.96	0.48
1:A:23:ASN:O	1:A:27:GLU:HG3	2.13	0.48
1:A:60:LYS:HE3	1:A:61:TYR:CZ	2.49	0.48
1:A:382:PHE:CE1	1:A:401:TRP:HZ3	2.31	0.48
1:B:381:SER:HA	1:B:384:VAL:HG22	1.96	0.48
1:A:29:ARG:HB3	2:W:38:PRO:HG3	1.96	0.47
1:A:388:SER:O	1:A:392:LEU:HD23	2.14	0.47
1:A:443:GLN:HG3	1:A:465:MSE:SE	2.65	0.46
1:B:222:ARG:HH22	1:B:355:TRP:HD1	1.63	0.46
1:B:395:PHE:O	1:B:399:ILE:HG12	2.15	0.46
1:A:364:ARG:O	1:A:368:ILE:HG23	2.15	0.46
1:B:214:LEU:HB3	1:B:230:HIS:ND1	2.29	0.46
1:A:249:LYS:HA	1:A:252:ILE:HG22	1.98	0.46
1:B:221:LEU:HD13	1:B:223:MSE:HE3	1.96	0.46
1:B:244:ARG:NH2	1:B:281:MSE:HG2	2.30	0.46
1:B:34:ILE:HD11	1:B:50:TRP:CD2	2.51	0.46
1:A:214:LEU:HD13	1:A:230:HIS:CE1	2.51	0.45
1:A:133:ARG:HH21	1:A:470:MSE:HG3	1.82	0.45
1:B:209:ARG:HG2	2:X:27:LYS:HB3	1.98	0.45
1:A:116:ARG:HG2	2:W:28:SER:HB2	1.99	0.45
1:B:265:ASP:O	1:B:268:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HG3	1:A:401:TRP:N	2.31	0.45
1:A:28:ALA:HB1	1:A:54:ASP:OD1	2.17	0.44
1:B:300:LYS:HA	1:B:303:GLU:OE1	2.17	0.44
1:A:181:LEU:H	1:A:181:LEU:HD12	1.81	0.44
1:B:95:LEU:HD13	1:B:110:ALA:HB3	2.00	0.44
1:A:58:SER:HA	1:A:62:LEU:HB2	1.98	0.44
1:A:249:LYS:O	1:A:252:ILE:HG22	2.17	0.44
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.88	0.44
1:B:94:HIS:CE1	1:B:106:GLU:HG3	2.52	0.44
1:A:109:ARG:HB3	2:W:31:ALA:HB1	1.99	0.44
1:B:455:PRO:HB2	1:B:456:SER:H	1.58	0.44
1:A:34:ILE:HG13	1:A:50:TRP:CD1	2.53	0.44
1:B:181:LEU:HD21	1:B:220:GLU:HG3	2.00	0.44
1:A:91:GLN:HB3	1:A:114:LEU:CD2	2.46	0.44
1:B:252:ILE:HG13	1:B:271:TYR:CE1	2.53	0.43
1:B:424:ASN:O	1:B:428:VAL:HG23	2.18	0.43
1:A:219:MSE:HE3	1:A:219:MSE:HB2	1.84	0.43
1:A:452:ALA:HB3	1:A:454:LEU:HD12	1.99	0.43
1:A:244:ARG:NH2	1:A:280:SER:O	2.52	0.43
1:B:32:ASN:HD22	1:B:32:ASN:C	2.25	0.43
1:A:105:VAL:HA	1:A:149:LEU:HD11	2.00	0.43
1:A:219:MSE:HB3	1:A:227:SER:OG	2.17	0.43
1:A:338:GLN:HE21	1:A:364:ARG:HH12	1.64	0.43
1:A:282:GLU:OE2	1:B:389:TYR:OH	2.27	0.42
1:B:222:ARG:NH2	1:B:355:TRP:HD1	2.18	0.42
1:B:256:GLU:OE1	2:X:22:THR:OG1	2.35	0.42
1:B:336:LEU:HG	1:B:372:LEU:HD21	2.01	0.42
1:B:346:ILE:CG2	1:B:361:TYR:HB2	2.50	0.42
1:A:390:GLN:HG3	1:A:391:LYS:N	2.35	0.42
1:A:374:ASP:O	1:A:378:LEU:HB2	2.19	0.41
1:A:184:ALA:O	1:A:188:LEU:HG	2.20	0.41
1:A:68:LEU:HD21	1:A:106:GLU:HG2	2.02	0.41
1:A:209:ARG:HH11	2:W:30:PRO:HD2	1.84	0.41
1:B:287:LEU:O	1:B:291:ILE:HG13	2.21	0.41
1:A:33:VAL:O	1:A:37:ILE:HG13	2.20	0.41
1:A:192:LEU:HD11	1:A:211:HIS:CE1	2.56	0.41
1:B:112:THR:HG22	1:B:142:ALA:HB1	2.03	0.41
1:B:345:LEU:HD12	1:B:345:LEU:HA	1.91	0.41
1:A:355:TRP:CZ2	1:A:391:LYS:HG3	2.56	0.41
1:B:382:PHE:O	1:B:385:ILE:HG22	2.21	0.41
1:B:419:ALA:O	1:B:423:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:HD11	1:B:294:ASN:ND2	2.36	0.40
1:A:449:ALA:HB1	1:A:457:VAL:HG23	2.02	0.40
1:B:214:LEU:HD13	1:B:230:HIS:CE1	2.57	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	456/531 (86%)	436 (96%)	20 (4%)	0	100	100
1	B	414/531 (78%)	398 (96%)	16 (4%)	0	100	100
2	W	24/45 (53%)	22 (92%)	2 (8%)	0	100	100
2	X	21/45 (47%)	20 (95%)	1 (5%)	0	100	100
All	All	915/1152 (79%)	876 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	349/441 (79%)	349 (100%)	0	100	100
1	B	303/441 (69%)	303 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	W	15/32 (47%)	15 (100%)	0	100	100
2	X	12/32 (38%)	12 (100%)	0	100	100
All	All	679/946 (72%)	679 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	212	HIS
1	A	213	ASN
1	A	272	GLN
1	A	276	ASN
1	A	338	GLN
1	A	390	GLN
1	A	469	HIS
1	B	113	GLN
1	B	180	ASN
1	B	196	ASN
1	B	212	HIS
1	B	230	HIS
1	B	475	ASN

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	449/531 (84%)	0.82	44 (9%) 13 8	4, 25, 58, 100	0
1	B	416/531 (78%)	0.94	48 (11%) 9 6	6, 30, 61, 77	0
2	W	28/45 (62%)	1.41	6 (21%) 2 2	11, 30, 50, 72	0
2	X	25/45 (55%)	0.80	0 100 100	8, 30, 36, 40	0
All	All	918/1152 (79%)	0.89	98 (10%) 11 6	4, 27, 60, 100	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	GLN	6.3
1	B	147	GLN	4.5
1	A	50	TRP	4.4
1	B	148	THR	4.3
1	B	483	GLN	4.3
1	A	158	SER	4.2
1	B	4	ASP	4.1
1	A	481	ARG	4.1
2	W	40	ARG	3.9
1	B	406	TRP	3.9
1	A	473	PHE	3.8
1	B	101	ALA	3.7
1	B	472	ARG	3.7
1	B	3	ARG	3.7
1	A	474	ASP	3.6
2	W	39	HIS	3.5
1	B	455	PRO	3.4
1	B	471	ILE	3.4
2	W	32	THR	3.4
1	B	439	LEU	3.4
1	B	330	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	482	LEU	3.4
1	B	128	ASP	3.4
1	A	111	CYS	3.3
1	A	439	LEU	3.3
1	B	459	LEU	3.3
1	A	471	ILE	3.3
2	W	4	LYS	3.1
1	A	4	ASP	3.1
1	B	440	ASP	3.1
1	B	475	ASN	3.0
1	B	111	CYS	3.0
1	B	146	ALA	3.0
1	A	482	LEU	2.9
1	B	327	GLY	2.9
1	B	390	GLN	2.9
1	A	483	GLN	2.9
1	A	5	GLU	2.8
1	A	130	TYR	2.8
1	A	303	GLU	2.8
1	B	464	ASN	2.7
1	B	9	SER	2.7
1	A	179	ASP	2.7
1	A	453	ASN	2.7
1	A	3	ARG	2.7
1	B	56	ASP	2.6
1	A	413	GLY	2.6
1	B	98	ALA	2.6
1	A	456	SER	2.6
2	W	33	GLY	2.6
1	A	435	TRP	2.6
1	B	122	PHE	2.6
1	B	473	PHE	2.6
1	B	481	ARG	2.6
1	B	410	LYS	2.5
1	B	329	SER	2.4
1	A	438	ALA	2.4
1	A	440	ASP	2.4
1	A	472	ARG	2.4
1	A	466	HIS	2.4
1	B	129	HIS	2.4
1	B	179	ASP	2.4
1	A	419	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	446	TYR	2.3
1	B	105	VAL	2.3
1	A	95	LEU	2.3
1	A	233	GLN	2.3
2	W	5	GLN	2.3
1	B	436	ALA	2.3
1	A	150	LYS	2.3
1	A	107	GLN	2.3
1	A	331	GLU	2.2
1	B	102	SER	2.2
1	B	91	GLN	2.2
1	A	241	ILE	2.2
1	A	208	SER	2.2
1	B	458	GLN	2.2
1	A	468	SER	2.2
1	B	418	GLN	2.2
1	A	216	ASN	2.2
1	A	100	ASP	2.1
1	B	48	LEU	2.1
1	A	441	ALA	2.1
1	A	20	GLU	2.1
1	B	407	GLU	2.1
1	B	32	ASN	2.1
1	B	170	ASN	2.1
1	B	195	CYS	2.1
1	B	412	ILE	2.1
1	A	2	GLY	2.1
1	A	27	GLU	2.1
1	A	388	SER	2.1
1	B	384	VAL	2.1
1	A	385	ILE	2.1
1	B	67	LEU	2.1
1	B	476	ILE	2.1
1	B	171	ILE	2.0
1	A	122	PHE	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.