W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2022 – 10:32 AM EDT

PDB ID	:	7T7T
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)

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

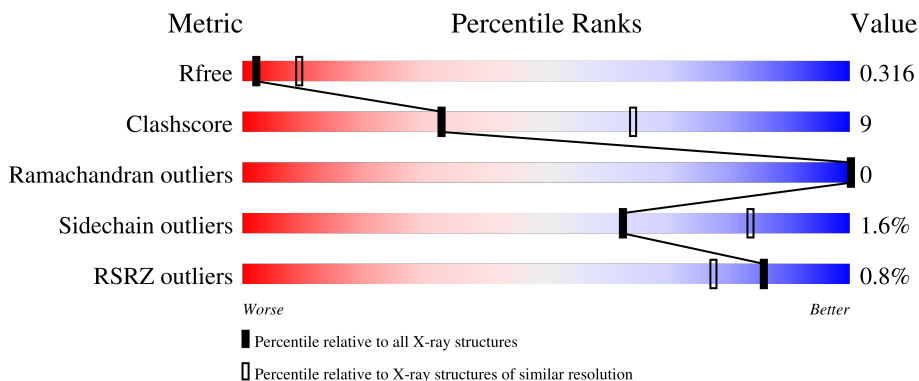|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	Percentile Ranks	Value
Rfree		0.316
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (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 <=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	70% 18% 12%
1	B	531	.% 66% 15% 19%
2	W	45	47% 16% 38%
2	X	45	51% • 44%

W O R L D W I D E

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PROTEIN DATA BANK

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 3586	C 2252	N 634	O 676	S 8	Se 16	0	0	0
1	B	432	Total 3246	C 2028	N 566	O 628	S 8	Se 16	0	0	0

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 159	C 97	N 32	O 30	0	0	0
2	W	28	Total 184	C 113	N 37	O 34	0	0	0

- Molecule 3 is water.

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

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.
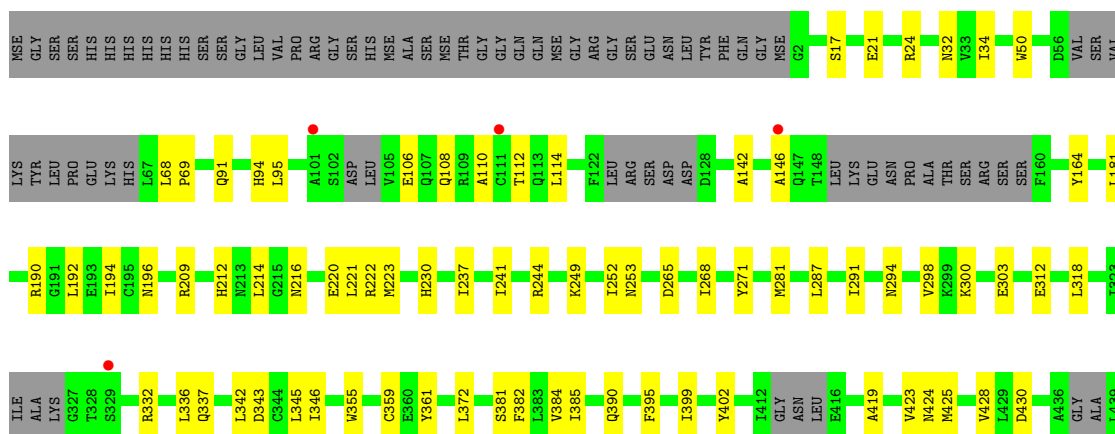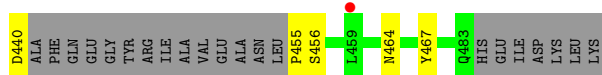
- Molecule 1: Protein TONSOKU

Chain A:
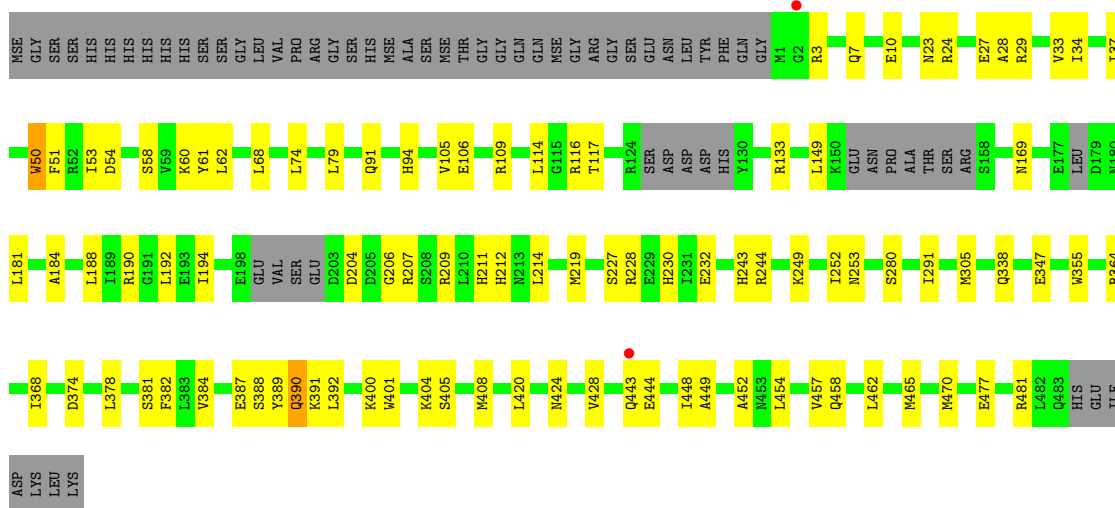
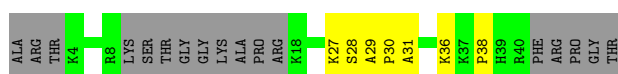- Molecule 1: Protein TONSOKU

Chain B:

D440 ALA PHE GLN GLU GLY TYR ARG ILE ALA VAL GLU ALA ASN LEU P455 S456 L459 N464 Y467 Q483 HIS GLU ILE ASP LYS LEU LYS

● Molecule 2: Histone H3.1

Chain X:

51% . 44%

ALA ARG T3 K9 SER THR GLY GLY LYS ALA PRO ARG LYS Q19 R26 K27 K36 LYS PRO HIS ARG PHE ARG PRO GLY THR

● Molecule 2: Histone H3.1

Chain W:

47% 16% 38%

ALA ARG THR K4 R8 LYS SER THR GLY GLY LYS ALA PRO ARG K18 K27 S28 A29 P30 A31 K36 K37 P38 H39 R40 PHE ARG PRO GLY THR

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 39.61 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.53-3.17) 97.5 (39.61-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.279 , 0.318 0.277 , 0.316	Depositor DCC
R_{free} test set	2000 reflections (7.31%)	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 , 45.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.27	0/3621	0.51	0/4847
1	B	0.27	0/3273	0.50	0/4386
2	W	0.30	0/184	0.60	0/246
2	X	0.28	0/158	0.63	0/211
All	All	0.27	0/7236	0.51	0/9690

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	70	0
1	B	3246	0	2931	50	0
2	W	184	0	185	9	0
2	X	159	0	157	3	0
3	B	1	0	0	0	0
All	All	7176	0	6671	120	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 (120) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:312:GLU:OE2	1:B:361:TYR:OH	2.28	0.47
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:A:400:LYS:HG3	1:A:401:TRP:N	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:222:ARG:NH2	1:B:355:TRP:HD1	2.18	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
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 ⓘ

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	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 ⓘ

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%)	342 (98%)	7 (2%)	55	79
1	B	303/441 (69%)	299 (99%)	4 (1%)	69	86
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%)	668 (98%)	11 (2%)	62	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	50	TRP

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Mol	Chain	Res	Type
1	A	243	HIS
1	A	305	MSE
1	A	347	GLU
1	A	389	TYR
1	A	390	GLN
1	B	24	ARG
1	B	32	ASN
1	B	343	ASP
1	B	359	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	212	HIS
1	A	213	ASN
1	A	338	GLN
1	B	196	ASN
1	B	212	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 ⓘ

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(Å²)	Q<0.9
1	A	449/531 (84%)	-0.15	2 (0%)	92	89	4, 25, 58, 100	0
1	B	416/531 (78%)	-0.05	5 (1%)	79	67	6, 30, 61, 77	0
2	W	28/45 (62%)	-0.11	0	100	100	11, 30, 50, 72	0
2	X	25/45 (55%)	-0.36	0	100	100	8, 30, 36, 40	0
All	All	918/1152 (79%)	-0.11	7 (0%)	86	77	4, 27, 60, 100	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	GLN	4.3
1	B	101	ALA	3.5
1	A	2	GLY	3.3
1	B	329	SER	2.8
1	B	146	ALA	2.7
1	B	459	LEU	2.7
1	B	111	CYS	2.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.5 Other polymers (i)

There are no such residues in this entry.