



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2026 – 02:12 PM EDT

PDB ID : 38NR / pdb_000038nr
Title : Structure of TONSOKU (TSK)/BRU1 TPR domain bound to Histone H3.1
K4me1K27ac
Authors : Davarinejad, H.; Couture, J.F.
Deposited on : 2026-09-08
Resolution : 3.09 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 Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

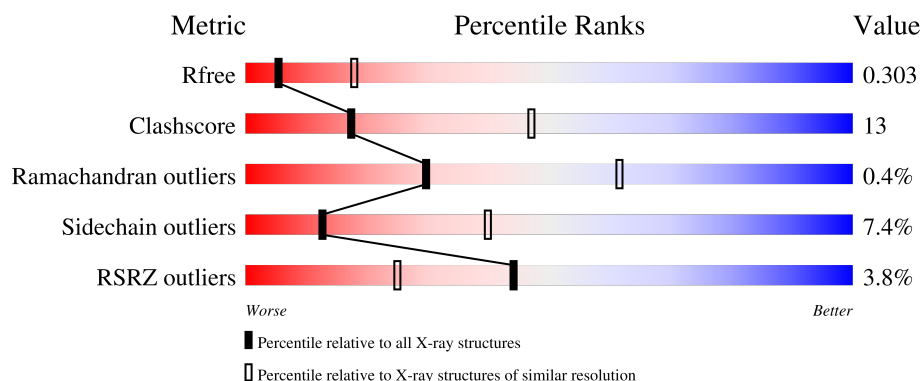
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	491	
1	B	491	
2	W	46	
2	X	46	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7067 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	470	Total	C	N	O	S	Se	0	0	0
			3495	2182	623	667	8	15			
1	B	456	Total	C	N	O	S	Se	0	0	0
			3198	1982	562	632	8	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	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	28	Total	C	N	O	0	0	0
			170	105	32	33			
2	W	33	Total	C	N	O	0	0	0
			204	126	38	40			

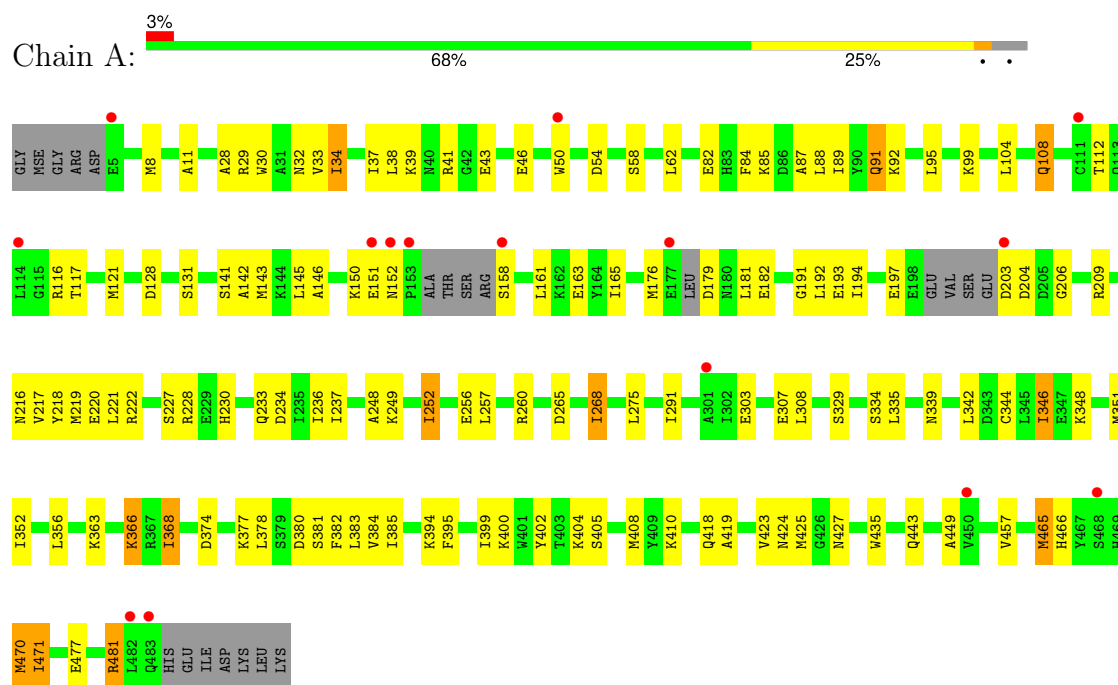
There are 2 discrepancies between the modelled and reference sequences:

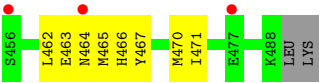
Chain	Residue	Modelled	Actual	Comment	Reference
X	46	TYR	-	expression tag	UNP P59226
W	46	TYR	-	expression tag	UNP P59226

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 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	84.11Å 92.80Å 206.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.24 – 3.09 55.24 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.0 (55.24-3.09) 97.0 (55.24-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.07Å)	Xtriage
Refinement program	PHENIX 2.1_6048	Depositor
R, R_{free}	0.262 , 0.300 0.264 , 0.303	Depositor DCC
R_{free} test set	1503 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 90.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: ALY, MLZ

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	0.44	0/3531	0.65	0/4749
1	B	0.43	0/3221	0.59	0/4343
2	W	0.32	0/180	0.51	0/244
2	X	0.45	0/146	0.61	0/196
All	All	0.44	0/7078	0.62	0/9532

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 [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	3495	0	3152	83	0
1	B	3198	0	2648	78	0
2	W	204	0	176	4	0
2	X	170	0	146	9	0
All	All	7067	0	6122	165	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 13.

All (165) 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:B:322:MSE:HE1	1:B:335:LEU:HD23	1.59	0.83
1:B:54:ASP:O	1:B:58:SER:HB2	1.83	0.79
1:A:351:MSE:HA	2:W:19:GLN:HG2	1.63	0.78
1:B:211:HIS:HD2	1:B:230:HIS:HD2	1.35	0.75
1:A:382:PHE:HB2	1:A:405:SER:HB3	1.72	0.71
1:A:95:LEU:O	1:A:99:LYS:HG2	1.92	0.70
2:W:4:MLZ:HCM3	2:W:4:MLZ:H	1.57	0.69
1:A:477:GLU:O	1:A:481:ARG:HG2	1.93	0.68
1:B:379:SER:HB3	1:B:408:MSE:HB3	1.76	0.68
1:A:87:ALA:O	1:A:91:GLN:HG2	1.95	0.67
1:A:58:SER:HA	1:A:62:LEU:HD12	1.77	0.67
1:A:112:THR:O	1:A:116:ARG:HG3	1.95	0.65
1:A:34:ILE:HD11	1:A:50:TRP:CD2	2.32	0.65
1:A:363:LYS:HG2	1:A:385:ILE:HD11	1.78	0.65
1:B:76:GLU:OE2	1:B:80:ARG:HD2	1.98	0.63
1:A:363:LYS:HD3	1:A:366:LYS:HE3	1.80	0.63
1:A:378:LEU:HB3	1:A:408:MSE:HE3	1.81	0.62
1:A:449:ALA:HB1	1:A:457:VAL:HG23	1.82	0.61
1:B:55:TYR:O	1:B:59:VAL:HG23	1.99	0.61
1:B:211:HIS:CD2	1:B:230:HIS:HD2	2.18	0.61
1:A:30:TRP:O	1:A:34:ILE:HG23	2.00	0.61
1:A:335:LEU:HD22	1:A:368:ILE:HG23	1.83	0.60
1:A:34:ILE:HD11	1:A:50:TRP:CE2	2.36	0.60
1:B:194:ILE:O	1:B:198:GLU:HG2	2.02	0.59
1:A:248:ALA:O	1:A:252:ILE:HG22	2.02	0.59
1:B:190:ARG:O	1:B:194:ILE:HG13	2.03	0.58
1:A:303:GLU:O	1:A:307:GLU:HG3	2.04	0.57
1:A:395:PHE:O	1:A:399:ILE:HG12	2.04	0.57
1:A:435:TRP:CZ3	1:A:471:ILE:HB	2.39	0.57
1:B:127:ASP:HA	1:B:470:MSE:HE1	1.87	0.57
1:B:246:GLY:HA2	2:X:27:ALY:HE3	1.87	0.57
1:B:251:TYR:CE1	1:B:273:LYS:HD2	2.40	0.56
1:A:400:LYS:O	1:A:404:LYS:HG3	2.06	0.56
1:A:424:ASN:O	1:A:427:ASN:HB2	2.05	0.56
1:B:462:LEU:HA	1:B:465:MSE:HE2	1.87	0.56
1:B:356:LEU:HD12	1:B:392:LEU:HD21	1.89	0.55
1:B:105:VAL:HG13	1:B:106:GLU:H	1.71	0.55
1:B:231:ILE:HD12	1:B:257:LEU:HD12	1.89	0.55
1:B:282:GLU:HG3	1:B:283:ASP:OD1	2.07	0.54
1:A:191:GLY:HA2	1:A:194:ILE:HD12	1.88	0.54
1:B:463:GLU:O	1:B:466:HIS:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:TRP:HZ3	1:A:471:ILE:HB	1.74	0.53
1:A:29:ARG:O	1:A:33:VAL:HG23	2.09	0.53
1:A:206:GLY:HA2	1:A:209:ARG:NH1	2.24	0.53
1:B:317:LYS:O	1:B:321:ASN:HB2	2.08	0.53
1:A:356:LEU:H	1:A:356:LEU:HD22	1.73	0.53
1:A:443:GLN:HG2	1:A:465:MSE:HE3	1.90	0.53
1:B:463:GLU:O	1:B:466:HIS:CB	2.57	0.53
1:B:315:LEU:HB2	1:B:341:SER:OG	2.10	0.52
1:B:113:GLN:HG2	2:X:31:ALA:HB2	1.91	0.52
1:A:181:LEU:HB3	1:A:221:LEU:HD21	1.91	0.52
1:A:8:MSE:HE1	1:A:34:ILE:HB	1.92	0.51
1:A:219:MSE:HE2	1:A:257:LEU:HB2	1.91	0.51
1:B:222:ARG:HB2	1:B:222:ARG:NH1	2.26	0.51
1:B:402:TYR:CZ	1:B:424:ASN:HB3	2.46	0.50
1:A:443:GLN:CG	1:A:465:MSE:HE3	2.41	0.50
1:A:228:ARG:HB2	1:A:257:LEU:HD21	1.93	0.50
1:A:161:LEU:O	1:A:165:ILE:HD12	2.12	0.49
1:B:29:ARG:O	1:B:33:VAL:HG23	2.13	0.49
1:B:287:LEU:O	1:B:291:ILE:HG13	2.12	0.49
1:A:193:GLU:O	1:A:197:GLU:HG3	2.13	0.49
2:W:4:MLZ:H	2:W:4:MLZ:CM	2.25	0.49
1:B:172:GLY:HA2	1:B:187:LEU:HD13	1.94	0.49
1:A:218:TYR:HE2	1:A:230:HIS:CD2	2.32	0.48
1:A:381:SER:O	1:A:385:ILE:HB	2.13	0.48
1:A:8:MSE:HE1	1:A:34:ILE:HD12	1.95	0.48
1:A:382:PHE:HE2	1:A:408:MSE:HE2	1.79	0.48
1:B:129:HIS:CB	1:B:470:MSE:HE2	2.44	0.48
1:A:95:LEU:HD11	1:A:99:LYS:HE3	1.96	0.48
1:A:383:LEU:HD12	1:A:402:TYR:HE1	1.77	0.48
1:B:26:GLU:O	1:B:30:TRP:HD1	1.97	0.48
1:B:408:MSE:HE3	1:B:408:MSE:HB2	1.75	0.48
1:A:28:ALA:HB1	1:A:54:ASP:OD1	2.14	0.48
1:A:382:PHE:CB	1:A:405:SER:HB3	2.44	0.48
1:B:389:TYR:CE1	1:B:397:LYS:HD2	2.49	0.47
1:B:214:LEU:HD13	1:B:230:HIS:CE1	2.49	0.47
1:A:220:GLU:C	1:A:222:ARG:H	2.22	0.47
1:B:305:MSE:HE3	1:B:309:LYS:HD3	1.96	0.47
1:B:303:GLU:O	1:B:307:GLU:HG3	2.14	0.47
1:B:430:ASP:OD2	1:B:467:TYR:HE1	1.98	0.47
1:A:249:LYS:HA	1:A:252:ILE:CG2	2.45	0.47
1:A:394:LYS:HD3	1:A:394:LYS:HA	1.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASP:O	1:A:384:VAL:HG23	2.15	0.46
1:B:390:GLN:HB2	1:B:428:VAL:HG22	1.96	0.46
1:B:356:LEU:CD1	1:B:392:LEU:HD21	2.45	0.46
1:A:256:GLU:O	1:A:260:ARG:HG3	2.15	0.46
1:A:34:ILE:HD11	1:A:50:TRP:CE3	2.50	0.46
1:A:466:HIS:NE2	1:A:470:MSE:HE1	2.30	0.45
1:A:143:MSE:HE3	1:A:146:ALA:HB3	1.98	0.45
1:A:233:GLN:O	1:A:237:ILE:HG22	2.16	0.45
1:A:382:PHE:O	1:A:385:ILE:HG22	2.15	0.45
1:B:305:MSE:HE1	1:B:357:LYS:NZ	2.31	0.45
1:A:88:LEU:HD12	1:A:121:MSE:HE1	1.98	0.45
1:A:88:LEU:HB3	1:A:92:LYS:HE2	1.99	0.45
1:A:176:MSE:O	1:A:179:ASP:HA	2.17	0.45
1:A:410:LYS:HA	1:A:418:GLN:OE1	2.17	0.45
1:B:176:MSE:SE	1:B:216:ASN:HB3	2.67	0.45
1:A:84:PHE:HB3	1:A:121:MSE:HE3	1.99	0.45
1:A:108:GLN:OE1	1:A:163:GLU:HG2	2.17	0.45
1:A:344:CYS:O	1:A:348:LYS:HG3	2.17	0.44
1:A:363:LYS:CD	1:A:366:LYS:HE3	2.46	0.44
1:A:275:LEU:HB2	1:A:291:ILE:HG21	1.98	0.44
1:A:11:ALA:HB1	1:A:34:ILE:HG22	1.98	0.44
1:B:346:ILE:HB	1:B:358:HIS:CD2	2.52	0.44
1:A:88:LEU:HG	1:A:117:THR:HG21	1.99	0.44
1:A:470:MSE:HE2	1:A:470:MSE:HB2	1.75	0.44
1:B:346:ILE:HG22	1:B:361:TYR:CB	2.47	0.44
2:X:19:GLN:O	2:X:20:LEU:HD23	2.18	0.44
1:B:181:LEU:HD22	1:B:221:LEU:CD2	2.48	0.44
1:B:261:VAL:HG12	1:B:263:LYS:HG3	2.00	0.44
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.70	0.43
1:B:462:LEU:HA	1:B:465:MSE:HB2	2.00	0.43
1:B:209:ARG:HH11	1:B:209:ARG:HG3	1.83	0.43
2:W:27:ALY:HE2	2:W:27:ALY:HH31	1.47	0.43
1:A:192:LEU:HD23	1:A:192:LEU:HA	1.70	0.43
1:B:75:GLY:HA3	1:B:91:GLN:HG2	2.01	0.43
1:B:66:HIS:O	1:B:69:PRO:HD2	2.17	0.43
1:B:382:PHE:HB2	1:B:405:SER:HB2	2.01	0.43
1:B:403:THR:HG23	1:B:425:MSE:SE	2.69	0.43
1:B:362:ALA:HB1	1:B:384:VAL:HG23	2.01	0.43
1:A:150:LYS:C	1:A:152:ASN:H	2.27	0.43
1:B:209:ARG:HE	2:X:29:ALA:HB2	1.84	0.43
1:B:211:HIS:HD2	1:B:230:HIS:CD2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:O	1:B:346:ILE:HG23	2.18	0.43
1:A:374:ASP:CG	1:A:377:LYS:HD2	2.44	0.42
1:B:471:ILE:HA	1:B:471:ILE:HD12	1.78	0.42
1:A:203:ASP:C	1:A:237:ILE:HD11	2.43	0.42
1:A:104:LEU:HA	1:A:104:LEU:HD13	1.79	0.42
1:B:32:ASN:HD22	1:B:51:PHE:HE1	1.66	0.42
1:B:176:MSE:HE3	1:B:176:MSE:HB2	1.98	0.42
1:B:183:GLU:O	1:B:187:LEU:HD12	2.20	0.42
1:A:108:GLN:NE2	1:A:163:GLU:HB3	2.34	0.42
1:A:419:ALA:O	1:A:423:VAL:HG23	2.19	0.42
1:A:204:ASP:N	1:A:237:ILE:HD11	2.35	0.42
1:B:219:MSE:HB2	1:B:227:SER:OG	2.18	0.42
1:A:38:LEU:HD13	1:A:46:GLU:O	2.20	0.42
1:A:39:LYS:HB3	1:A:39:LYS:HE2	1.87	0.42
1:A:84:PHE:CB	1:A:121:MSE:HE3	2.50	0.42
1:B:435:TRP:CZ3	1:B:471:ILE:HG21	2.55	0.42
1:B:94:HIS:ND1	1:B:110:ALA:HB2	2.35	0.42
1:B:173:MSE:HE1	2:X:28:SER:CB	2.50	0.42
1:B:212:HIS:ND1	2:X:27:ALY:HB3	2.35	0.42
1:B:346:ILE:HG21	1:B:346:ILE:HD13	1.73	0.42
1:B:68:LEU:HB2	1:B:69:PRO:HD3	2.02	0.41
1:B:382:PHE:O	1:B:385:ILE:HG22	2.19	0.41
1:B:311:GLU:OE2	1:B:314:ASN:HB3	2.20	0.41
1:A:32:ASN:HB2	1:A:54:ASP:OD2	2.20	0.41
1:A:141:SER:O	1:A:145:LEU:HD12	2.20	0.41
1:B:214:LEU:HD22	1:B:230:HIS:CE1	2.56	0.41
1:B:219:MSE:HG2	1:B:260:ARG:HH11	1.85	0.41
1:B:335:LEU:HD23	1:B:335:LEU:HA	1.92	0.41
1:B:32:ASN:HB2	1:B:54:ASP:OD2	2.20	0.41
1:B:464:ASN:HB3	2:X:4:MLZ:HA	2.02	0.41
1:B:403:THR:O	1:B:407:GLU:HG2	2.21	0.41
1:A:112:THR:HG23	1:A:142:ALA:HB1	2.03	0.41
1:B:383:LEU:HD12	1:B:383:LEU:HA	1.86	0.41
1:B:464:ASN:HD22	2:X:5:GLN:H	1.69	0.41
1:A:37:ILE:O	1:A:41:ARG:HG3	2.21	0.40
1:A:128:ASP:HB3	1:A:131:SER:OG	2.21	0.40
1:B:165:ILE:O	1:B:168:HIS:HB2	2.20	0.40
1:B:271:TYR:CE2	1:B:294:ASN:HB3	2.56	0.40
1:A:265:ASP:O	1:A:268:ILE:HG13	2.22	0.40
1:A:342:LEU:O	1:A:346:ILE:HG12	2.22	0.40
1:B:346:ILE:HG22	1:B:361:TYR:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:HE	2:X:29:ALA:CB	2.33	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	462/491 (94%)	432 (94%)	28 (6%)	2 (0%)	30	61
1	B	438/491 (89%)	401 (92%)	35 (8%)	2 (0%)	24	57
2	W	27/46 (59%)	25 (93%)	2 (7%)	0	100	100
2	X	22/46 (48%)	18 (82%)	4 (18%)	0	100	100
All	All	949/1074 (88%)	876 (92%)	69 (7%)	4 (0%)	30	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	329	SER
1	B	242	GLU
1	B	373	CYS

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	319/413 (77%)	291 (91%)	28 (9%)	9	33
1	B	260/413 (63%)	245 (94%)	15 (6%)	18	48
2	W	11/31 (36%)	11 (100%)	0	100	100
2	X	8/31 (26%)	7 (88%)	1 (12%)	4	19
All	All	598/888 (67%)	554 (93%)	44 (7%)	13	40

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	43	GLU
1	A	82	GLU
1	A	85	LYS
1	A	89	ILE
1	A	91	GLN
1	A	108	GLN
1	A	158	SER
1	A	182	GLU
1	A	216	ASN
1	A	217	VAL
1	A	227	SER
1	A	234	ASP
1	A	236	ILE
1	A	252	ILE
1	A	268	ILE
1	A	308	LEU
1	A	334	SER
1	A	339	ASN
1	A	346	ILE
1	A	352	ILE
1	A	366	LYS
1	A	368	ILE
1	A	425	MSE
1	A	465	MSE
1	A	470	MSE
1	A	471	ILE
1	A	481	ARG
1	B	4	ASP
1	B	58	SER
1	B	86	ASP
1	B	105	VAL
1	B	176	MSE

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Mol	Chain	Res	Type
1	B	200	VAL
1	B	214	LEU
1	B	216	ASN
1	B	289	SER
1	B	295	ILE
1	B	379	SER
1	B	403	THR
1	B	405	SER
1	B	408	MSE
1	B	425	MSE
2	X	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	258	HIS
1	B	211	HIS
1	B	230	HIS
1	B	253	ASN
1	B	464	ASN
1	B	466	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLZ	W	4	2	8,9,10	0.69	0	4,9,11	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLZ	X	4	2	8,9,10	0.81	0	4,9,11	0.60	0
2	ALY	W	27	2	10,11,12	0.54	0	7,12,14	0.52	0
2	ALY	X	27	2	10,11,12	0.52	0	7,12,14	1.67	2 (28%)

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	MLZ	W	4	2	-	1/7/8/10	-
2	MLZ	X	4	2	-	0/7/8/10	-
2	ALY	W	27	2	-	5/9/10/12	-
2	ALY	X	27	2	-	7/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	27	ALY	CD-CE-NZ	-3.29	102.98	112.20
2	X	27	ALY	CE-NZ-CH	2.74	126.60	122.56

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	27	ALY	C-CA-CB-CG
2	X	27	ALY	O-C-CA-CB
2	W	4	MLZ	CD-CE-NZ-CM
2	W	27	ALY	C-CA-CB-CG
2	X	27	ALY	CG-CD-CE-NZ
2	X	27	ALY	OH-CH-NZ-CE
2	X	27	ALY	CH3-CH-NZ-CE
2	W	27	ALY	OH-CH-NZ-CE
2	W	27	ALY	CH3-CH-NZ-CE
2	W	27	ALY	CG-CD-CE-NZ
2	W	27	ALY	CE-CD-CG-CB
2	X	27	ALY	CE-CD-CG-CB
2	X	27	ALY	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	W	4	MLZ	2	0
2	X	4	MLZ	1	0
2	W	27	ALY	1	0
2	X	27	ALY	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	454/491 (92%)	0.08	15 (3%)	49	29	66, 93, 129, 172	0
1	B	440/491 (89%)	0.23	19 (4%)	40	22	69, 102, 148, 183	0
2	W	31/46 (67%)	0.13	1 (3%)	50	30	76, 99, 119, 134	0
2	X	26/46 (56%)	0.34	1 (3%)	44	25	79, 105, 116, 126	0
All	All	951/1074 (88%)	0.15	36 (3%)	44	25	66, 97, 137, 183	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	PRO	3.8
1	A	483	GLN	3.8
1	B	464	ASN	3.7
1	B	450	VAL	3.4
1	A	152	ASN	3.1
1	B	148	THR	3.1
1	B	477	GLU	3.1
1	B	127	ASP	3.1
1	B	416	GLU	3.0
1	B	2	GLY	2.9
1	A	151	GLU	2.9
1	B	64	GLU	2.8
1	A	482	LEU	2.8
1	B	107	GLN	2.8
1	B	418	GLN	2.7
1	B	122	PHE	2.6
1	A	158	SER	2.6
1	A	177	GLU	2.5
1	B	170	ASN	2.5
1	A	468	SER	2.5
1	A	301	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	2.4
1	B	111	CYS	2.4
1	A	111	CYS	2.4
1	B	160	PHE	2.3
1	A	5	GLU	2.3
1	B	47	ALA	2.3
2	X	5	GLN	2.3
1	B	183	GLU	2.3
1	A	50	TRP	2.2
1	B	60	LYS	2.2
1	A	450	VAL	2.2
2	W	11	THR	2.1
1	A	203	ASP	2.1
1	B	456	SER	2.1
1	B	245	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ALY	X	27	12/13	0.90	0.18	76,80,85,88	0
2	MLZ	W	4	10/11	0.90	0.12	97,104,107,109	0
2	MLZ	X	4	10/11	0.92	0.14	80,110,116,119	0
2	ALY	W	27	12/13	0.96	0.12	71,77,83,83	0

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.