Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2026 – 06:10 PM EDT

PDB ID	:	38NQ / pdb_000038nq
Title	:	Structure of TONSOKU (TSK)/BRU1 TPR domain bound to Histone H3.1 K27ac
Authors	:	Davarinejad, H.; Couture, J.F.
Deposited on	:	2026-09-08
Resolution	:	2.79 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:

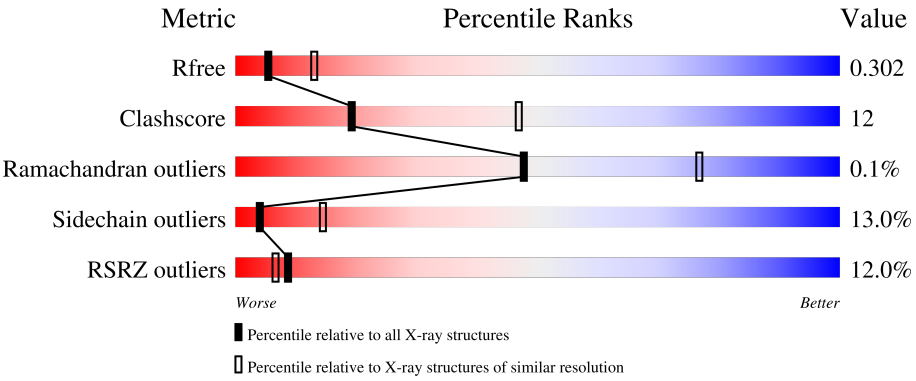
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	491	9% 67% 25% • 5%
1	B	491	11% 69% 19% • 8%
2	W	46	13% 54% 13% • 30%
2	X	46	17% 50% 7% 43%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7027 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	468	Total	C	N	O	S	Se	0	0	0
			3474	2179	614	658	8	15			
1	B	452	Total	C	N	O	S	Se	0	0	0
			3197	1988	561	624	8	16			

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	26	Total	C	N	O	0	0	0
			159	95	31	33			
2	W	32	Total	C	N	O	0	0	0
			197	120	38	39			

There are 2 discrepancies between the modelled and reference sequences:

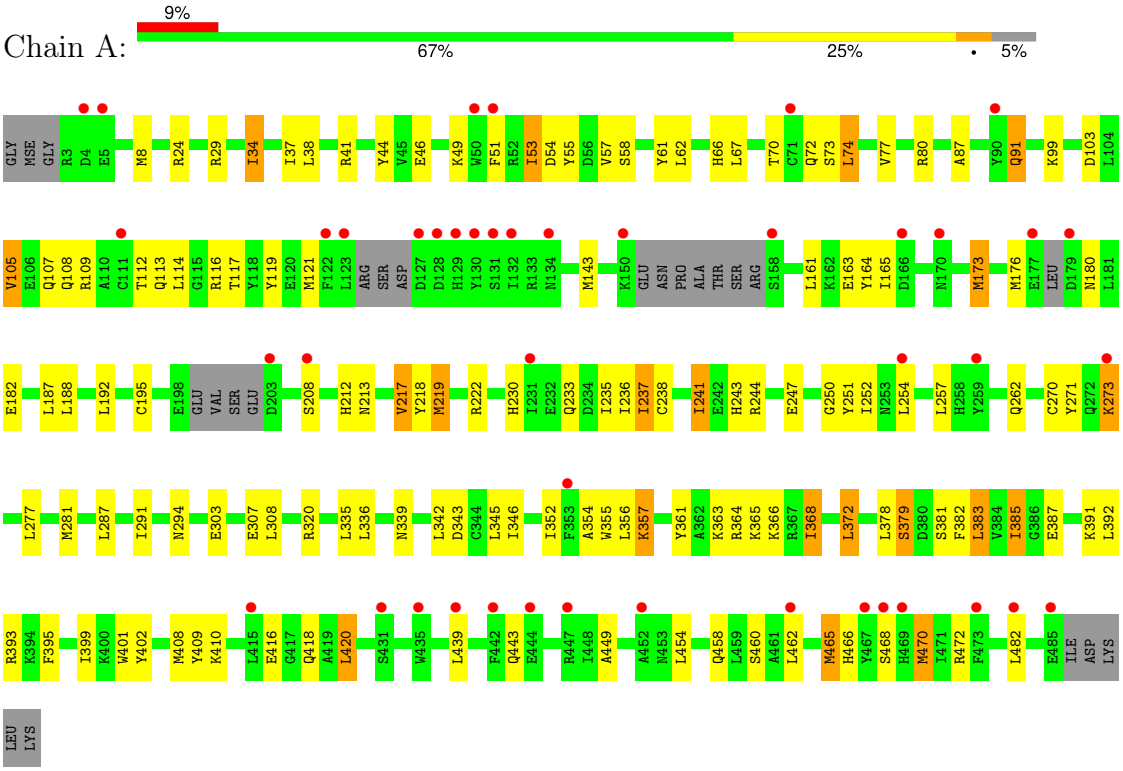
Chain	Residue	Modelled	Actual	Comment	Reference
X	46	TYR	-	expression tag	UNP P59226
W	46	TYR	-	expression tag	UNP P59226

3 Residue-property plots (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.

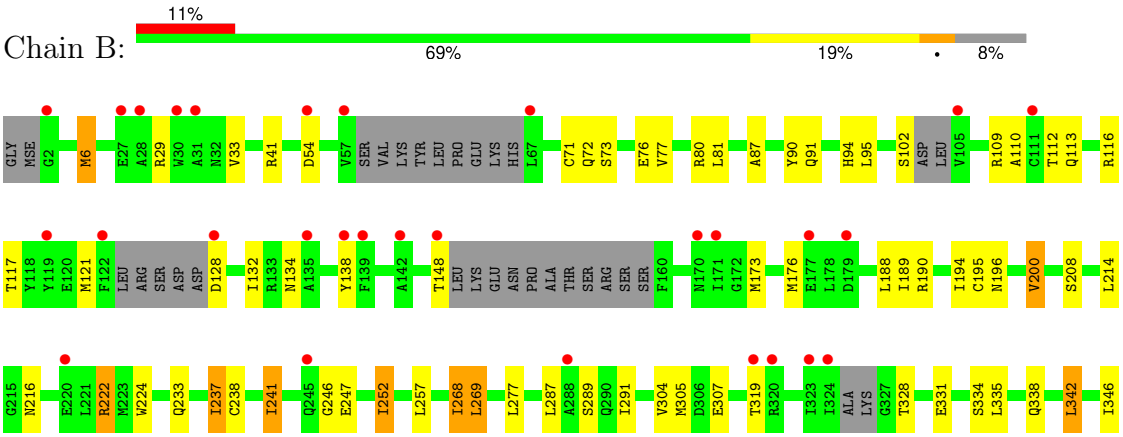
• Molecule 1: Protein TONSOKU

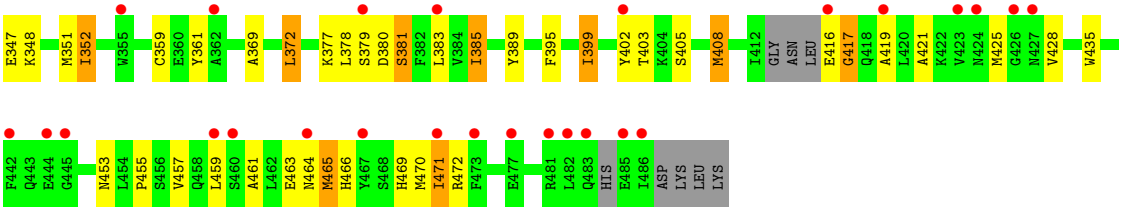
Chain A:



• Molecule 1: Protein TONSOKU

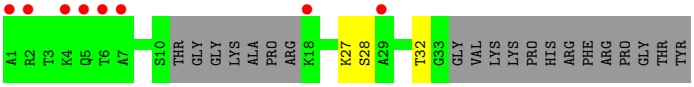
Chain B:





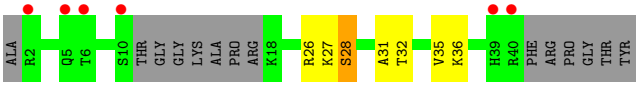
• Molecule 2: Histone H3.1





• Molecule 2: Histone H3.1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.93Å 92.36Å 207.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.35 – 2.79 40.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.35-2.79) 97.8 (40.35-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.81Å)	Xtriage
Refinement program	PHENIX 2.1_6048	Depositor
R, R_{free}	0.256 , 0.299 0.261 , 0.302	Depositor DCC
R_{free} test set	2016 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	100.3	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 102.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7027	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: ALY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.39	0/3508	0.62	1/4717 (0.0%)
1	B	0.37	0/3223	0.59	1/4348 (0.0%)
2	W	0.35	0/184	0.68	0/250
2	X	0.36	0/145	0.57	0/196
All	All	0.38	0/7060	0.61	2/9511 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	ILE	N-CA-C	-6.92	102.51	110.05
1	B	352	ILE	N-CA-C	-5.39	104.17	110.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	222	ARG	Sidechain

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	3474	0	3143	90	0
1	B	3197	0	2682	63	0
2	W	197	0	170	10	0
2	X	159	0	138	4	0
All	All	7027	0	6133	154	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 12.

All (154) 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:173:MSE:HE1	2:W:28:SER:HA	1.44	0.97
1:B:208:SER:HB2	1:B:237:ILE:HD13	1.49	0.92
1:A:116:ARG:HD2	2:W:28:SER:HB2	1.66	0.76
1:A:108:GLN:HE21	1:A:163:GLU:HB3	1.51	0.74
1:A:462:LEU:HA	1:A:465:MSE:HE2	1.68	0.74
1:B:252:ILE:HD11	1:B:291:ILE:HG12	1.69	0.71
1:A:58:SER:HA	1:A:62:LEU:HD12	1.73	0.70
1:A:342:LEU:HD11	1:A:364:ARG:HG2	1.74	0.68
1:B:348:LYS:HA	1:B:351:MSE:HE3	1.75	0.68
1:A:238:CYS:HB3	1:A:247:GLU:HB3	1.75	0.68
1:A:247:GLU:HG3	1:A:277:LEU:HD13	1.76	0.65
1:A:112:THR:O	1:A:116:ARG:HG3	1.96	0.65
1:A:364:ARG:O	1:A:368:ILE:HG23	1.97	0.65
1:A:51:PHE:HB3	1:A:74:LEU:HD13	1.77	0.65
1:A:87:ALA:O	1:A:91:GLN:HG2	1.99	0.63
1:A:66:HIS:HD1	2:W:36:LYS:HE3	1.64	0.63
1:A:449:ALA:HB1	1:A:458:GLN:HG3	1.81	0.63
1:B:233:GLN:O	1:B:237:ILE:HG22	1.99	0.62
1:B:347:GLU:HG2	1:B:351:MSE:HE2	1.80	0.62
1:A:241:ILE:HG22	1:A:243:HIS:HB2	1.81	0.62
1:A:382:PHE:O	1:A:385:ILE:HG22	2.00	0.61
1:A:212:HIS:CD2	2:W:27:ALY:HB3	2.36	0.61
1:B:342:LEU:HD12	1:B:361:TYR:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:O	1:B:291:ILE:HG13	2.02	0.60
1:A:368:ILE:O	1:A:372:LEU:HB2	2.00	0.60
1:A:24:ARG:HD2	1:A:61:TYR:CD2	2.37	0.59
1:A:222:ARG:HH21	1:A:355:TRP:HD1	1.51	0.59
1:A:91:GLN:OE1	1:A:113:GLN:HB3	2.03	0.58
1:A:343:ASP:O	1:A:346:ILE:HG13	2.04	0.58
1:B:94:HIS:ND1	1:B:110:ALA:HB2	2.18	0.58
1:B:402:TYR:HB3	1:B:425:MSE:HE2	1.86	0.58
1:A:161:LEU:O	1:A:165:ILE:HD12	2.05	0.56
1:A:462:LEU:HD23	1:A:465:MSE:HE3	1.87	0.56
1:B:379:SER:HB3	1:B:408:MSE:HB3	1.87	0.56
1:A:58:SER:HB3	1:A:67:LEU:HD22	1.88	0.56
1:A:235:ILE:HG12	1:A:250:GLY:HA3	1.88	0.56
1:B:435:TRP:CE3	1:B:471:ILE:HG21	2.40	0.56
1:B:195:CYS:O	1:B:200:VAL:HG13	2.06	0.55
1:B:29:ARG:O	1:B:33:VAL:HG23	2.06	0.55
1:A:163:GLU:HG3	2:W:32:THR:HB	1.89	0.55
1:B:116:ARG:HG2	2:X:28:SER:HB2	1.89	0.55
1:B:91:GLN:NE2	1:B:113:GLN:HG3	2.22	0.55
1:A:117:THR:O	1:A:121:MSE:HG3	2.08	0.54
1:B:247:GLU:HG3	1:B:277:LEU:HD13	1.89	0.54
1:A:109:ARG:HG2	2:W:31:ALA:HB1	1.90	0.54
1:B:73:SER:O	1:B:77:VAL:HG12	2.08	0.53
1:B:419:ALA:HB1	1:B:457:VAL:HG11	1.89	0.53
1:B:381:SER:O	1:B:385:ILE:HG22	2.09	0.53
1:A:38:LEU:CD2	1:A:46:GLU:HB3	2.38	0.53
1:A:365:LYS:HD3	1:A:381:SER:HB3	1.90	0.53
1:A:466:HIS:NE2	1:A:470:MSE:HE2	2.23	0.53
1:A:354:ALA:HB1	1:A:357:LYS:CE	2.39	0.53
1:A:219:MSE:HE2	1:A:257:LEU:HD13	1.90	0.52
1:B:87:ALA:O	1:B:91:GLN:HG2	2.10	0.52
1:B:190:ARG:O	1:B:194:ILE:HG13	2.08	0.52
1:B:472:ARG:NH1	1:B:472:ARG:HA	2.25	0.52
1:A:233:GLN:O	1:A:237:ILE:HG22	2.10	0.52
1:A:58:SER:HA	1:A:62:LEU:HB2	1.92	0.52
1:B:76:GLU:OE2	1:B:80:ARG:HD2	2.09	0.52
1:B:472:ARG:HA	1:B:472:ARG:CZ	2.40	0.52
1:A:208:SER:CB	1:A:237:ILE:HD13	2.40	0.51
1:B:95:LEU:HD23	1:B:110:ALA:HB3	1.93	0.51
1:A:99:LYS:HA	1:A:107:GLN:OE1	2.10	0.51
1:A:244:ARG:HB2	1:A:281:MSE:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:HIS:CE1	1:A:470:MSE:HE2	2.46	0.50
1:A:335:LEU:HD22	1:A:368:ILE:HB	1.93	0.50
1:B:246:GLY:HA2	2:X:27:ALY:HE3	1.93	0.50
1:A:387:GLU:O	1:A:391:LYS:HG2	2.12	0.50
1:B:222:ARG:HG3	1:B:224:TRP:CZ2	2.47	0.49
1:B:94:HIS:HD1	1:B:110:ALA:HB2	1.76	0.49
1:A:24:ARG:HD2	1:A:61:TYR:CE2	2.48	0.49
1:A:466:HIS:CE1	1:A:482:LEU:HD22	2.48	0.49
1:B:91:GLN:HE22	1:B:113:GLN:HG3	1.77	0.48
1:A:143:MSE:HE1	1:A:164:TYR:CD1	2.49	0.48
1:A:383:LEU:HD11	1:A:420:LEU:HB3	1.94	0.48
1:B:395:PHE:O	1:B:399:ILE:HG12	2.13	0.48
1:B:453:ASN:O	1:B:455:PRO:HD3	2.14	0.48
1:A:53:ILE:HG13	1:A:54:ASP:N	2.28	0.47
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.80	0.47
1:A:416:GLU:HG2	1:A:420:LEU:HD23	1.96	0.47
1:B:463:GLU:O	1:B:466:HIS:HB3	2.14	0.47
1:A:254:LEU:HD23	1:A:270:CYS:SG	2.55	0.47
1:B:331:GLU:O	1:B:335:LEU:HD23	2.14	0.47
1:A:53:ILE:O	1:A:57:VAL:HG23	2.15	0.47
1:A:308:LEU:HD21	1:A:361:TYR:OH	2.15	0.46
1:A:468:SER:O	1:A:472:ARG:HB2	2.16	0.46
1:A:192:LEU:O	1:A:195:CYS:HB2	2.15	0.46
1:A:368:ILE:O	1:A:368:ILE:HG13	2.11	0.46
1:B:377:LYS:HA	1:B:380:ASP:HB2	1.96	0.46
1:B:109:ARG:HE	2:X:32:THR:HB	1.80	0.46
1:B:268:ILE:HG13	1:B:269:LEU:N	2.31	0.46
1:A:271:TYR:CE2	1:A:294:ASN:HB3	2.51	0.46
1:A:87:ALA:HB1	1:A:91:GLN:HE21	1.81	0.46
1:A:91:GLN:HB3	1:A:114:LEU:HD22	1.97	0.45
1:A:218:TYR:HE2	1:A:230:HIS:HD2	1.64	0.45
1:B:237:ILE:O	1:B:241:ILE:HG13	2.17	0.45
1:A:303:GLU:O	1:A:307:GLU:HG3	2.16	0.45
1:B:399:ILE:HG23	1:B:428:VAL:HG11	1.99	0.45
1:A:49:LYS:O	1:A:53:ILE:HG23	2.17	0.45
1:A:393:ARG:CZ	1:A:395:PHE:HZ	2.29	0.45
1:B:471:ILE:O	1:B:472:ARG:HD2	2.17	0.45
1:A:37:ILE:O	1:A:41:ARG:HG3	2.17	0.45
2:W:27:ALY:HH31	2:W:27:ALY:HE2	1.55	0.45
1:A:287:LEU:HD12	1:A:287:LEU:HA	1.79	0.44
1:A:339:ASN:HB2	1:A:368:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:MSE:O	1:B:176:MSE:HG2	2.18	0.44
1:A:72:GLN:NE2	2:W:31:ALA:HB3	2.33	0.43
1:A:213:ASN:O	1:A:217:VAL:HG12	2.18	0.43
1:A:44:TYR:HB3	1:A:77:VAL:HG13	2.00	0.43
1:B:134:ASN:O	1:B:138:TYR:HD2	2.01	0.43
1:A:8:MSE:SE	1:A:34:ILE:HG22	2.68	0.43
1:A:51:PHE:CZ	1:A:73:SER:HB3	2.52	0.43
1:A:222:ARG:NH2	1:A:355:TRP:HD1	2.15	0.43
1:A:382:PHE:CE2	1:A:408:MSE:HE3	2.54	0.43
1:B:238:CYS:HB3	1:B:247:GLU:HB3	2.01	0.43
1:A:379:SER:HB2	1:A:409:TYR:CE1	2.53	0.43
1:B:369:ALA:HB3	1:B:378:LEU:HD13	1.99	0.43
1:A:119:TYR:OH	2:W:26:ARG:HG3	2.18	0.43
1:B:335:LEU:HB3	1:B:372:LEU:HD23	2.01	0.43
1:B:109:ARG:NE	2:X:32:THR:HB	2.34	0.42
1:A:346:ILE:HG22	1:A:361:TYR:HB2	2.00	0.42
1:A:354:ALA:HB1	1:A:357:LYS:HE2	2.02	0.42
1:B:72:GLN:HB2	1:B:94:HIS:HD2	1.85	0.42
1:A:143:MSE:HE1	1:A:164:TYR:CE1	2.54	0.42
1:B:77:VAL:O	1:B:81:LEU:HD12	2.20	0.42
1:B:461:ALA:O	1:B:465:MSE:HB2	2.20	0.42
1:B:416:GLU:O	1:B:417:GLY:C	2.63	0.42
1:B:421:ALA:O	1:B:425:MSE:HB2	2.19	0.41
1:A:173:MSE:HE3	1:A:173:MSE:HB3	1.61	0.41
1:A:218:TYR:CE2	1:A:230:HIS:HD2	2.37	0.41
1:B:128:ASP:HB3	1:B:470:MSE:HE1	2.01	0.41
1:B:188:LEU:HB3	1:B:214:LEU:HD13	2.02	0.41
1:A:357:LYS:CE	1:A:357:LYS:H	2.33	0.41
1:A:383:LEU:HD23	1:A:402:TYR:HE1	1.84	0.41
1:A:29:ARG:HA	2:W:36:LYS:HD3	2.02	0.41
1:B:379:SER:HB3	1:B:408:MSE:CB	2.50	0.41
1:B:399:ILE:HG12	1:B:399:ILE:H	1.74	0.41
1:B:6:MSE:HE3	1:B:6:MSE:HB2	1.93	0.41
1:B:117:THR:O	1:B:121:MSE:HG3	2.20	0.41
1:A:55:TYR:HA	1:A:70:THR:HG21	2.03	0.41
1:A:103:ASP:O	1:A:105:VAL:HG12	2.21	0.41
1:A:439:LEU:O	1:A:443:GLN:HG3	2.20	0.41
1:B:304:VAL:O	1:B:307:GLU:HB2	2.21	0.41
1:B:402:TYR:O	1:B:405:SER:HB2	2.21	0.41
1:A:366:LYS:HE2	1:A:401:TRP:CH2	2.56	0.41
1:A:410:LYS:HA	1:A:418:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:CZ	1:A:273:LYS:HD2	2.56	0.40
1:B:71:CYS:HB3	1:B:90:TYR:O	2.21	0.40
1:B:128:ASP:O	1:B:132:ILE:HG22	2.22	0.40
1:B:188:LEU:CB	1:B:214:LEU:HD13	2.52	0.40
1:B:385:ILE:HD11	1:B:389:TYR:CE2	2.55	0.40
1:B:305:MSE:HA	1:B:305:MSE:HE2	2.02	0.40
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.86	0.40
1:A:382:PHE:HE2	1:A:408:MSE:HE3	1.86	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	458/491 (93%)	438 (96%)	20 (4%)	0	100	100
1	B	436/491 (89%)	413 (95%)	22 (5%)	1 (0%)	43	72
2	W	27/46 (59%)	24 (89%)	3 (11%)	0	100	100
2	X	21/46 (46%)	20 (95%)	1 (5%)	0	100	100
All	All	942/1074 (88%)	895 (95%)	46 (5%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	417	GLY

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	315/413 (76%)	276 (88%)	39 (12%)	4 16
1	B	264/413 (64%)	227 (86%)	37 (14%)	3 12
2	W	12/32 (38%)	10 (83%)	2 (17%)	2 8
2	X	9/32 (28%)	9 (100%)	0	100 100
All	All	600/890 (67%)	522 (87%)	78 (13%)	4 14

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	53	ILE
1	A	74	LEU
1	A	80	ARG
1	A	91	GLN
1	A	105	VAL
1	A	173	MSE
1	A	176	MSE
1	A	180	ASN
1	A	182	GLU
1	A	188	LEU
1	A	217	VAL
1	A	219	MSE
1	A	236	ILE
1	A	237	ILE
1	A	241	ILE
1	A	252	ILE
1	A	262	GLN
1	A	273	LYS
1	A	291	ILE
1	A	320	ARG
1	A	336	LEU
1	A	345	LEU
1	A	356	LEU
1	A	357	LYS
1	A	363	LYS
1	A	368	ILE
1	A	372	LEU
1	A	378	LEU
1	A	379	SER

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Mol	Chain	Res	Type
1	A	383	LEU
1	A	385	ILE
1	A	392	LEU
1	A	399	ILE
1	A	420	LEU
1	A	454	LEU
1	A	460	SER
1	A	465	MSE
1	A	470	MSE
1	B	6	MSE
1	B	41	ARG
1	B	54	ASP
1	B	102	SER
1	B	112	THR
1	B	148	THR
1	B	189	ILE
1	B	196	ASN
1	B	200	VAL
1	B	216	ASN
1	B	237	ILE
1	B	241	ILE
1	B	252	ILE
1	B	257	LEU
1	B	268	ILE
1	B	269	LEU
1	B	289	SER
1	B	319	THR
1	B	328	THR
1	B	334	SER
1	B	338	GLN
1	B	342	LEU
1	B	346	ILE
1	B	352	ILE
1	B	359	CYS
1	B	372	LEU
1	B	381	SER
1	B	383	LEU
1	B	385	ILE
1	B	399	ILE
1	B	403	THR
1	B	408	MSE
1	B	459	LEU

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Mol	Chain	Res	Type
1	B	464	ASN
1	B	465	MSE
1	B	469	HIS
1	B	471	ILE
2	W	28	SER
2	W	35	VAL

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

Mol	Chain	Res	Type
1	A	25	GLN
1	A	72	GLN
1	A	91	GLN
1	A	169	ASN
1	A	213	ASN
1	A	253	ASN
1	A	358	HIS
1	A	390	GLN
1	A	418	GLN
1	A	466	HIS
1	B	91	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	ALY	W	27	2	10,11,12	0.49	0	7,12,14	0.55	0
2	ALY	X	27	2	10,11,12	0.54	0	7,12,14	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALY	W	27	2	-	7/9/10/12	-
2	ALY	X	27	2	-	6/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	27	ALY	O-C-CA-CB
2	W	27	ALY	N-CA-CB-CG
2	W	27	ALY	C-CA-CB-CG
2	W	27	ALY	O-C-CA-CB
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	X	27	ALY	CG-CD-CE-NZ
2	W	27	ALY	CG-CD-CE-NZ
2	X	27	ALY	CE-CD-CG-CB
2	W	27	ALY	CE-CD-CG-CB
2	X	27	ALY	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

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, 95^{th} 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	452/491 (92%)	0.64	44 (9%) 13 10	78, 102, 134, 142	0
1	B	436/491 (88%)	0.88	55 (12%) 8 6	80, 116, 152, 166	0
2	W	31/46 (67%)	0.96	6 (19%) 3 2	82, 107, 130, 143	0
2	X	25/46 (54%)	1.26	8 (32%) 1 1	85, 112, 139, 147	0
All	All	944/1074 (87%)	0.78	113 (11%) 9 6	78, 107, 145, 166	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLY	4.9
1	A	485	GLU	4.6
1	B	485	GLU	4.5
1	B	467	TYR	4.4
1	A	71	CYS	4.4
1	B	122	PHE	4.3
1	A	127	ASP	4.2
1	B	111	CYS	4.0
1	B	138	TYR	4.0
1	B	31	ALA	4.0
1	A	4	ASP	4.0
1	A	150	LYS	3.9
1	A	50	TRP	3.9
1	A	111	CYS	3.9
1	A	128	ASP	3.8
1	B	67	LEU	3.8
2	W	10	SER	3.7
1	B	464	ASN	3.6
1	A	482	LEU	3.6
1	B	319	THR	3.6
1	B	323	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	245	GLN	3.5
1	A	90	TYR	3.4
1	B	148	THR	3.4
1	A	208	SER	3.4
1	B	220	GLU	3.4
1	A	177	GLU	3.4
1	A	439	LEU	3.4
1	B	486	ILE	3.3
2	X	2	ARG	3.3
2	W	2	ARG	3.2
1	B	27	GLU	3.2
1	A	179	ASP	3.1
1	B	324	ILE	3.1
1	B	423	VAL	3.1
1	B	179	ASP	3.0
1	B	30	TRP	2.9
1	A	203	ASP	2.9
1	B	142	ALA	2.9
2	W	40	ARG	2.9
1	B	105	VAL	2.9
1	B	355	TRP	2.9
1	B	460	SER	2.9
1	A	170	ASN	2.9
1	B	54	ASP	2.9
1	B	28	ALA	2.9
1	A	122	PHE	2.9
1	B	427	ASN	2.9
1	B	471	ILE	2.9
1	B	482	LEU	2.9
1	A	123	LEU	2.8
1	A	415	LEU	2.8
1	B	459	LEU	2.8
1	A	452	ALA	2.8
1	A	51	PHE	2.8
1	B	481	ARG	2.8
1	A	158	SER	2.8
1	B	402	TYR	2.8
1	B	320	ARG	2.7
2	X	4	LYS	2.7
2	X	5	GLN	2.7
1	B	419	ALA	2.6
1	A	473	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	468	SER	2.6
1	B	177	GLU	2.5
2	X	7	ALA	2.5
1	B	57	VAL	2.5
1	B	139	PHE	2.5
1	A	131	SER	2.5
1	B	477	GLU	2.4
2	W	5	GLN	2.4
1	A	442	PHE	2.4
2	X	1	ALA	2.4
1	A	231	ILE	2.4
1	B	424	ASN	2.4
1	A	132	ILE	2.4
1	B	171	ILE	2.3
2	X	6	THR	2.3
1	A	444	GLU	2.3
2	W	6	THR	2.3
1	B	416	GLU	2.3
1	A	353	PHE	2.3
1	A	462	LEU	2.3
1	A	467	TYR	2.3
1	A	5	GLU	2.3
1	B	170	ASN	2.3
1	A	130	TYR	2.3
1	B	362	ALA	2.2
1	A	166	ASP	2.2
1	B	128	ASP	2.2
1	A	435	TRP	2.2
1	B	383	LEU	2.2
1	A	273	LYS	2.2
1	B	119	TYR	2.2
1	B	426	GLY	2.2
1	B	379	SER	2.2
1	A	431	SER	2.1
1	B	442	PHE	2.1
2	W	39	HIS	2.1
1	B	135	ALA	2.1
1	A	134	ASN	2.1
1	A	129	HIS	2.1
1	A	259	TYR	2.1
1	B	473	PHE	2.1
1	B	288	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	444	GLU	2.1
2	X	18	LYS	2.1
1	B	483	GLN	2.1
1	A	254	LEU	2.1
2	X	29	ALA	2.0
1	A	469	HIS	2.0
1	B	445	GLY	2.0
1	A	447	ARG	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, 95^{th} 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	0.93	0.14	89,92,96,101	0
2	ALY	W	27	12/13	0.95	0.12	86,91,93,93	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.