



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2026 – 12:27 PM JST

PDB ID : 9UJU / pdb_00009uju
Title : The structure of Egalitarian in complex with the K10 mRNA localization signal reveals a modular binding surface required for function
Authors : Hong, Z.; Muehle, J.; Bono, F.
Deposited on : 2025-04-17
Resolution : 3.08 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
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

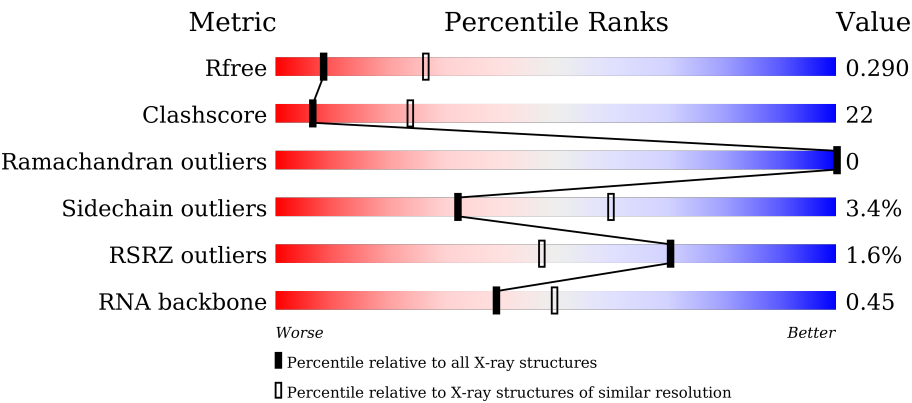
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)
RNA backbone	3983	1054 (3.30-2.86)

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	B	48	<div><div></div><div>31%35%27%. .</div></div>
1	D	48	<div><div></div><div>33%44%23%</div></div>
2	A	308	<div><div>%</div><div>58%26%.14%</div></div>
2	C	308	<div><div>%</div><div>60%23%.13%</div></div>

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Mol	Chain	Length	Quality of chain
3	X	5	<div><div>40%</div><div>100%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5828 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 RNA chain called RNA (46-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	46	Total	C	N	O	P	0	0	0
			964	435	161	323	45			
1	D	48	Total	C	N	O	P	0	0	0
			990	445	166	332	47			

- Molecule 2 is a protein called Egalitarian, isoform B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	267	Total	C	N	O	S	0	0	0
			1941	1234	334	363	10			
2	A	266	Total	C	N	O	S	0	0	0
			1883	1192	317	364	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	781	ASN	VAL	conflict	UNP Q9W1K4
A	784	ASN	VAL	conflict	UNP Q9W1K4

- Molecule 3 is a protein called ALA-LEU-GLU-PHE-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	X	5	Total	C	N	O	0	0	0
			25	15	5	5			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		
4	C	5	Total	Ca	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total 2	O 2	0	0
5	D	4	Total 4	O 4	0	0
5	C	5	Total 5	O 5	0	0
5	A	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

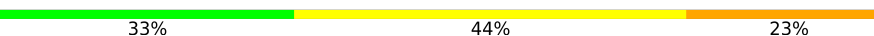
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

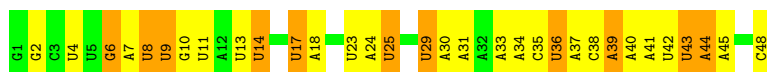
- Molecule 1: RNA (46-MER)

Chain B: 



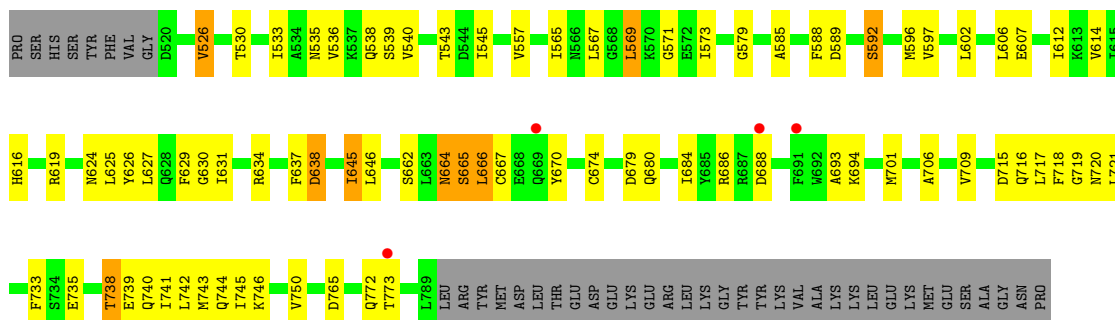
- Molecule 1: RNA (46-MER)

Chain D: 



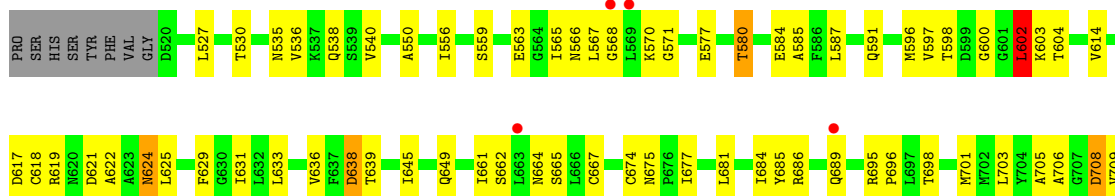
- Molecule 2: Egalitarian, isoform B

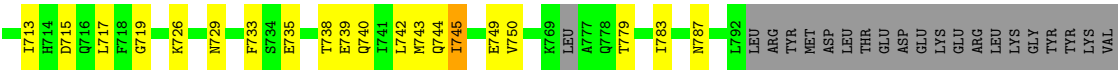
Chain C: 



- Molecule 2: Egalitarian, isoform B

Chain A: 





● Molecule 3: ALA-LEU-GLU-PHE-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.50Å 106.80Å 139.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.48 – 3.08 44.48 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.48-3.08) 99.9 (44.48-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.240 , 0.292 0.242 , 0.290	Depositor DCC
R_{free} test set	982 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 99.0	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	0.94	EDS
Total number of atoms	5828	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	B	0.58	0/1075	1.07	10/1667 (0.6%)
1	D	0.63	0/1104	1.09	9/1713 (0.5%)
2	A	1.16	1/1910 (0.1%)	1.68	11/2614 (0.4%)
2	C	1.16	3/1969 (0.2%)	1.75	13/2688 (0.5%)
3	X	1.23	0/24	1.72	0/32
All	All	1.00	4/6082 (0.1%)	1.50	43/8714 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	741	ILE	C-O	7.29	1.32	1.24
2	C	616	HIS	C-O	-6.01	1.16	1.24
2	A	617	ASP	C-O	5.89	1.32	1.23
2	C	746	LYS	N-CA	5.04	1.50	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	G	C2'-C3'-O3'	-9.27	99.79	113.70
2	C	746	LYS	CB-CA-C	7.74	117.73	111.00
1	D	4	U	C3'-C2'-O2'	7.64	122.16	110.70
1	B	25	U	C4'-C3'-O3'	7.38	124.06	113.00
2	C	738	THR	CA-CB-OG1	-7.22	98.77	109.60
1	D	4	U	C4'-C3'-O3'	-6.94	102.59	113.00
1	D	6	G	C3'-C2'-O2'	6.50	120.44	110.70
1	B	48	C	C3'-C2'-O2'	6.40	120.30	110.70
2	C	638	ASP	CA-CB-CG	-6.39	106.21	112.60
1	D	8	U	C3'-C2'-O2'	6.32	120.18	110.70
1	B	30	A	C2'-C3'-O3'	-6.23	104.35	113.70
1	B	16	U	C2'-C3'-O3'	-6.17	104.45	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	C	C3'-C2'-O2'	6.09	119.84	110.70
2	C	750	VAL	CA-C-O	-6.05	114.44	120.85
1	B	9	U	C3'-C2'-O2'	6.03	119.74	110.70
2	A	708	ASP	CA-CB-CG	5.92	118.52	112.60
2	A	638	ASP	CA-CB-CG	-5.85	106.75	112.60
1	B	5	U	C3'-C2'-O2'	-5.83	101.95	110.70
2	C	545	ILE	N-CA-C	-5.83	105.05	110.53
2	A	580	THR	CA-CB-OG1	-5.74	100.99	109.60
2	A	779	THR	CA-C-N	5.71	128.98	120.87
2	A	779	THR	C-N-CA	5.71	128.98	120.87
2	C	569	LEU	N-CA-C	-5.65	105.12	111.28
1	D	2	G	C4'-C3'-O3'	-5.59	104.61	113.00
1	B	16	U	C4'-C3'-O3'	5.58	121.36	113.00
2	C	664	ASN	N-CA-C	-5.53	106.49	113.18
2	A	602	LEU	CA-C-O	-5.51	115.21	121.00
2	C	765	ASP	CA-C-O	-5.48	115.07	120.82
1	D	44	A	C1'-C2'-O2'	5.48	116.61	108.40
2	A	591	GLN	N-CA-C	-5.44	105.26	111.14
2	C	664	ASN	CB-CA-C	5.43	120.75	109.95
2	C	571	GLY	CA-C-O	-5.42	116.17	121.76
2	A	565	ILE	CB-CA-C	5.38	117.04	111.23
1	B	5	U	C2'-C3'-O3'	-5.30	105.74	113.70
1	D	43	U	C1'-C2'-O2'	5.30	116.36	108.40
1	D	36	U	C4'-C3'-O3'	5.28	120.92	113.00
1	B	6	G	C4'-C3'-C2'	-5.24	97.36	102.60
2	C	745	ILE	CA-C-N	-5.21	117.21	122.83
2	C	745	ILE	C-N-CA	-5.21	117.21	122.83
2	A	735	GLU	CB-CG-CD	5.13	121.33	112.60
2	C	741	ILE	O-C-N	5.06	127.35	121.94
2	A	598	THR	CA-CB-OG1	-5.01	102.08	109.60
2	A	624	ASN	N-CA-C	-5.00	104.83	112.04

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	B	964	0	490	51	1
1	D	990	0	500	50	1
2	A	1883	0	1677	61	0
2	C	1941	0	1797	64	0
3	X	25	0	18	0	0
4	A	2	0	0	0	0
4	C	5	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	2	0
5	B	2	0	0	0	0
5	C	5	0	0	0	0
5	D	4	0	0	0	0
All	All	5828	0	4482	221	1

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 22.

All (221) 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)
2:C:662:SER:OG	2:C:665:SER:HB3	1.55	1.05
1:D:33:A:H2'	1:D:34:A:C8	2.02	0.94
2:A:563:GLU:OE1	5:A:1001:HOH:O	1.89	0.91
1:D:30:A:H2'	1:D:31:A:C8	2.09	0.88
2:C:645:ILE:HD13	2:C:733:PHE:HB2	1.57	0.87
1:B:38:C:H2'	1:B:39:A:C8	2.15	0.81
1:D:8:U:O2	1:D:41:A:N1	2.14	0.81
2:C:716:GLN:O	2:C:720:ASN:ND2	2.14	0.80
2:C:670:TYR:HB3	2:C:720:ASN:HD22	1.45	0.80
2:C:645:ILE:CD1	2:C:733:PHE:HA	2.13	0.79
2:C:526:VAL:O	2:C:530:THR:HG23	1.84	0.77
2:C:645:ILE:HD11	2:C:733:PHE:HA	1.67	0.76
1:D:38:C:H2'	1:D:39:A:C8	2.22	0.75
2:C:664:ASN:HA	2:C:667:CYS:SG	2.29	0.73
2:C:565:ILE:HD11	2:C:693:ALA:HB2	1.70	0.72
2:C:533:ILE:HG22	2:C:596:MET:HE3	1.72	0.72
2:A:662:SER:OG	2:A:665:SER:HB3	1.90	0.71
1:D:30:A:H2'	1:D:31:A:H8	1.53	0.70
2:A:536:VAL:O	2:A:540:VAL:HG23	1.91	0.70
1:B:38:C:H2'	1:B:39:A:N9	2.06	0.70
1:B:39:A:O5'	1:B:39:A:H8	1.74	0.70
1:D:33:A:C2	1:D:34:A:C2	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:530:THR:HG22	2:A:585:ALA:HB3	1.72	0.69
2:C:614:VAL:HG11	2:C:718:PHE:CD1	2.28	0.69
2:C:742:LEU:O	2:C:743:MET:C	2.36	0.69
1:D:33:A:H2'	1:D:34:A:N9	2.10	0.67
2:A:739:GLU:HB2	2:A:750:VAL:HG13	1.75	0.67
2:A:638:ASP:OD2	2:A:740:GLN:HG2	1.94	0.67
1:B:10:G:N2	1:B:39:A:C2	2.63	0.67
1:D:10:G:N2	1:D:39:A:C2	2.64	0.66
2:A:649:GLN:HE22	2:A:726:LYS:H	1.43	0.66
2:C:645:ILE:HD13	2:C:733:PHE:CB	2.25	0.66
2:A:717:LEU:C	2:A:717:LEU:HD23	2.21	0.65
2:C:569:LEU:HA	2:C:627:LEU:HD12	1.79	0.64
1:B:16:U:O2'	1:B:17:U:H5'	1.98	0.64
2:C:638:ASP:OD1	2:C:638:ASP:C	2.40	0.62
1:D:33:A:C6	1:D:34:A:C6	2.87	0.62
1:D:30:A:C2	1:D:31:A:C4	2.89	0.61
1:B:9:U:O2	1:B:40:A:H2	1.82	0.61
2:A:559:SER:OG	2:A:709:VAL:O	2.15	0.61
2:A:738:THR:HG22	2:A:742:LEU:HD12	1.83	0.61
1:B:1:G:N2	2:A:566:ASN:OD1	2.30	0.61
2:C:626:TYR:O	2:C:630:GLY:HA2	2.01	0.60
1:B:16:U:C2	1:B:17:U:C5	2.90	0.59
2:A:667:CYS:SG	2:A:717:LEU:HD12	2.43	0.59
1:D:39:A:C2	1:D:40:A:C5	2.91	0.59
1:D:8:U:H2'	1:D:9:U:C6	2.38	0.58
2:C:717:LEU:C	2:C:717:LEU:HD23	2.28	0.58
1:B:9:U:O2	1:B:40:A:C2	2.55	0.58
1:B:21:U:C2	1:B:22:U:C5	2.92	0.58
2:C:645:ILE:CD1	2:C:733:PHE:CA	2.82	0.58
1:D:9:U:H3'	1:D:10:G:H8	1.69	0.58
1:B:1:G:H1'	2:A:689:GLN:NE2	2.20	0.57
1:B:39:A:C2	1:B:40:A:C5	2.92	0.57
2:A:638:ASP:OD1	2:A:638:ASP:C	2.48	0.57
1:D:36:U:C2	1:D:37:A:C8	2.93	0.57
1:B:38:C:C4	1:B:39:A:N6	2.73	0.57
1:D:42:U:C2	1:D:43:U:C6	2.93	0.56
2:A:645:ILE:CD1	2:A:733:PHE:HA	2.35	0.56
2:A:708:ASP:OD2	5:A:1001:HOH:O	2.17	0.56
1:B:38:C:N3	1:B:39:A:C6	2.73	0.56
1:D:13:U:H2'	1:D:14:U:C6	2.41	0.56
1:B:10:G:N2	1:B:39:A:H2	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:U:C4	1:D:43:U:C5	2.94	0.55
2:C:569:LEU:CA	2:C:627:LEU:HD12	2.36	0.55
1:D:33:A:C2'	1:D:34:A:C8	2.84	0.55
1:D:6:G:H1	1:D:43:U:H3	1.53	0.55
1:B:42:U:C2	1:B:43:U:C6	2.96	0.54
1:D:34:A:C6	1:D:35:C:N4	2.76	0.54
2:C:645:ILE:HD11	2:C:733:PHE:CA	2.38	0.54
2:C:735:GLU:O	2:C:739:GLU:HG3	2.08	0.54
2:C:530:THR:HA	2:C:585:ALA:O	2.08	0.53
1:B:10:G:C2	1:B:39:A:H2	2.26	0.53
2:A:559:SER:OG	2:A:709:VAL:HG22	2.09	0.53
2:A:625:LEU:HD12	2:A:633:LEU:HD21	1.91	0.53
2:A:783:ILE:O	2:A:787:ASN:N	2.39	0.53
1:D:41:A:H2'	1:D:42:U:H6	1.73	0.52
2:C:597:VAL:HG11	2:C:629:PHE:HB3	1.90	0.52
2:C:573:ILE:HD12	2:C:625:LEU:HD23	1.91	0.52
2:C:694:LYS:CB	2:C:701:MET:HE1	2.39	0.52
1:D:35:C:C2	1:D:36:U:C5	2.98	0.52
1:D:24:A:C6	1:D:25:U:C4	2.97	0.52
1:B:42:U:N3	1:B:43:U:C5	2.78	0.51
2:C:667:CYS:HB2	2:C:674:CYS:SG	2.50	0.51
1:B:21:U:N3	1:B:22:U:C4	2.79	0.51
2:C:588:PHE:HD2	2:C:596:MET:HE2	1.74	0.51
2:A:698:THR:H	2:A:701:MET:HE3	1.74	0.51
1:B:38:C:C4	1:B:39:A:C6	2.98	0.51
2:A:622:ALA:HA	2:A:633:LEU:HD23	1.92	0.51
1:B:40:A:H2'	1:B:41:A:H8	1.75	0.51
1:D:24:A:C4	1:D:25:U:C5	2.99	0.51
1:D:33:A:N1	1:D:34:A:N1	2.58	0.51
2:A:742:LEU:O	2:A:745:ILE:O	2.28	0.51
1:D:42:U:N3	1:D:43:U:C5	2.78	0.51
1:B:10:G:C2	1:B:39:A:C2	2.99	0.51
2:C:567:LEU:HA	2:C:624:ASN:HD22	1.76	0.51
2:A:580:THR:HG21	2:A:584:GLU:OE1	2.11	0.51
2:A:649:GLN:HE21	2:A:729:ASN:HD21	1.59	0.50
1:D:37:A:H2'	1:D:38:C:C6	2.47	0.50
1:B:29:U:H2'	1:B:30:A:C8	2.47	0.50
1:D:36:U:N3	1:D:37:A:C8	2.80	0.50
2:C:662:SER:HG	2:C:665:SER:HB3	1.72	0.50
1:D:24:A:C5	1:D:25:U:C5	3.00	0.50
1:D:34:A:H2'	1:D:35:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:715:ASP:O	2:C:719:GLY:HA3	2.12	0.49
2:A:577:GLU:HG2	2:A:705:ALA:HB1	1.94	0.49
2:A:618:CYS:O	2:A:619:ARG:C	2.56	0.49
2:A:695:ARG:CB	2:A:696:PRO:HD3	2.43	0.49
2:A:739:GLU:O	2:A:743:MET:N	2.46	0.49
1:B:39:A:H8	1:B:39:A:P	2.36	0.49
1:D:41:A:C4	1:D:42:U:C5	3.02	0.48
2:A:530:THR:HG21	2:A:706:ALA:HB2	1.96	0.48
2:C:533:ILE:CG2	2:C:596:MET:HE3	2.43	0.48
1:B:6:G:H2'	1:B:7:A:O4'	2.14	0.48
1:B:30:A:N1	1:B:31:A:C5	2.81	0.48
2:C:530:THR:HG21	2:C:706:ALA:CB	2.44	0.48
2:A:571:GLY:C	2:A:624:ASN:HD21	2.22	0.48
1:D:34:A:H2'	1:D:35:C:H6	1.79	0.47
2:A:645:ILE:CD1	2:A:733:PHE:HB2	2.44	0.47
2:C:619:ARG:HG3	2:C:740:GLN:NE2	2.29	0.47
1:D:24:A:H2'	1:D:25:U:H6	1.79	0.47
2:A:527:LEU:HD11	2:A:703:LEU:HD11	1.96	0.47
1:B:38:C:C2'	1:B:39:A:C8	2.94	0.47
2:A:597:VAL:HA	2:A:602:LEU:HB3	1.97	0.47
1:B:30:A:C2'	1:B:31:A:O5'	2.63	0.47
1:D:34:A:C4	1:D:35:C:C5	3.02	0.47
2:A:530:THR:HG21	2:A:706:ALA:CB	2.43	0.47
1:B:41:A:C4	1:B:42:U:C5	3.03	0.47
1:D:44:A:H2'	1:D:45:A:O5'	2.14	0.47
2:C:666:LEU:HD21	2:C:721:LEU:HD21	1.96	0.47
2:C:597:VAL:HG13	2:C:631:ILE:HD11	1.97	0.47
2:A:567:LEU:HD21	2:A:621:ASP:OD1	2.15	0.47
2:A:629:PHE:HB2	2:A:631:ILE:HG13	1.97	0.47
2:A:645:ILE:HD13	2:A:733:PHE:HB2	1.97	0.47
1:B:8:U:O2	1:B:41:A:N1	2.48	0.47
2:A:568:GLY:H	2:A:624:ASN:HD22	1.61	0.46
1:B:39:A:N1	1:B:40:A:C6	2.84	0.46
1:D:39:A:O5'	1:D:39:A:H8	1.98	0.46
1:B:38:C:N4	1:B:39:A:N6	2.63	0.46
2:C:667:CYS:CB	2:C:674:CYS:HG	2.29	0.46
2:C:684:ILE:O	2:C:688:ASP:N	2.47	0.46
2:A:622:ALA:HA	2:A:633:LEU:CD2	2.46	0.46
1:B:1:G:N7	2:A:686:ARG:HG2	2.31	0.46
2:A:535:ASN:HD21	2:A:538:GLN:HG3	1.81	0.46
1:B:8:U:O2	1:B:41:A:C2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:A:H2'	1:B:41:A:C8	2.51	0.46
2:C:536:VAL:O	2:C:540:VAL:HG23	2.16	0.46
2:C:742:LEU:O	2:C:744:GLN:N	2.48	0.46
2:A:550:ALA:HA	2:A:556:ILE:HG12	1.97	0.46
1:D:7:A:H61	1:D:41:A:N6	2.14	0.45
2:C:646:LEU:HD12	2:C:670:TYR:OH	2.17	0.45
1:B:30:A:H2'	1:B:31:A:O5'	2.17	0.45
1:D:35:C:H2'	1:D:36:U:C6	2.52	0.45
1:B:3:C:OP1	2:A:570:LYS:NZ	2.50	0.45
1:D:34:A:C6	1:D:35:C:C4	3.05	0.44
1:B:27:C:H2'	1:B:28:U:C6	2.52	0.44
1:D:36:U:N3	1:D:37:A:N7	2.65	0.44
2:C:530:THR:HG21	2:C:706:ALA:HB2	1.97	0.44
2:C:772:GLN:O	2:C:773:THR:C	2.59	0.44
1:D:29:U:H2'	1:D:30:A:C8	2.52	0.44
1:D:35:C:H2'	1:D:36:U:H6	1.82	0.44
2:C:588:PHE:HD2	2:C:596:MET:CE	2.31	0.44
1:B:21:U:H2'	1:B:22:U:C6	2.52	0.44
2:C:614:VAL:HG12	2:C:637:PHE:HB3	2.00	0.44
2:C:539:SER:HB2	2:C:596:MET:HE3	2.00	0.44
2:A:580:THR:HG22	2:A:584:GLU:O	2.18	0.44
2:A:675:ASN:OD1	2:A:677:ILE:HG12	2.18	0.44
1:B:30:A:C2	1:B:31:A:C4	3.06	0.43
1:B:35:C:H4'	1:B:36:U:OP1	2.18	0.43
2:C:619:ARG:HD3	2:C:743:MET:HE3	2.00	0.43
2:A:596:MET:HA	2:A:600:GLY:HA3	2.00	0.43
1:B:16:U:C2'	1:B:17:U:H5'	2.48	0.43
2:C:557:VAL:HG22	2:C:612:ILE:HD12	2.01	0.43
2:C:579:GLY:HA3	2:C:709:VAL:HG22	2.00	0.43
2:A:661:ILE:HG22	2:A:662:SER:O	2.19	0.43
2:C:667:CYS:CB	2:C:674:CYS:SG	3.06	0.43
1:B:21:U:N3	1:B:22:U:C5	2.86	0.43
2:C:597:VAL:HG21	2:C:629:PHE:CD1	2.54	0.43
2:A:664:ASN:HB2	2:A:674:CYS:HB3	2.00	0.43
2:C:602:LEU:O	2:C:606:LEU:HG	2.19	0.43
2:A:681:LEU:HA	2:A:684:ILE:HD12	2.01	0.43
2:C:535:ASN:HD21	2:C:538:GLN:HG3	1.84	0.43
2:A:559:SER:HB3	2:A:713:ILE:HB	2.01	0.43
1:D:17:U:H2'	1:D:18:A:C8	2.54	0.42
1:B:48:C:C4	2:A:685:TYR:CD2	3.07	0.42
1:B:3:C:H2'	1:B:4:U:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:A:C8	1:B:39:A:O5'	2.64	0.42
1:D:41:A:H2'	1:D:42:U:C6	2.52	0.42
1:D:7:A:N6	1:D:41:A:H61	2.18	0.42
2:C:667:CYS:HB2	2:C:674:CYS:HG	1.84	0.42
2:A:638:ASP:OD1	2:A:639:THR:N	2.52	0.42
2:C:607:GLU:HB3	2:C:634:ARG:NH2	2.33	0.42
2:A:596:MET:O	2:A:600:GLY:HA3	2.19	0.42
1:B:27:C:H2'	1:B:28:U:H6	1.84	0.42
1:B:41:A:H2'	1:B:42:U:H6	1.85	0.42
2:A:577:GLU:HG2	2:A:587:LEU:HD22	2.01	0.42
1:B:25:U:C2	1:B:26:U:H5'	2.54	0.42
2:C:740:GLN:OE1	2:C:740:GLN:HA	2.20	0.42
1:B:42:U:C4	1:B:43:U:C5	3.08	0.42
2:C:539:SER:O	2:C:543:THR:HG23	2.20	0.42
2:C:679:ASP:OD1	2:C:680:GLN:HG3	2.19	0.42
1:D:41:A:C6	1:D:42:U:C4	3.08	0.41
2:C:716:GLN:O	2:C:720:ASN:CG	2.62	0.41
2:C:567:LEU:HA	2:C:624:ASN:ND2	2.36	0.41
2:C:579:GLY:N	2:C:709:VAL:CG2	2.83	0.41
2:A:603:LYS:O	2:A:604:THR:C	2.62	0.41
2:A:596:MET:O	2:A:600:GLY:CA	2.69	0.41
1:B:7:A:N6	1:B:41:A:H61	2.19	0.41
1:D:39:A:N1	1:D:40:A:C6	2.89	0.41
2:C:626:TYR:HA	2:C:631:ILE:O	2.21	0.41
1:D:7:A:H61	1:D:41:A:H61	1.69	0.41
2:C:614:VAL:CG1	2:C:718:PHE:CD1	3.02	0.41
2:A:633:LEU:HB3	2:A:636:VAL:CG2	2.51	0.41
2:A:645:ILE:HD12	2:A:733:PHE:HD1	1.86	0.41
2:A:717:LEU:C	2:A:717:LEU:CD2	2.90	0.41
1:D:33:A:N1	1:D:34:A:C2	2.89	0.40
2:C:638:ASP:OD2	2:C:740:GLN:CG	2.69	0.40
2:C:589:ASP:CG	2:C:592:SER:OG	2.64	0.40
2:A:625:LEU:HB3	2:A:631:ILE:HB	2.02	0.40
2:A:715:ASP:O	2:A:719:GLY:N	2.55	0.40
1:D:44:A:C2'	1:D:45:A:O5'	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:U:O4'	1:D:23:U:OP2[3_444]	1.72	0.48

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	
2	A	262/308 (85%)	242 (92%)	20 (8%)	0	100	100
2	C	263/308 (85%)	245 (93%)	18 (7%)	0	100	100
3	X	3/5 (60%)	3 (100%)	0	0	100	100
All	All	528/621 (85%)	490 (93%)	38 (7%)	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	
2	A	172/274 (63%)	167 (97%)	5 (3%)	37	63
2	C	183/274 (67%)	176 (96%)	7 (4%)	29	57
All	All	355/548 (65%)	343 (97%)	12 (3%)	32	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	526	VAL
2	C	592	SER
2	C	645	ILE
2	C	665	SER
2	C	666	LEU
2	C	686	ARG
2	C	738	THR

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Mol	Chain	Res	Type
2	A	602	LEU
2	A	614	VAL
2	A	744	GLN
2	A	745	ILE
2	A	749	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	535	ASN
2	C	538	GLN
2	C	624	ASN
2	C	643	HIS
2	C	649	GLN
2	C	689	GLN
2	C	729	ASN
2	A	535	ASN
2	A	538	GLN
2	A	624	ASN
2	A	649	GLN
2	A	680	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	44/48 (91%)	10 (22%)	0
1	D	45/48 (93%)	7 (15%)	0
All	All	89/96 (92%)	17 (19%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	9	U
1	B	10	G
1	B	17	U
1	B	26	U
1	B	27	C
1	B	31	A
1	B	32	A
1	B	35	C

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Mol	Chain	Res	Type
1	B	36	U
1	B	45	A
1	D	9	U
1	D	11	U
1	D	14	U
1	D	17	U
1	D	25	U
1	D	29	U
1	D	39	A

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	773:THR	C	777:SER	N	8.62

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	B	46/48 (95%)	-0.16	0	100	100	66, 185, 260, 324	0
1	D	48/48 (100%)	-0.38	0	100	100	52, 192, 269, 285	0
2	A	266/308 (86%)	0.18	4 (1%)	72	50	62, 91, 130, 167	0
2	C	267/308 (86%)	0.06	4 (1%)	72	50	55, 84, 122, 145	0
3	X	5/5 (100%)	2.24	2 (40%)	1	0	223, 226, 243, 256	0
All	All	632/717 (88%)	0.08	10 (1%)	70	47	52, 91, 214, 324	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	663	LEU	4.1
2	C	773	THR	3.2
3	X	-137	LEU	3.2
2	C	669	GLN	3.1
2	A	568	GLY	2.7
2	A	569	LEU	2.5
3	X	-134	ALA	2.4
2	C	691	PHE	2.3
2	A	689	GLN	2.2
2	C	688	ASP	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	D	101	1/1	0.56	0.26	202,202,202,202	0
4	CA	C	904	1/1	0.84	0.19	141,141,141,141	0
4	CA	C	905	1/1	0.87	0.20	175,175,175,175	0
4	CA	A	902	1/1	0.89	0.13	144,144,144,144	0
4	CA	A	901	1/1	0.90	0.12	122,122,122,122	0
4	CA	C	901	1/1	0.92	0.25	125,125,125,125	0
4	CA	C	902	1/1	0.93	0.19	127,127,127,127	0
4	CA	C	903	1/1	0.93	0.16	142,142,142,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.