



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:27 PM EDT

PDB ID : 3BX2
Title : Puf4 RNA binding domain bound to HO endonuclease RNA 3' UTR recognition sequence
Authors : Miller, M.T.; Higgin, J.J.; Hall, T.M.T.
Deposited on : 2008-01-11
Resolution : 2.84 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

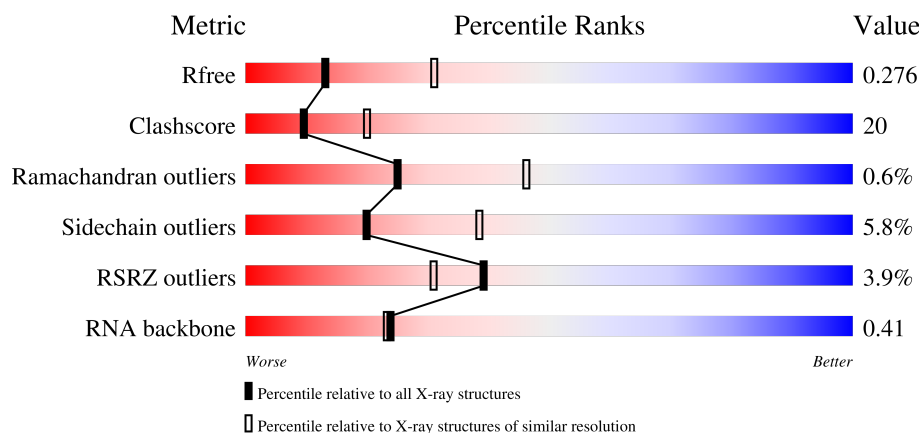
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)
RNA backbone	3102	1077 (3.10-2.58)

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	C	9	<div> <div>22%</div> <div>44%</div> <div>44%</div> <div>11%</div> </div>
1	D	9	<div> <div>33%</div> <div>33%</div> <div>56%</div> <div>11%</div> </div>
2	A	335	<div> <div>%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
2	B	335	<div> <div>5%</div> <div>58%</div> <div>35%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	952	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5653 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.

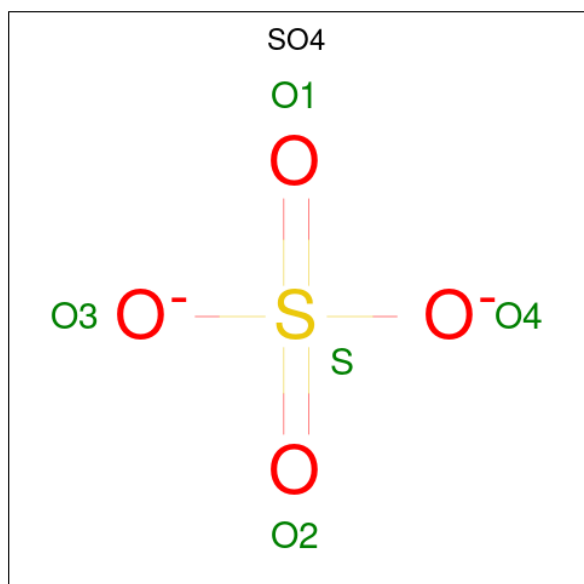
- Molecule 1 is a RNA chain called HO endonuclease 3' UTR binding sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	9	Total	C	N	O	P	0	0	0
			186	85	30	63	8			
1	D	9	Total	C	N	O	P	0	0	0
			186	85	30	63	8			

- Molecule 2 is a protein called Protein PUF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	328	Total	C	N	O	S	0	0	0
			2611	1658	446	494	13			
2	B	323	Total	C	N	O	S	0	0	0
			2570	1631	439	487	13			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Na 2 2	0	0

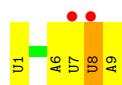
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	D	3	Total O 3 3	0	0
5	A	37	Total O 37 37	0	0
5	B	17	Total O 17 17	0	0

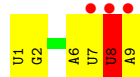
3 Residue-property plots [i](#)

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.

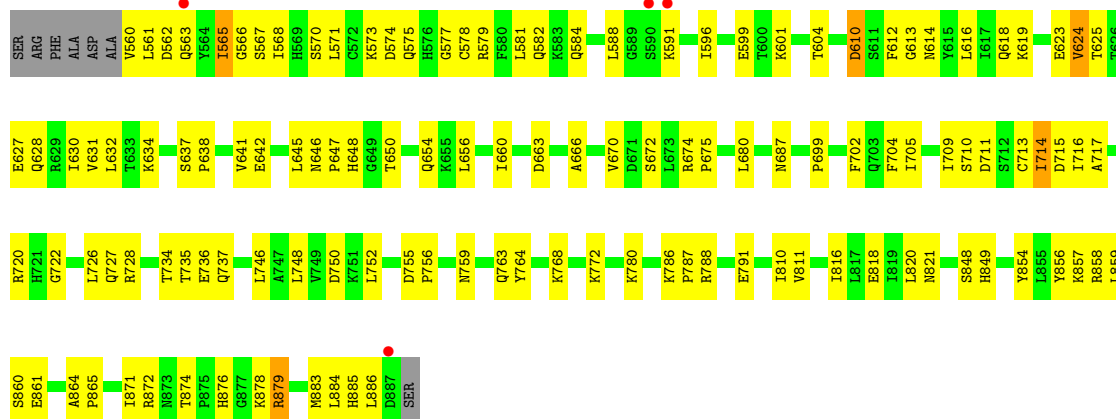
- Molecule 1: HO endonuclease 3' UTR binding sequence



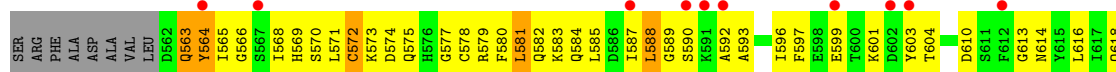
- Molecule 1: HO endonuclease 3' UTR binding sequence

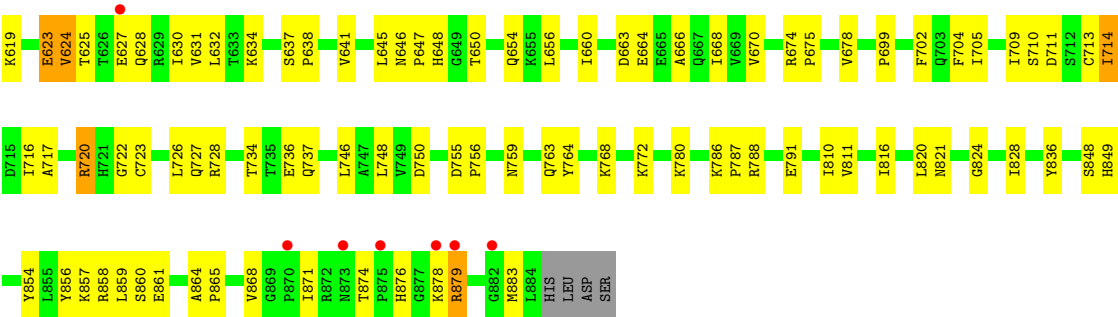


- Molecule 2: Protein PUF4



- Molecule 2: Protein PUF4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.86Å 136.18Å 158.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.90 – 2.84 14.90 – 2.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (14.90-2.84) 93.6 (14.90-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.280 0.239 , 0.276	Depositor DCC
R_{free} test set	1645 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5653	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: NA, SO4

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	C	0.58	0/207	1.14	1/320 (0.3%)
1	D	0.60	0/207	1.12	1/320 (0.3%)
2	A	0.43	0/2655	0.59	0/3592
2	B	0.38	0/2613	0.57	0/3534
All	All	0.42	0/5682	0.64	2/7766 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	8	U	P-O3'-C3'	-5.43	113.18	119.70
1	C	9	A	O4'-C1'-N9	5.10	112.28	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	588	LEU	Peptide

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	C	186	0	96	5	0
1	D	186	0	96	7	0
2	A	2611	0	2654	99	0
2	B	2570	0	2612	114	0
3	A	20	0	0	0	0
3	B	20	0	0	1	0
4	B	2	0	0	0	0
5	A	37	0	0	2	0
5	B	17	0	0	2	0
5	C	1	0	0	1	0
5	D	3	0	0	0	0
All	All	5653	0	5458	216	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 20.

All (216) 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:B:624:VAL:HG13	2:B:628:GLN:HB2	1.43	0.97
2:A:624:VAL:HG13	2:A:628:GLN:HB2	1.43	0.96
2:B:734:THR:HG22	2:B:736:GLU:H	1.29	0.96
2:A:734:THR:HG22	2:A:736:GLU:H	1.31	0.93
2:A:704:PHE:CZ	2:A:705:ILE:HG13	2.12	0.84
2:A:578:CYS:O	2:A:582:GLN:HG3	1.77	0.83
2:B:704:PHE:CZ	2:B:705:ILE:HG13	2.14	0.82
2:B:572:CYS:HB3	2:B:616:LEU:HD22	1.60	0.81
2:B:584:GLN:HB3	2:B:592:ALA:HB1	1.61	0.81
2:A:562:ASP:HB3	2:A:565:ILE:HG13	1.62	0.79
2:A:575:GLN:HB2	2:A:612:PHE:CE1	2.17	0.79
2:A:714:ILE:HD11	2:A:748:LEU:HD13	1.66	0.75
2:B:720:ARG:HG2	5:B:966:HOH:O	1.85	0.75
2:B:734:THR:HG22	2:B:736:GLU:N	2.01	0.75
2:B:570:SER:HA	2:B:573:LYS:HE2	1.67	0.74
2:B:714:ILE:HD11	2:B:748:LEU:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:THR:HG21	2:B:632:LEU:HD22	1.69	0.73
2:A:604:THR:HG21	2:A:632:LEU:HD22	1.70	0.73
2:B:568:ILE:HG23	2:B:599:GLU:HB3	1.71	0.72
2:B:624:VAL:CG1	2:B:628:GLN:HB2	2.20	0.71
2:A:810:ILE:HD12	2:A:811:VAL:HG13	1.71	0.71
2:A:734:THR:HG22	2:A:736:GLU:N	2.05	0.70
2:A:650:THR:O	2:A:654:GLN:HG3	1.91	0.70
1:D:1:U:N3	2:B:876:HIS:HB3	2.06	0.69
2:B:810:ILE:HD12	2:B:811:VAL:HG13	1.75	0.69
2:A:704:PHE:CE1	2:A:705:ILE:HG13	2.28	0.68
2:B:704:PHE:CE1	2:B:705:ILE:HG13	2.30	0.67
2:B:584:GLN:HB3	2:B:592:ALA:CB	2.25	0.66
2:A:575:GLN:HE21	2:A:579:ARG:HE	1.44	0.65
2:A:610:ASP:HB2	5:A:961:HOH:O	1.97	0.65
2:A:705:ILE:CG2	2:A:709:ILE:HD12	2.28	0.64
2:B:585:LEU:O	2:B:623:GLU:HG2	1.97	0.64
2:B:746:LEU:HD21	2:B:780:LYS:HB3	1.80	0.64
2:A:714:ILE:CD1	2:A:748:LEU:HD13	2.27	0.64
2:A:624:VAL:CG1	2:A:628:GLN:HB2	2.23	0.63
2:B:582:GLN:HG2	2:B:616:LEU:CD1	2.29	0.62
2:B:705:ILE:CG2	2:B:709:ILE:HD12	2.29	0.62
2:A:570:SER:HA	2:A:573:LYS:HE3	1.81	0.62
2:B:714:ILE:CD1	2:B:748:LEU:HD13	2.29	0.61
2:B:864:ALA:HB3	2:B:865:PRO:HD3	1.82	0.61
2:A:874:THR:O	2:A:878:LYS:HG3	2.00	0.61
2:B:650:THR:O	2:B:654:GLN:HG3	2.00	0.61
2:A:864:ALA:HB3	2:A:865:PRO:HD3	1.83	0.61
2:A:604:THR:HG21	2:A:632:LEU:CD2	2.30	0.61
2:B:582:GLN:HG2	2:B:616:LEU:HD13	1.83	0.61
2:B:816:ILE:HD13	2:B:848:SER:HB3	1.83	0.60
2:B:879:ARG:NH1	5:B:970:HOH:O	2.34	0.60
1:C:6:A:H4'	5:C:10:HOH:O	2.02	0.60
2:B:874:THR:O	2:B:878:LYS:HG3	2.02	0.60
2:B:759:ASN:O	2:B:763:GLN:HG3	2.01	0.60
2:B:705:ILE:HG22	2:B:709:ILE:HD12	1.83	0.59
2:B:604:THR:HG21	2:B:632:LEU:CD2	2.32	0.59
2:B:674:ARG:HB3	2:B:675:PRO:HD3	1.85	0.59
1:C:8:U:H5''	1:C:8:U:H6	1.68	0.59
2:B:575:GLN:NE2	2:B:579:ARG:HH21	2.01	0.59
2:A:562:ASP:CB	2:A:565:ILE:HG13	2.31	0.58
2:B:734:THR:HB	2:B:737:GLN:HG3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:746:LEU:HD21	2:A:780:LYS:HB3	1.85	0.58
2:B:734:THR:HG23	3:B:953:SO4:O1	2.03	0.58
2:A:674:ARG:HB3	2:A:675:PRO:HD3	1.85	0.57
2:A:759:ASN:O	2:A:763:GLN:HG3	2.05	0.57
2:A:705:ILE:HG22	2:A:709:ILE:HD12	1.87	0.57
2:B:584:GLN:CB	2:B:592:ALA:HB1	2.34	0.56
2:A:567:SER:O	2:A:571:LEU:HD23	2.06	0.56
2:A:571:LEU:O	2:A:577:GLY:HA3	2.06	0.56
2:A:613:GLY:O	2:A:616:LEU:N	2.39	0.56
2:A:699:PRO:HA	2:A:702:PHE:CZ	2.40	0.56
1:D:8:U:H5''	1:D:8:U:H6	1.71	0.55
2:B:568:ILE:HG23	2:B:599:GLU:CB	2.35	0.55
2:B:820:LEU:HD21	2:B:859:LEU:HD23	1.89	0.55
2:A:716:ILE:HG23	2:A:722:GLY:CA	2.36	0.55
2:A:849:HIS:CE1	2:A:886:LEU:HB3	2.41	0.55
2:A:638:PRO:HB3	2:B:678:VAL:HG11	1.90	0.54
2:A:857:LYS:O	2:A:861:GLU:HG2	2.08	0.54
2:B:572:CYS:HB3	2:B:616:LEU:CD2	2.33	0.54
2:B:587:ILE:HD12	2:B:588:LEU:H	1.73	0.54
2:B:714:ILE:CG1	2:B:748:LEU:HD13	2.37	0.54
2:A:601:LYS:HA	2:A:604:THR:HG23	1.90	0.54
2:B:699:PRO:HA	2:B:702:PHE:CZ	2.43	0.53
2:A:768:LYS:O	2:A:772:LYS:HG3	2.08	0.53
2:B:569:HIS:CD2	2:B:603:TYR:CZ	2.97	0.53
2:A:704:PHE:CZ	2:A:705:ILE:CG1	2.89	0.53
2:B:849:HIS:HB2	2:B:856:TYR:CD1	2.43	0.53
2:A:816:ILE:HD13	2:A:848:SER:HB3	1.91	0.53
2:A:641:VAL:O	2:A:645:LEU:HG	2.07	0.53
2:B:568:ILE:CG2	2:B:599:GLU:HB3	2.37	0.53
2:B:601:LYS:HA	2:B:604:THR:HG23	1.90	0.53
2:B:704:PHE:CZ	2:B:705:ILE:CG1	2.91	0.52
1:D:2:G:HO2'	2:B:836:TYR:HE1	1.56	0.52
2:A:627:GLU:O	2:A:631:VAL:HG23	2.09	0.52
2:A:709:ILE:HG12	2:A:716:ILE:HD12	1.92	0.52
2:A:714:ILE:CG1	2:A:748:LEU:HD13	2.39	0.52
2:B:849:HIS:HB2	2:B:856:TYR:CE1	2.44	0.52
2:A:820:LEU:HD21	2:A:859:LEU:HD23	1.91	0.52
2:A:614:ASN:ND2	2:A:648:HIS:HB3	2.25	0.52
2:A:849:HIS:HB2	2:A:856:TYR:CD1	2.45	0.52
2:B:587:ILE:HD12	2:B:588:LEU:N	2.25	0.51
2:B:710:SER:O	2:B:713:CYS:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:710:SER:O	2:A:713:CYS:HB2	2.10	0.51
2:B:578:CYS:O	2:B:582:GLN:HG3	2.11	0.51
2:B:768:LYS:O	2:B:772:LYS:HG3	2.09	0.51
1:D:2:G:H1'	2:B:836:TYR:CD1	2.46	0.51
2:A:699:PRO:HA	2:A:702:PHE:CE2	2.46	0.51
2:B:755:ASP:OD1	2:B:756:PRO:HD2	2.11	0.51
2:A:849:HIS:HB2	2:A:856:TYR:CE1	2.46	0.50
2:B:569:HIS:CE1	2:B:603:TYR:CE1	3.00	0.50
2:A:666:ALA:O	2:A:670:VAL:HG13	2.11	0.50
2:B:585:LEU:C	2:B:589:GLY:HA2	2.31	0.50
2:A:734:THR:HB	2:A:737:GLN:HG3	1.92	0.50
2:A:642:GLU:HB3	2:B:714:ILE:HB	1.94	0.50
2:B:641:VAL:O	2:B:645:LEU:HG	2.12	0.50
2:A:563:GLN:N	2:A:563:GLN:CD	2.66	0.50
2:B:613:GLY:O	2:B:616:LEU:N	2.45	0.50
2:A:601:LYS:O	2:A:604:THR:HG23	2.12	0.49
2:B:716:ILE:HG23	2:B:722:GLY:CA	2.42	0.49
2:B:709:ILE:HG12	2:B:716:ILE:HD12	1.93	0.49
2:A:561:LEU:N	2:A:561:LEU:HD12	2.27	0.49
2:B:584:GLN:O	2:B:589:GLY:HA2	2.12	0.49
2:B:614:ASN:ND2	2:B:648:HIS:HB3	2.27	0.49
2:B:656:LEU:O	2:B:660:ILE:HG23	2.13	0.49
2:A:656:LEU:O	2:A:660:ILE:HG23	2.13	0.49
2:B:857:LYS:O	2:B:861:GLU:HG2	2.13	0.49
2:A:656:LEU:C	2:A:656:LEU:HD23	2.33	0.48
2:B:624:VAL:CG1	2:B:625:THR:N	2.76	0.48
2:B:568:ILE:HG23	2:B:599:GLU:CG	2.44	0.48
2:A:614:ASN:O	2:A:618:GLN:HG3	2.13	0.48
2:A:755:ASP:OD1	2:A:756:PRO:HD2	2.13	0.48
2:B:578:CYS:SG	2:B:616:LEU:HB2	2.53	0.48
1:D:2:G:H1'	2:B:836:TYR:HD1	1.77	0.47
2:A:637:SER:HB2	2:A:672:SER:OG	2.14	0.47
1:C:6:A:C8	1:C:6:A:H3'	2.49	0.47
2:A:568:ILE:HB	2:A:599:GLU:OE1	2.14	0.47
2:B:727:GLN:HG2	2:B:764:TYR:CD2	2.49	0.47
1:D:6:A:C8	1:D:6:A:H3'	2.49	0.47
2:A:704:PHE:CG	2:A:705:ILE:N	2.83	0.47
2:A:646:ASN:HA	2:A:647:PRO:HD3	1.77	0.47
2:A:734:THR:HG22	2:A:735:THR:N	2.29	0.47
2:B:666:ALA:O	2:B:670:VAL:HG13	2.14	0.47
2:A:705:ILE:HG23	2:A:709:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:PHE:CG	2:B:705:ILE:N	2.83	0.46
2:B:786:LYS:HB3	2:B:787:PRO:HD3	1.97	0.46
2:A:614:ASN:HD22	2:A:648:HIS:HB3	1.80	0.46
2:A:630:ILE:O	2:A:634:LYS:HG3	2.16	0.46
2:B:585:LEU:CD2	2:B:593:ALA:HA	2.45	0.46
2:B:627:GLU:O	2:B:631:VAL:HG23	2.15	0.46
2:B:637:SER:OG	2:B:638:PRO:HD3	2.15	0.46
2:A:565:ILE:CG2	2:A:566:GLY:N	2.78	0.46
2:B:563:GLN:O	2:B:564:TYR:CD1	2.69	0.46
2:B:585:LEU:O	2:B:589:GLY:CA	2.64	0.46
2:B:585:LEU:HG	2:B:596:ILE:HD12	1.96	0.46
2:B:714:ILE:HG12	2:B:748:LEU:HD13	1.97	0.45
2:A:568:ILE:HD13	2:A:596:ILE:HG12	1.99	0.45
2:B:574:ASP:O	2:B:578:CYS:HB2	2.15	0.45
2:A:637:SER:OG	2:A:638:PRO:HD3	2.16	0.45
2:B:585:LEU:O	2:B:623:GLU:CG	2.64	0.45
2:B:624:VAL:HG13	2:B:625:THR:N	2.31	0.45
2:B:646:ASN:HA	2:B:647:PRO:HD3	1.76	0.45
2:B:824:GLY:O	2:B:828:ILE:HG13	2.16	0.45
2:B:565:ILE:HG22	2:B:566:GLY:N	2.32	0.44
1:C:8:U:O2	2:A:614:ASN:ND2	2.50	0.44
2:A:714:ILE:HG12	2:A:748:LEU:HD13	1.99	0.44
2:B:630:ILE:O	2:B:634:LYS:HG3	2.17	0.44
2:B:699:PRO:HA	2:B:702:PHE:CE2	2.51	0.44
2:B:727:GLN:HG2	2:B:764:TYR:CG	2.53	0.44
2:B:568:ILE:HD13	2:B:599:GLU:CD	2.38	0.44
2:B:577:GLY:O	2:B:581:LEU:HB2	2.17	0.44
2:A:734:THR:CG2	2:A:735:THR:N	2.80	0.43
2:A:748:LEU:O	2:A:752:LEU:HG	2.18	0.43
2:B:582:GLN:HG2	2:B:616:LEU:HD12	2.00	0.43
2:A:849:HIS:NE2	2:A:886:LEU:HB3	2.33	0.43
2:B:717:ALA:HB2	2:B:726:LEU:CD1	2.48	0.43
2:A:578:CYS:SG	2:A:612:PHE:HB2	2.58	0.43
2:A:624:VAL:CG1	2:A:625:THR:N	2.81	0.43
2:A:854:TYR:O	2:A:858:ARG:HG2	2.19	0.43
2:A:879:ARG:O	2:A:883:MET:HG3	2.19	0.43
2:B:656:LEU:C	2:B:656:LEU:HD23	2.38	0.43
2:A:728:ARG:HD3	2:A:728:ARG:HA	1.85	0.43
2:B:601:LYS:O	2:B:604:THR:HG23	2.18	0.43
2:A:786:LYS:HB3	2:A:787:PRO:HD3	1.99	0.43
2:B:854:TYR:O	2:B:858:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:591:LYS:NZ	5:A:987:HOH:O	2.45	0.43
2:B:585:LEU:O	2:B:589:GLY:HA3	2.19	0.43
2:B:664:GLU:O	2:B:668:ILE:HG13	2.19	0.43
2:A:858:ARG:HA	2:A:858:ARG:HD3	1.79	0.43
2:B:585:LEU:HB3	2:B:623:GLU:HG2	2.00	0.43
2:B:614:ASN:O	2:B:618:GLN:HG3	2.18	0.42
1:D:1:U:C2	2:B:876:HIS:HB3	2.54	0.42
2:A:884:LEU:HD23	2:A:884:LEU:HA	1.82	0.42
2:B:619:LYS:HA	2:B:619:LYS:HD2	1.91	0.42
2:A:818:GLU:OE1	2:A:818:GLU:HA	2.20	0.42
2:A:885:HIS:C	2:A:886:LEU:HD12	2.39	0.42
2:B:585:LEU:HD21	2:B:596:ILE:HD12	2.01	0.42
2:A:619:LYS:HD2	2:A:619:LYS:HA	1.87	0.42
2:A:727:GLN:HG2	2:A:764:TYR:CD2	2.54	0.42
2:A:581:LEU:O	2:A:584:GLN:HB2	2.20	0.42
2:B:580:PHE:O	2:B:583:LYS:HB2	2.20	0.42
2:B:728:ARG:HD3	2:B:728:ARG:HA	1.85	0.42
2:B:788:ARG:HD2	2:B:791:GLU:CD	2.39	0.41
2:A:624:VAL:HG13	2:A:625:THR:N	2.36	0.41
2:A:849:HIS:HE1	2:A:886:LEU:O	2.04	0.41
2:B:858:ARG:HA	2:B:858:ARG:HD3	1.81	0.41
2:B:717:ALA:HA	2:B:726:LEU:HD12	2.03	0.41
2:A:717:ALA:HA	2:A:726:LEU:HD12	2.03	0.41
2:A:788:ARG:HD2	2:A:791:GLU:CD	2.42	0.41
2:A:849:HIS:CE1	2:A:886:LEU:O	2.74	0.41
2:B:585:LEU:CD2	2:B:596:ILE:HD12	2.51	0.41
2:B:585:LEU:CG	2:B:596:ILE:HD12	2.51	0.41
2:B:588:LEU:O	2:B:590:SER:N	2.54	0.41
2:A:872:ARG:HH11	2:A:872:ARG:HD2	1.75	0.41
2:B:581:LEU:O	2:B:596:ILE:HD11	2.21	0.40
2:A:588:LEU:HD23	2:A:588:LEU:HA	1.71	0.40
2:A:849:HIS:CE1	2:A:886:LEU:CB	3.04	0.40
2:A:883:MET:HA	2:A:886:LEU:HD11	2.03	0.40
2:A:768:LYS:HB3	2:A:768:LYS:HE2	1.85	0.40
2:B:879:ARG:O	2:B:883:MET:HG3	2.21	0.40
1:C:1:U:N3	2:A:876:HIS:HB3	2.36	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	
2	A	326/335 (97%)	309 (95%)	15 (5%)	2 (1%)	25	46
2	B	321/335 (96%)	301 (94%)	18 (6%)	2 (1%)	25	46
All	All	647/670 (97%)	610 (94%)	33 (5%)	4 (1%)	25	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	821	ASN
2	A	565	ILE
2	A	821	ASN
2	B	597	PHE

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	
2	A	298/303 (98%)	282 (95%)	16 (5%)	22	42
2	B	293/303 (97%)	275 (94%)	18 (6%)	18	36
All	All	591/606 (98%)	557 (94%)	34 (6%)	20	38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	560	VAL
2	A	574	ASP

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Mol	Chain	Res	Type
2	A	610	ASP
2	A	623	GLU
2	A	624	VAL
2	A	663	ASP
2	A	680	LEU
2	A	687	ASN
2	A	711	ASP
2	A	714	ILE
2	A	715	ASP
2	A	720	ARG
2	A	750	ASP
2	A	860	SER
2	A	871	ILE
2	A	879	ARG
2	B	563	GLN
2	B	564	TYR
2	B	571	LEU
2	B	572	CYS
2	B	581	LEU
2	B	610	ASP
2	B	623	GLU
2	B	624	VAL
2	B	663	ASP
2	B	711	ASP
2	B	714	ILE
2	B	720	ARG
2	B	723	CYS
2	B	750	ASP
2	B	860	SER
2	B	868	VAL
2	B	871	ILE
2	B	879	ARG

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

Mol	Chain	Res	Type
2	A	575	GLN
2	A	648	HIS
2	A	849	HIS
2	B	569	HIS
2	B	575	GLN
2	B	773	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	8/9 (88%)	2 (25%)	0
1	D	8/9 (88%)	3 (37%)	0
All	All	16/18 (88%)	5 (31%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	7	U
1	C	8	U
1	D	7	U
1	D	8	U
1	D	9	A

There are no RNA pucker outliers to report.

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 ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
3	SO4	B	953	-	4,4,4	0.22	0	6,6,6	0.15	0
3	SO4	A	958	-	4,4,4	0.62	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	956	-	4,4,4	0.20	0	6,6,6	0.13	0
3	SO4	B	952	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	A	957	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	B	955	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	951	-	4,4,4	0.27	0	6,6,6	0.23	0
3	SO4	B	954	-	4,4,4	0.27	0	6,6,6	0.12	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	953	SO4	1	0

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 [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	C	9/9 (100%)	1.61	2 (22%) 0 0	46, 55, 104, 157	0
1	D	9/9 (100%)	1.38	3 (33%) 0 0	48, 66, 94, 159	0
2	A	328/335 (97%)	-0.37	4 (1%) 79 76	12, 28, 69, 111	0
2	B	323/335 (96%)	-0.05	17 (5%) 26 20	13, 35, 93, 133	0
All	All	669/688 (97%)	-0.16	26 (3%) 39 31	12, 32, 88, 159	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	U	6.2
1	D	7	U	5.3
2	B	567	SER	5.0
2	B	873	ASN	4.9
2	B	592	ALA	3.8
2	B	590	SER	3.7
2	B	882	GLY	3.5
2	B	870	PRO	3.1
2	B	627	GLU	3.1
2	A	591	LYS	3.0
2	B	879	ARG	2.7
2	B	599	GLU	2.7
2	A	887	ASP	2.6
2	B	602	ASP	2.6
2	B	875	PRO	2.6
2	B	591	LYS	2.6
2	A	563	GLN	2.5
2	B	878	LYS	2.5
2	B	612	PHE	2.4
1	C	8	U	2.4
2	A	590	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	8	U	2.2
2	B	603	TYR	2.2
2	B	587	ILE	2.0
2	B	564	TYR	2.0
1	D	9	A	2.0

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 monosaccharides 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
3	SO4	A	957	5/5	0.76	0.26	113,113,124,127	0
3	SO4	B	952	5/5	0.76	0.42	134,135,137,142	0
3	SO4	B	954	5/5	0.81	0.25	100,101,111,128	0
3	SO4	B	953	5/5	0.88	0.26	104,105,109,120	0
3	SO4	B	955	5/5	0.89	0.29	109,112,114,118	0
4	NA	B	901	1/1	0.90	0.12	30,30,30,30	0
3	SO4	A	951	5/5	0.93	0.17	41,55,72,73	0
3	SO4	A	956	5/5	0.95	0.20	95,106,113,117	0
3	SO4	A	958	5/5	0.96	0.41	30,30,30,30	0
4	NA	B	902	1/1	0.98	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.