WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 01:04 AM EDT

PDB ID	:	3BX3
Title	:	Puf4 T650C/C724R Mutant bound to Cox17 RNA 3' UTR recognition sequence
Authors	:	Miller, M.T.; Higgin, J.J.; Hall, T.M.T.
Deposited on	:	2008-01-11
Resolution	:	3.00 Å(reported)

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

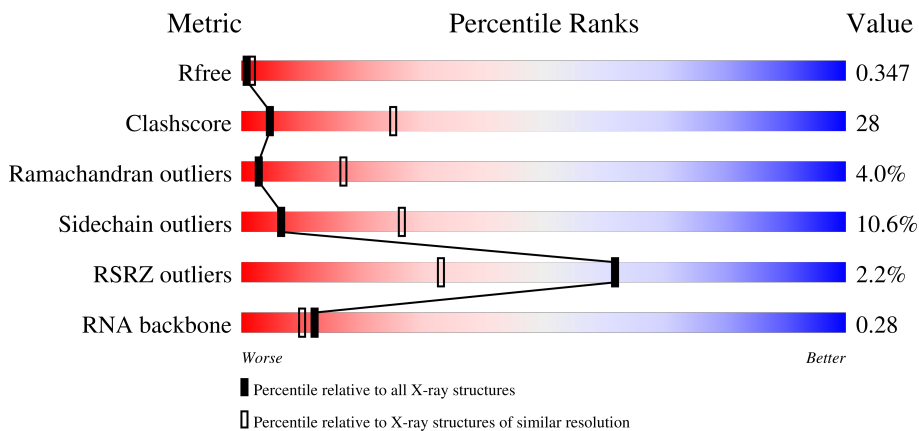|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.347
Clashscore		28
Ramachandran outliers		4.0%
Sidechain outliers		10.6%
RSRZ outliers		2.2%
RNA backbone		0.28

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	C	8	25% / 38% / 50% / 12%
1	D	8	25% / 38% / 50% / 12%
2	A	335	% / 42% / 45% / 10% ·
2	B	335	2% / 45% / 37% / 7% / 10%

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2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5349 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 COX17 RNA target sequence.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	8	Total	C	N	O	P	0	0	0
			166	76	28	55	7			
1	D	8	Total	C	N	O	P	0	0	0
			166	76	28	55	7			

- Molecule 2 is a protein called Protein PUF4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	325	Total	C	N	O	S	0	0	0
			2592	1645	446	488	13			
2	B	300	Total	C	N	O	S	0	0	0
			2380	1511	408	450	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	650	CYS	THR	engineered mutation	UNP P25339
A	724	ARG	CYS	engineered mutation	UNP P25339
B	650	CYS	THR	engineered mutation	UNP P25339
B	724	ARG	CYS	engineered mutation	UNP P25339

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
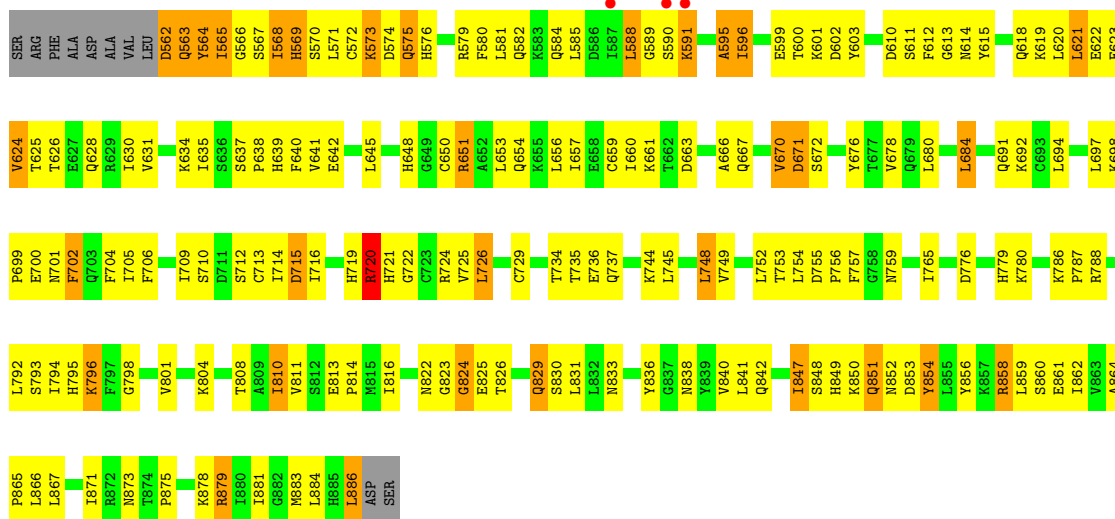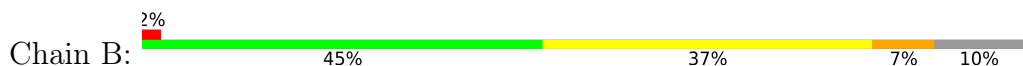
- Molecule 1: COX17 RNA target sequence
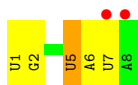
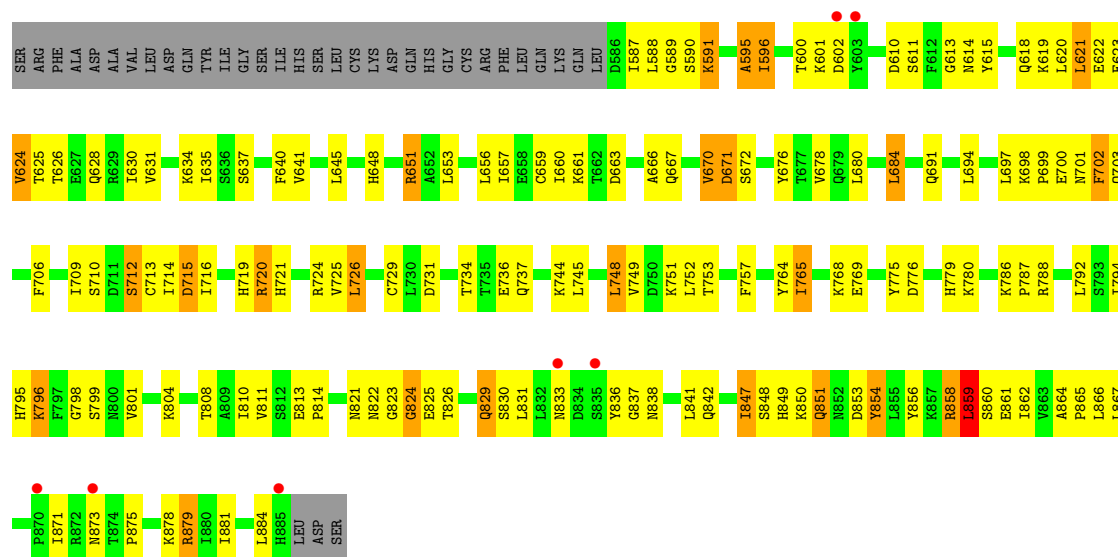- Molecule 1: COX17 RNA target sequence
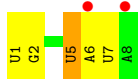
- Molecule 2: Protein PUF4

- 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	66.06Å 137.12Å 160.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.40 – 3.00 24.41 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.40-3.00) 97.9 (24.41-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.14 (at 2.99Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.290 , 0.350 0.291 , 0.347	Depositor DCC
R_{free} test set	1500 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.2	EDS
L-test for twinning[2]	$< |L| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	5349	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7354e-03.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.76	0/185	1.48	4/286 (1.4%)
1	D	0.74	0/185	1.43	4/286 (1.4%)
2	A	0.49	0/2636	0.76	3/3564 (0.1%)
2	B	0.46	0/2420	0.72	4/3275 (0.1%)
All	All	0.50	0/5426	0.82	15/7411 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	651	ARG	NE-CZ-NH2	-13.33	113.63	120.30
2	A	651	ARG	NE-CZ-NH1	12.37	126.48	120.30
2	B	651	ARG	NE-CZ-NH1	-11.76	114.42	120.30
2	B	651	ARG	NE-CZ-NH2	11.47	126.03	120.30
1	D	5	U	C1'-O4'-C4'	-7.12	104.21	109.90
1	C	5	U	O4'-C1'-N1	7.00	113.80	108.20
1	D	2	G	O4'-C1'-N9	6.80	113.64	108.20
1	C	5	U	C1'-O4'-C4'	-6.71	104.53	109.90
2	A	651	ARG	CD-NE-CZ	6.48	132.67	123.60
1	D	5	U	O4'-C1'-N1	6.35	113.28	108.20
2	B	651	ARG	CD-NE-CZ	6.02	132.03	123.60
1	C	2	G	O4'-C1'-N9	5.68	112.75	108.20
1	C	5	U	C4'-C3'-C2'	-5.13	97.47	102.60
2	B	859	LEU	CA-CB-CG	5.08	126.99	115.30
1	D	5	U	C4'-C3'-C2'	-5.08	97.52	102.60

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	C	166	0	86	11	0
1	D	166	0	86	8	0
2	A	2592	0	2636	181	0
2	B	2380	0	2415	133	0
3	A	25	0	0	1	0
3	B	20	0	0	1	0
All	All	5349	0	5223	297	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 28.

All (297) 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:A:642:GLU:HG3	2:B:714:ILE:CG2	1.60	1.31
2:B:753:THR:HG23	2:B:801:VAL:HG21	1.31	1.12
2:A:642:GLU:HG3	2:B:714:ILE:HG22	1.09	1.09
2:A:753:THR:HG23	2:A:801:VAL:HG21	1.31	1.07
2:B:734:THR:HG22	2:B:736:GLU:H	1.21	1.04
2:A:734:THR:HG22	2:A:736:GLU:H	1.20	1.02
2:B:808:THR:HG22	2:B:811:VAL:HG22	1.47	0.97
2:B:714:ILE:HD13	2:B:748:LEU:HD13	1.47	0.97
2:A:642:GLU:CG	2:B:714:ILE:HG22	1.94	0.97
2:A:714:ILE:HD13	2:A:748:LEU:HD13	1.51	0.93
2:A:808:THR:HG22	2:A:811:VAL:HG22	1.48	0.92
1:C:1:U:H3	2:A:838:ASN:ND2	1.67	0.92
2:A:575:GLN:HE22	2:A:579:ARG:HE	1.12	0.90
1:C:5:U:N3	2:A:724:ARG:HD3	1.89	0.85
2:A:572:CYS:O	2:A:573:LYS:HG3	1.76	0.85
2:A:734:THR:HG22	2:A:736:GLU:N	1.91	0.85
1:C:1:U:H3	2:A:838:ASN:HD21	1.25	0.85
2:A:753:THR:HG23	2:A:801:VAL:CG2	2.09	0.83
2:B:734:THR:HG22	2:B:736:GLU:N	1.93	0.82
2:A:588:LEU:HB3	2:A:589:GLY:CA	2.09	0.82
2:B:753:THR:HG23	2:B:801:VAL:CG2	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:883:MET:O	2:A:886:LEU:HD22	1.85	0.77
1:D:1:U:H3	2:B:838:ASN:HD21	1.33	0.77
2:B:864:ALA:HB3	2:B:865:PRO:HD3	1.65	0.76
2:A:849:HIS:HE1	2:A:886:LEU:C	1.89	0.75
2:A:621:LEU:N	2:A:621:LEU:HD23	2.01	0.74
2:A:676:TYR:OH	2:B:719:HIS:HD2	1.69	0.74
2:A:642:GLU:HG3	2:B:714:ILE:HG21	1.63	0.74
2:A:735:THR:HG21	3:A:905:SO4:O2	1.88	0.74
2:B:621:LEU:HD23	2:B:621:LEU:N	2.03	0.74
2:A:864:ALA:HB3	2:A:865:PRO:HD3	1.68	0.74
1:D:5:U:N3	2:B:724:ARG:HD3	2.03	0.73
2:A:582:GLN:HE22	2:A:615:TYR:HB3	1.54	0.73
2:A:588:LEU:HB3	2:A:589:GLY:HA2	1.71	0.72
2:A:794:ILE:O	2:A:836:TYR:HD2	1.74	0.71
2:B:808:THR:HG22	2:B:811:VAL:CG2	2.20	0.71
2:A:588:LEU:CB	2:A:589:GLY:HA2	2.20	0.70
2:A:588:LEU:HD22	2:A:589:GLY:HA2	1.73	0.70
1:C:7:U:H3	2:A:618:GLN:HE22	1.40	0.69
2:B:794:ILE:O	2:B:836:TYR:HD2	1.76	0.69
2:A:849:HIS:CE1	2:A:886:LEU:HB3	2.28	0.69
2:B:734:THR:CG2	2:B:736:GLU:H	2.01	0.69
2:A:808:THR:HG22	2:A:811:VAL:CG2	2.21	0.68
2:A:667:GLN:O	2:A:671:ASP:OD1	2.13	0.67
2:A:849:HIS:CE1	2:A:886:LEU:CB	2.78	0.67
2:A:571:LEU:HD23	2:A:571:LEU:N	2.09	0.67
2:B:678:VAL:HG22	2:B:716:ILE:HD11	1.74	0.67
2:A:678:VAL:HG22	2:A:716:ILE:HD11	1.77	0.66
1:C:5:U:C2	2:A:724:ARG:HD3	2.30	0.65
2:A:715:ASP:O	2:A:719:HIS:HB2	1.98	0.64
2:B:611:SER:HA	2:B:648:HIS:CE1	2.32	0.64
2:A:588:LEU:CD2	2:A:589:GLY:HA2	2.28	0.63
2:B:813:GLU:HB2	2:B:814:PRO:HD3	1.81	0.63
2:B:610:ASP:OD2	2:B:613:GLY:N	2.32	0.63
2:B:829:GLN:HG2	2:B:866:LEU:HD13	1.80	0.63
2:A:611:SER:HA	2:A:648:HIS:CE1	2.34	0.62
2:B:715:ASP:OD1	2:B:715:ASP:N	2.32	0.62
2:A:564:TYR:CG	2:A:565:ILE:N	2.66	0.62
2:B:831:LEU:HD23	2:B:841:LEU:HB2	1.80	0.62
2:A:734:THR:CG2	2:A:736:GLU:H	2.03	0.62
2:B:734:THR:H	2:B:737:GLN:HB2	1.64	0.62
2:A:574:ASP:HB3	2:A:576:HIS:HD2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:715:ASP:O	2:B:719:HIS:HB2	2.01	0.61
2:A:610:ASP:OD2	2:A:613:GLY:N	2.34	0.60
2:A:676:TYR:OH	2:B:719:HIS:CD2	2.52	0.60
2:A:625:THR:HG23	2:A:628:GLN:OE1	2.02	0.60
2:B:776:ASP:O	2:B:780:LYS:HG3	2.01	0.59
2:B:875:PRO:O	2:B:879:ARG:HG2	2.01	0.59
2:A:829:GLN:HE22	2:A:833:ASN:ND2	2.00	0.59
2:B:667:GLN:O	2:B:671:ASP:OD1	2.21	0.58
2:B:700:GLU:CD	2:B:700:GLU:H	2.05	0.58
2:A:829:GLN:HG2	2:A:866:LEU:HD13	1.84	0.58
2:A:715:ASP:OD1	2:A:715:ASP:N	2.33	0.58
2:A:813:GLU:HB2	2:A:814:PRO:HD3	1.85	0.58
2:B:698:LYS:HE3	2:B:700:GLU:OE1	2.03	0.58
1:D:1:U:H3	2:B:838:ASN:ND2	1.99	0.58
2:A:699:PRO:HA	2:A:702:PHE:CE2	2.39	0.58
2:A:776:ASP:O	2:A:780:LYS:HG3	2.03	0.58
2:A:875:PRO:O	2:A:879:ARG:HG2	2.03	0.58
2:A:734:THR:H	2:A:737:GLN:HB2	1.68	0.57
2:B:823:GLY:O	2:B:824:GLY:O	2.22	0.57
2:B:625:THR:HG23	2:B:628:GLN:OE1	2.03	0.57
2:A:640:PHE:HD2	2:A:672:SER:HB3	1.68	0.57
2:B:698:LYS:O	2:B:701:ASN:HB2	2.04	0.57
2:B:829:GLN:HE22	2:B:833:ASN:ND2	2.02	0.57
1:C:7:U:C4	2:A:651:ARG:HD2	2.40	0.56
2:A:700:GLU:CD	2:A:700:GLU:H	2.07	0.56
2:B:656:LEU:C	2:B:656:LEU:HD23	2.26	0.56
2:A:584:GLN:O	2:A:588:LEU:HB2	2.05	0.56
2:A:614:ASN:O	2:A:618:GLN:HG3	2.06	0.56
2:A:788:ARG:NH2	2:A:792:LEU:HD21	2.21	0.56
2:A:831:LEU:HD23	2:A:841:LEU:HB2	1.86	0.56
2:A:698:LYS:O	2:A:701:ASN:HB2	2.05	0.55
2:B:858:ARG:NH1	2:B:861:GLU:OE2	2.39	0.55
2:A:779:HIS:NE2	2:A:810:ILE:HD12	2.22	0.55
2:B:699:PRO:HA	2:B:702:PHE:CE2	2.41	0.55
2:A:574:ASP:HB3	2:A:576:HIS:CD2	2.42	0.55
2:A:858:ARG:NH1	2:A:861:GLU:OE2	2.40	0.55
2:B:749:VAL:HA	2:B:752:LEU:HB2	1.88	0.55
2:B:796:LYS:HE2	2:B:836:TYR:CE2	2.41	0.55
2:A:626:THR:O	2:A:630:ILE:HG13	2.07	0.54
2:A:656:LEU:C	2:A:656:LEU:HD23	2.27	0.54
2:A:564:TYR:CE2	2:A:565:ILE:HB	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:588:LEU:CB	2:A:589:GLY:CA	2.80	0.54
2:B:640:PHE:HD2	2:B:672:SER:HB3	1.72	0.54
1:D:7:U:C4	2:B:651:ARG:HD3	2.43	0.54
2:B:788:ARG:NH2	2:B:792:LEU:HD21	2.22	0.54
1:C:5:U:C2	2:A:724:ARG:CD	2.91	0.54
2:B:858:ARG:HH11	2:B:858:ARG:HG3	1.71	0.54
2:A:645:LEU:HD13	2:B:751:LYS:HD2	1.90	0.54
2:A:619:LYS:HA	2:A:622:GLU:HG3	1.90	0.53
2:A:676:TYR:HB2	2:A:680:LEU:HD12	1.90	0.53
2:A:698:LYS:HE3	2:A:700:GLU:OE1	2.08	0.53
2:A:749:VAL:HA	2:A:752:LEU:HB2	1.89	0.53
2:B:776:ASP:OD1	2:B:780:LYS:HE3	2.08	0.53
2:B:858:ARG:NH1	2:B:858:ARG:HG3	2.24	0.53
2:A:822:ASN:C	2:A:824:GLY:H	2.12	0.53
2:B:619:LYS:HA	2:B:622:GLU:HG3	1.91	0.52
2:A:706:PHE:CZ	2:A:729:CYS:HB3	2.45	0.52
2:A:719:HIS:O	2:A:721:HIS:N	2.42	0.52
2:A:564:TYR:CZ	2:A:565:ILE:HB	2.44	0.52
2:A:666:ALA:O	2:A:670:VAL:HG13	2.10	0.52
2:A:776:ASP:OD1	2:A:780:LYS:HE3	2.10	0.52
2:A:796:LYS:HE2	2:A:836:TYR:CE2	2.44	0.52
2:B:626:THR:O	2:B:630:ILE:HG13	2.10	0.52
2:A:676:TYR:O	2:A:680:LEU:HD12	2.10	0.52
2:A:691:GLN:HA	2:A:694:LEU:HD12	1.92	0.51
2:B:726:LEU:HD23	2:B:745:LEU:HD11	1.92	0.51
2:B:873:ASN:O	2:B:878:LYS:HE3	2.10	0.51
2:A:849:HIS:CE1	2:A:886:LEU:C	2.79	0.51
2:A:726:LEU:HD23	2:A:745:LEU:HD11	1.92	0.51
2:A:867:LEU:HD13	2:A:881:ILE:HG12	1.93	0.51
2:B:795:HIS:CD2	3:B:903:SO4:O2	2.64	0.51
2:A:825:GLU:HG3	2:A:862:ILE:HG23	1.91	0.51
2:B:826:THR:O	2:B:829:GLN:N	2.40	0.51
2:A:786:LYS:HB3	2:A:787:PRO:HD3	1.92	0.51
2:A:704:PHE:CZ	2:A:705:ILE:HG13	2.46	0.50
2:A:719:HIS:O	2:A:720:ARG:C	2.50	0.50
2:A:653:LEU:O	2:A:657:ILE:HG13	2.10	0.50
2:A:709:ILE:HD11	2:A:725:VAL:HG12	1.91	0.50
2:A:793:SER:HB3	2:A:840:VAL:HG21	1.93	0.50
2:B:666:ALA:O	2:B:670:VAL:HG13	2.12	0.50
2:B:847:ILE:HG23	2:B:851:GLN:HG3	1.92	0.50
2:B:822:ASN:C	2:B:824:GLY:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:630:ILE:HG22	2:A:634:LYS:HE3	1.94	0.50
2:B:786:LYS:HB3	2:B:787:PRO:HD3	1.93	0.50
1:C:6:A:H2	2:A:654:GLN:HE22	1.58	0.49
2:A:564:TYR:CE2	2:A:565:ILE:HD13	2.47	0.49
2:B:867:LEU:HD13	2:B:881:ILE:HG12	1.94	0.49
2:A:624:VAL:HG22	2:A:628:GLN:OE1	2.12	0.49
2:A:568:ILE:HB	2:A:599:GLU:OE1	2.12	0.49
2:A:641:VAL:O	2:A:645:LEU:HG	2.13	0.49
2:B:660:ILE:O	2:B:660:ILE:HG13	2.13	0.49
2:B:753:THR:HG22	2:B:798:GLY:HA2	1.93	0.49
1:C:7:U:N3	2:A:651:ARG:HD2	2.27	0.49
2:A:575:GLN:O	2:A:579:ARG:HB2	2.13	0.49
2:B:825:GLU:O	2:B:825:GLU:HG2	2.12	0.49
2:B:849:HIS:HB2	2:B:856:TYR:CD1	2.47	0.49
2:B:630:ILE:HG22	2:B:634:LYS:HE3	1.94	0.49
2:A:575:GLN:HE22	2:A:579:ARG:NE	1.95	0.49
2:A:753:THR:HG22	2:A:798:GLY:HA2	1.94	0.49
2:B:825:GLU:HG3	2:B:862:ILE:HG23	1.94	0.49
2:A:709:ILE:HD11	2:A:725:VAL:CG1	2.42	0.48
2:B:710:SER:HB3	2:B:744:LYS:NZ	2.28	0.48
2:A:585:LEU:HD21	2:A:596:ILE:CD1	2.44	0.48
2:A:826:THR:O	2:A:829:GLN:N	2.44	0.48
2:A:568:ILE:O	2:A:569:HIS:C	2.52	0.48
2:B:614:ASN:O	2:B:618:GLN:HG3	2.12	0.48
2:B:825:GLU:HG3	2:B:862:ILE:CG2	2.43	0.48
2:B:640:PHE:HD2	2:B:672:SER:CB	2.26	0.48
2:A:631:VAL:O	2:A:635:ILE:HG13	2.13	0.48
2:A:659:CYS:O	2:A:661:LYS:HG3	2.13	0.48
2:A:849:HIS:HB2	2:A:856:TYR:CD1	2.49	0.48
2:B:631:VAL:O	2:B:635:ILE:HG13	2.13	0.48
2:B:720:ARG:HA	2:B:757:PHE:CE1	2.49	0.47
2:A:847:ILE:HG22	2:A:848:SER:N	2.30	0.47
2:A:847:ILE:HG23	2:A:851:GLN:HG3	1.96	0.47
1:C:7:U:H3	2:A:618:GLN:NE2	2.11	0.47
2:A:575:GLN:HB2	2:A:612:PHE:CD1	2.50	0.47
2:B:779:HIS:NE2	2:B:810:ILE:HD12	2.29	0.47
1:C:7:U:C2	2:A:651:ARG:HD2	2.49	0.47
2:B:590:SER:C	2:B:591:LYS:HD3	2.34	0.47
2:A:710:SER:HB3	2:A:744:LYS:NZ	2.29	0.47
2:B:656:LEU:HD23	2:B:656:LEU:O	2.14	0.47
2:A:590:SER:C	2:A:591:LYS:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:823:GLY:O	2:A:824:GLY:O	2.32	0.47
2:B:796:LYS:H	2:B:796:LYS:HG2	1.51	0.46
2:A:569:HIS:ND1	2:A:570:SER:N	2.63	0.46
2:B:847:ILE:O	2:B:850:LYS:N	2.49	0.46
2:A:568:ILE:HG23	2:A:581:LEU:HD22	1.97	0.46
2:B:676:TYR:HB2	2:B:680:LEU:HD12	1.98	0.46
2:A:676:TYR:CZ	2:B:719:HIS:HD2	2.34	0.46
2:A:873:ASN:O	2:A:878:LYS:HE3	2.15	0.46
2:A:565:ILE:HG23	2:A:565:ILE:O	2.16	0.46
2:A:794:ILE:O	2:A:836:TYR:CD2	2.63	0.46
2:B:641:VAL:O	2:B:645:LEU:HG	2.15	0.46
2:A:600:THR:C	2:A:602:ASP:H	2.19	0.46
2:A:640:PHE:HD2	2:A:672:SER:CB	2.28	0.46
2:A:642:GLU:HG3	2:B:714:ILE:CB	2.38	0.46
2:A:656:LEU:HD23	2:A:656:LEU:O	2.16	0.46
2:A:676:TYR:HB2	2:A:680:LEU:CD1	2.46	0.46
2:B:624:VAL:HG22	2:B:628:GLN:OE1	2.14	0.46
2:B:796:LYS:HE2	2:B:836:TYR:HE2	1.80	0.46
2:A:640:PHE:CE1	2:A:653:LEU:CD1	2.99	0.46
2:A:884:LEU:HD23	2:A:884:LEU:HA	1.68	0.46
2:B:624:VAL:HG22	2:B:628:GLN:HB2	1.98	0.46
2:A:582:GLN:NE2	2:A:615:TYR:HB3	2.26	0.45
2:A:720:ARG:HA	2:A:757:PHE:CE1	2.51	0.45
2:B:709:ILE:HD11	2:B:725:VAL:HG12	1.97	0.45
1:D:7:U:N3	2:B:651:ARG:HD3	2.31	0.45
2:B:847:ILE:HG22	2:B:848:SER:N	2.31	0.45
2:B:854:TYR:CD1	2:B:854:TYR:C	2.89	0.45
2:A:642:GLU:OE1	2:B:712:SER:HA	2.16	0.45
2:A:660:ILE:O	2:A:660:ILE:HG13	2.16	0.45
2:B:659:CYS:O	2:B:661:LYS:HG3	2.16	0.45
2:A:838:ASN:C	2:A:838:ASN:OD1	2.54	0.45
1:D:7:U:C2	2:B:651:ARG:HD3	2.52	0.45
2:A:624:VAL:HG22	2:A:628:GLN:HB2	1.98	0.45
2:A:642:GLU:OE2	2:B:715:ASP:OD1	2.34	0.45
2:B:595:ALA:O	2:B:596:ILE:C	2.55	0.45
2:B:615:TYR:O	2:B:619:LYS:HG2	2.17	0.45
2:A:639:HIS:CD2	2:B:712:SER:HG	2.35	0.45
2:A:595:ALA:O	2:A:596:ILE:C	2.56	0.45
2:A:858:ARG:HG3	2:A:858:ARG:HH11	1.82	0.45
2:A:754:LEU:HD22	2:A:795:HIS:CD2	2.52	0.45
2:B:703:GLN:OE1	2:B:737:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:590:SER:O	2:A:591:LYS:HD3	2.17	0.44
2:A:615:TYR:O	2:A:619:LYS:HG2	2.17	0.44
2:A:755:ASP:HA	2:A:756:PRO:HD3	1.84	0.44
2:A:849:HIS:CE1	2:A:886:LEU:HB2	2.50	0.44
2:B:706:PHE:CZ	2:B:729:CYS:HB3	2.52	0.44
2:B:709:ILE:HD11	2:B:725:VAL:CG1	2.47	0.44
2:B:769:GLU:OE1	2:B:775:TYR:HA	2.18	0.44
2:A:639:HIS:HD2	2:B:712:SER:HA	1.81	0.44
2:B:600:THR:C	2:B:602:ASP:H	2.20	0.44
2:A:596:ILE:H	2:A:596:ILE:HG13	1.59	0.44
2:A:825:GLU:HG3	2:A:862:ILE:CG2	2.46	0.44
2:B:859:LEU:C	2:B:861:GLU:H	2.21	0.44
2:A:562:ASP:O	2:A:563:GLN:O	2.36	0.44
2:B:823:GLY:O	2:B:824:GLY:C	2.56	0.44
2:B:590:SER:O	2:B:591:LYS:HD3	2.18	0.44
2:A:801:VAL:O	2:A:804:LYS:HB3	2.18	0.43
2:A:716:ILE:HG22	2:A:722:GLY:O	2.19	0.43
2:A:816:ILE:HD13	2:A:848:SER:HB3	1.99	0.43
2:B:884:LEU:HD23	2:B:884:LEU:HA	1.68	0.43
2:A:574:ASP:HB3	2:A:576:HIS:H	1.83	0.43
2:A:847:ILE:O	2:A:850:LYS:N	2.52	0.43
2:B:691:GLN:HA	2:B:694:LEU:HD12	2.01	0.43
2:B:660:ILE:HD11	2:B:697:LEU:HD21	2.01	0.43
2:B:849:HIS:HB2	2:B:856:TYR:CE1	2.54	0.43
2:B:764:TYR:O	2:B:765:ILE:C	2.57	0.43
2:B:671:ASP:OD1	2:B:671:ASP:N	2.52	0.43
2:A:858:ARG:NH1	2:A:858:ARG:HG3	2.33	0.43
2:A:562:ASP:OD1	2:A:562:ASP:N	2.51	0.42
2:A:660:ILE:HD11	2:A:697:LEU:HD21	2.01	0.42
2:A:565:ILE:HG13	2:A:566:GLY:O	2.18	0.42
2:A:638:PRO:O	2:B:712:SER:HB3	2.19	0.42
2:A:849:HIS:HB2	2:A:856:TYR:CE1	2.55	0.42
2:A:575:GLN:O	2:A:575:GLN:CD	2.58	0.42
2:A:641:VAL:HG21	2:B:715:ASP:HB3	2.02	0.42
2:A:862:ILE:O	2:A:862:ILE:HG22	2.19	0.42
2:B:620:LEU:O	2:B:624:VAL:HB	2.20	0.42
2:A:639:HIS:CD2	2:B:712:SER:HA	2.54	0.42
2:A:684:LEU:HD12	2:A:684:LEU:O	2.20	0.42
2:B:719:HIS:O	2:B:721:HIS:N	2.53	0.42
2:A:640:PHE:CD2	2:A:672:SER:HB3	2.52	0.42
1:D:7:U:H3	2:B:618:GLN:HE22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:653:LEU:O	2:B:657:ILE:HG13	2.19	0.42
2:B:801:VAL:O	2:B:804:LYS:HB3	2.20	0.42
2:A:825:GLU:O	2:A:825:GLU:HG2	2.19	0.41
2:B:719:HIS:O	2:B:720:ARG:C	2.58	0.41
2:A:580:PHE:CZ	2:A:584:GLN:HG2	2.55	0.41
2:B:660:ILE:HD11	2:B:697:LEU:CD2	2.50	0.41
2:B:640:PHE:CE1	2:B:653:LEU:CD1	3.03	0.41
2:B:786:LYS:O	2:B:787:PRO:C	2.58	0.41
2:B:837:GLY:O	2:B:838:ASN:C	2.56	0.41
1:D:6:A:C6	2:B:651:ARG:NH1	2.88	0.41
2:A:567:SER:O	2:A:568:ILE:C	2.58	0.41
2:A:854:TYR:CD1	2:A:854:TYR:C	2.93	0.41
2:A:650:CYS:O	2:A:654:GLN:HG3	2.21	0.41
2:A:641:VAL:CG2	2:B:715:ASP:HB3	2.51	0.41
2:B:684:LEU:HD12	2:B:684:LEU:O	2.21	0.41
2:A:692:LYS:HE2	2:A:692:LYS:HB2	1.77	0.41
2:A:755:ASP:O	2:A:759:ASN:HB3	2.21	0.41
2:B:714:ILE:HD12	2:B:714:ILE:HA	1.94	0.41
2:A:575:GLN:H	2:A:576:HIS:CD2	2.38	0.41
2:B:808:THR:CG2	2:B:811:VAL:HG22	2.33	0.41
2:A:569:HIS:HD2	2:A:603:TYR:CE2	2.39	0.41
2:A:582:GLN:HE22	2:A:615:TYR:CB	2.29	0.40
2:A:852:ASN:C	2:A:852:ASN:OD1	2.60	0.40
2:B:829:GLN:NE2	2:B:833:ASN:ND2	2.68	0.40
2:A:575:GLN:NE2	2:A:579:ARG:HE	1.96	0.40
2:A:620:LEU:O	2:A:624:VAL:HB	2.21	0.40
2:B:709:ILE:O	2:B:710:SER:C	2.58	0.40
2:B:731:ASP:HA	2:B:768:LYS:HE3	2.03	0.40
2:A:709:ILE:O	2:A:710:SER:C	2.59	0.40
2:B:804:LYS:HA	2:B:804:LYS:HD2	1.93	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	323/335 (96%)	258 (80%)	51 (16%)	14 (4%)	2	15
2	B	298/335 (89%)	247 (83%)	40 (13%)	11 (4%)	3	19
All	All	621/670 (93%)	505 (81%)	91 (15%)	25 (4%)	3	17

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	563	GLN
2	A	588	LEU
2	A	824	GLY
2	A	853	ASP
2	B	824	GLY
2	B	853	ASP
2	A	568	ILE
2	A	596	ILE
2	B	587	ILE
2	B	596	ILE
2	A	565	ILE
2	A	569	HIS
2	B	588	LEU
2	A	573	LYS
2	A	720	ARG
2	A	860	SER
2	B	799	SER
2	B	860	SER
2	A	595	ALA
2	A	765	ILE
2	B	595	ALA
2	A	601	LYS
2	B	601	LYS
2	B	765	ILE
2	B	589	GLY

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	295/303 (97%)	263 (89%)	32 (11%)	6	26
2	B	269/303 (89%)	241 (90%)	28 (10%)	7	27
All	All	564/606 (93%)	504 (89%)	60 (11%)	6	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	562	ASP
2	A	564	TYR
2	A	575	GLN
2	A	591	LYS
2	A	621	LEU
2	A	623	GLU
2	A	624	VAL
2	A	637	SER
2	A	663	ASP
2	A	670	VAL
2	A	671	ASP
2	A	684	LEU
2	A	702	PHE
2	A	712	SER
2	A	713	CYS
2	A	715	ASP
2	A	720	ARG
2	A	726	LEU
2	A	748	LEU
2	A	796	LYS
2	A	810	ILE
2	A	829	GLN
2	A	830	SER
2	A	842	GLN
2	A	847	ILE
2	A	851	GLN
2	A	854	TYR
2	A	858	ARG
2	A	859	LEU
2	A	871	ILE
2	A	879	ARG
2	A	886	LEU
2	B	591	LYS
2	B	621	LEU

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Mol	Chain	Res	Type
2	B	623	GLU
2	B	624	VAL
2	B	637	SER
2	B	663	ASP
2	B	670	VAL
2	B	671	ASP
2	B	684	LEU
2	B	702	PHE
2	B	712	SER
2	B	713	CYS
2	B	715	ASP
2	B	720	ARG
2	B	726	LEU
2	B	748	LEU
2	B	796	LYS
2	B	821	ASN
2	B	829	GLN
2	B	830	SER
2	B	842	GLN
2	B	847	ILE
2	B	851	GLN
2	B	854	TYR
2	B	858	ARG
2	B	859	LEU
2	B	871	ILE
2	B	879	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	575	GLN
2	A	576	HIS
2	A	582	GLN
2	A	614	ASN
2	A	618	GLN
2	A	654	GLN
2	A	679	GLN
2	A	688	HIS
2	A	821	ASN
2	A	833	ASN
2	A	838	ASN
2	B	614	ASN

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Mol	Chain	Res	Type
2	B	618	GLN
2	B	648	HIS
2	B	679	GLN
2	B	688	HIS
2	B	719	HIS
2	B	821	ASN
2	B	829	GLN
2	B	838	ASN
2	B	873	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	7/8 (87%)	0	0
1	D	7/8 (87%)	0	0
All	All	14/16 (87%)	0	0

There are no RNA backbone outliers to report.

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 ⓘ

9 ligands 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	$\#|Z| > 2$
3	SO4	B	903	-	4,4,4	0.17	0	6,6,6	0.36	0
3	SO4	B	909	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	A	906	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	A	905	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	A	901	-	4,4,4	0.13	0	6,6,6	0.26	0
3	SO4	A	902	-	4,4,4	0.29	0	6,6,6	0.31	0
3	SO4	A	904	-	4,4,4	0.16	0	6,6,6	0.14	0
3	SO4	B	907	-	4,4,4	0.07	0	6,6,6	0.36	0
3	SO4	B	908	-	4,4,4	0.14	0	6,6,6	0.18	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	903	SO4	1	0
3	A	905	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	C	8/8 (100%)	1.20	2 (25%)	0	0	40, 49, 89, 90	0
1	D	8/8 (100%)	1.70	2 (25%)	0	0	41, 51, 90, 91	0
2	A	325/335 (97%)	-0.24	3 (0%)	84	63	15, 34, 79, 107	0
2	B	300/335 (89%)	-0.18	7 (2%)	60	31	14, 34, 70, 106	0
All	All	641/686 (93%)	-0.17	14 (2%)	62	33	14, 34, 79, 107	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	A	3.7
2	B	885	HIS	3.3
2	A	590	SER	3.3
2	A	587	ILE	2.9
2	A	591	LYS	2.8
2	B	602	ASP	2.8
2	B	873	ASN	2.6
2	B	833	ASN	2.6
2	B	870	PRO	2.4
1	D	6	A	2.4
2	B	835	SER	2.4
1	C	8	A	2.2
2	B	603	TYR	2.1
1	C	7	U	2.0

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

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

6.3 Carbohydrates (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	B	909	5/5	0.83	0.17	42,44,61,98	0
3	SO4	B	903	5/5	0.90	0.28	21,22,50,65	0
3	SO4	A	901	5/5	0.90	0.33	13,30,97,111	0
3	SO4	B	907	5/5	0.91	0.28	44,44,77,89	0
3	SO4	A	905	5/5	0.94	0.20	41,41,50,73	0
3	SO4	A	902	5/5	0.95	0.28	8,13,86,96	0
3	SO4	B	908	5/5	0.96	0.21	43,45,73,79	0
3	SO4	A	904	5/5	0.96	0.19	47,63,80,86	0
3	SO4	A	906	5/5	0.97	0.13	35,43,69,71	0

6.5 Other polymers (i)

There are no such residues in this entry.