



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:32 am BST

PDB ID : 4HL8
Title : Re-refinement of the vault ribonucleoprotein particle
Authors : Casanas, A.; Querol-Audi, J.; Guerra, P.; Pous, J.; Tanaka, H.; Tsukihara, T.; Verdaguer, V.; Fita, I.
Deposited on : 2012-10-16
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

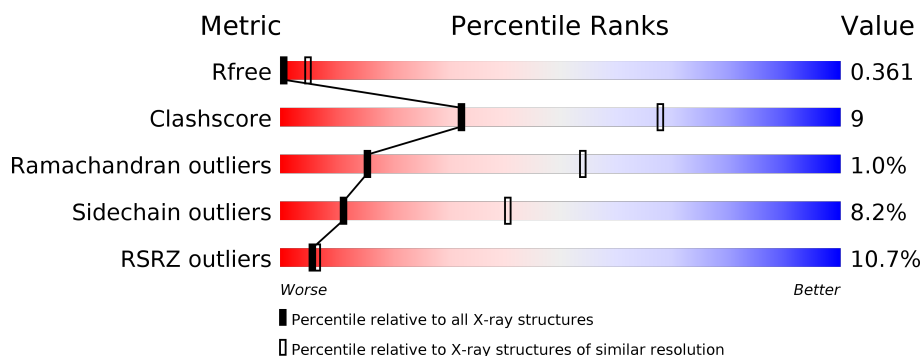
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	861	<div> <div>10%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>9%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6157 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 Major vault protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	782	6157	3874	1101	1167	15	0	0	0

- Molecule 1: Major vault protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	702.25Å 383.80Å 598.48Å 90.00° 124.69° 90.00°	Depositor
Resolution (Å)	200.00 – 3.50 203.54 – 3.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (200.00-3.50) 91.4 (203.54-3.47)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.352 , 0.354 0.359 , 0.361	Depositor DCC
R_{free} test set	76647 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	104.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6157	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.91% 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

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	1/6262 (0.0%)	0.88	58/8484 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	815	PRO	N-CD	22.60	1.79	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	PRO	CB-CA-C	-13.78	77.55	112.00
1	A	814	GLY	C-N-CD	-13.49	90.91	120.60
1	A	606	PHE	N-CA-C	-12.77	76.52	111.00
1	A	186	GLU	N-CA-CB	-12.77	87.62	110.60
1	A	24	ASN	CB-CA-C	-12.44	85.52	110.40
1	A	125	ALA	CB-CA-C	11.42	127.23	110.10
1	A	339	PRO	N-CA-C	11.14	141.05	112.10
1	A	815	PRO	CA-N-CD	-11.11	95.95	111.50
1	A	186	GLU	CB-CA-C	-11.03	88.35	110.40
1	A	642	SER	N-CA-CB	-10.47	94.80	110.50
1	A	344	GLU	CB-CA-C	-10.38	89.64	110.40
1	A	623	ARG	N-CA-CB	-10.06	92.48	110.60
1	A	513	ALA	N-CA-CB	9.54	123.45	110.10
1	A	512	ARG	N-CA-C	-9.53	85.27	111.00
1	A	607	GLU	N-CA-CB	-9.15	94.13	110.60
1	A	352	GLN	CB-CA-C	9.13	128.66	110.40
1	A	641	GLN	CB-CA-C	8.46	127.32	110.40
1	A	607	GLU	N-CA-C	8.37	133.60	111.00
1	A	345	SER	N-CA-CB	8.30	122.95	110.50
1	A	139	ALA	CB-CA-C	8.16	122.34	110.10
1	A	93	ALA	CB-CA-C	8.14	122.31	110.10
1	A	510	ALA	N-CA-CB	-8.07	98.80	110.10
1	A	466	ALA	N-CA-CB	-7.58	99.49	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	LYS	CB-CA-C	7.46	125.33	110.40
1	A	340	LEU	N-CA-CB	7.37	125.15	110.40
1	A	622	ALA	N-CA-C	-7.32	91.23	111.00
1	A	85	HIS	N-CA-C	-7.05	91.96	111.00
1	A	509	HIS	CB-CA-C	-7.05	96.31	110.40
1	A	203	ALA	CB-CA-C	6.98	120.56	110.10
1	A	512	ARG	CB-CA-C	6.69	123.78	110.40
1	A	510	ALA	N-CA-C	6.67	129.00	111.00
1	A	337	LEU	CB-CA-C	6.65	122.83	110.20
1	A	608	MET	CB-CA-C	-6.60	97.20	110.40
1	A	642	SER	N-CA-C	6.52	128.61	111.00
1	A	509	HIS	N-CA-C	6.48	128.50	111.00
1	A	101	PRO	N-CA-C	-6.38	95.52	112.10
1	A	513	ALA	N-CA-C	-6.37	93.81	111.00
1	A	338	GLN	N-CA-CB	-6.29	99.29	110.60
1	A	371	VAL	N-CA-CB	-6.21	97.84	111.50
1	A	187	GLY	N-CA-C	6.16	128.51	113.10
1	A	609	SER	N-CA-CB	6.05	119.58	110.50
1	A	200	SER	CB-CA-C	6.02	121.53	110.10
1	A	351	HIS	CB-CA-C	5.86	122.11	110.40
1	A	620	PRO	N-CA-CB	5.80	110.26	103.30
1	A	477	ARG	N-CA-CB	-5.75	100.26	110.60
1	A	344	GLU	N-CA-C	5.63	126.20	111.00
1	A	185	ARG	CB-CA-C	5.59	121.58	110.40
1	A	623	ARG	N-CA-C	5.47	125.77	111.00
1	A	25	VAL	N-CA-CB	5.46	123.51	111.50
1	A	102	GLY	N-CA-C	5.46	126.75	113.10
1	A	345	SER	N-CA-C	-5.43	96.33	111.00
1	A	320	ILE	N-CA-C	5.41	125.62	111.00
1	A	25	VAL	N-CA-C	-5.28	96.75	111.00
1	A	189	GLY	N-CA-C	-5.22	100.04	113.10
1	A	93	ALA	N-CA-C	-5.21	96.93	111.00
1	A	815	PRO	N-CA-C	5.19	125.60	112.10
1	A	352	GLN	N-CA-C	-5.08	97.30	111.00
1	A	186	GLU	N-CA-C	5.01	124.53	111.00

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	A	6157	0	6183	109	0
All	All	6157	0	6183	109	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 9.

All (109) 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:815:PRO:N	1:A:815:PRO:CD	1.79	1.35
1:A:320:ILE:HG22	1:A:320:ILE:O	1.52	1.09
1:A:814:GLY:C	1:A:815:PRO:CD	2.26	1.04
1:A:188:LYS:HB2	1:A:190:ARG:NH1	1.72	1.03
1:A:516:LEU:CD1	1:A:518:LEU:HD21	1.90	1.01
1:A:516:LEU:CD1	1:A:518:LEU:CD2	2.42	0.97
1:A:188:LYS:CB	1:A:190:ARG:NH1	2.28	0.96
1:A:518:LEU:HD22	1:A:547:PHE:CG	2.01	0.95
1:A:516:LEU:HD11	1:A:518:LEU:HD21	1.48	0.93
1:A:168:ILE:HD11	1:A:174:LEU:HB2	1.51	0.93
1:A:518:LEU:CD2	1:A:547:PHE:CD1	2.61	0.83
1:A:340:LEU:HA	1:A:351:HIS:O	1.77	0.83
1:A:516:LEU:HD11	1:A:518:LEU:CD2	2.07	0.83
1:A:320:ILE:CG2	1:A:320:ILE:O	2.24	0.83
1:A:518:LEU:HD22	1:A:547:PHE:CD1	2.14	0.82
1:A:606:PHE:O	1:A:622:ALA:HA	1.80	0.82
1:A:344:GLU:O	1:A:344:GLU:HG2	1.84	0.78
1:A:529:ILE:HD11	1:A:539:LEU:HD11	1.68	0.76
1:A:549:LEU:HD11	1:A:561:LEU:HD11	1.66	0.75
1:A:518:LEU:HD23	1:A:547:PHE:CD1	2.25	0.70
1:A:184:ASP:OD2	1:A:190:ARG:NE	2.24	0.69
1:A:188:LYS:HB2	1:A:190:ARG:CZ	2.22	0.69
1:A:516:LEU:HD12	1:A:518:LEU:HD21	1.77	0.67
1:A:518:LEU:HD23	1:A:547:PHE:CE1	2.30	0.66
1:A:518:LEU:HD11	1:A:561:LEU:HD22	1.78	0.65
1:A:188:LYS:HB2	1:A:190:ARG:HH11	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:HD11	1:A:174:LEU:CB	2.26	0.63
1:A:338:GLN:HB3	1:A:339:PRO:HD2	1.83	0.60
1:A:188:LYS:O	1:A:190:ARG:HD3	2.01	0.59
1:A:188:LYS:HB3	1:A:190:ARG:NH1	2.16	0.58
1:A:168:ILE:CD1	1:A:174:LEU:HB2	2.29	0.58
1:A:25:VAL:HG21	1:A:79:GLY:HA3	1.86	0.57
1:A:67:ARG:HD3	1:A:71:SER:O	2.05	0.56
1:A:631:ASN:H	1:A:631:ASN:HD22	1.52	0.56
1:A:80:GLN:HE22	1:A:101:PRO:HB2	1.71	0.56
1:A:516:LEU:CD1	1:A:518:LEU:CG	2.83	0.55
1:A:518:LEU:HD21	1:A:561:LEU:HD22	1.88	0.55
1:A:505:PRO:HB3	1:A:526:VAL:HG12	1.87	0.55
1:A:518:LEU:CD2	1:A:547:PHE:CE1	2.89	0.54
1:A:468:VAL:HG21	1:A:487:VAL:HG21	1.90	0.54
1:A:604:PHE:HB3	1:A:626:ALA:HB2	1.91	0.54
1:A:22:ASN:HB2	1:A:40:ASN:HD22	1.73	0.53
1:A:529:ILE:HD12	1:A:583:VAL:HG11	1.89	0.53
1:A:606:PHE:O	1:A:622:ALA:CA	2.53	0.53
1:A:423:VAL:HG13	1:A:452:ARG:HD3	1.91	0.52
1:A:516:LEU:CD1	1:A:518:LEU:HG	2.40	0.52
1:A:518:LEU:CD2	1:A:561:LEU:CD2	2.88	0.52
1:A:518:LEU:HD21	1:A:561:LEU:CD2	2.41	0.51
1:A:518:LEU:CD1	1:A:561:LEU:HD22	2.41	0.51
1:A:344:GLU:O	1:A:344:GLU:CG	2.47	0.51
1:A:516:LEU:HD13	1:A:518:LEU:HG	1.91	0.50
1:A:529:ILE:CD1	1:A:539:LEU:HD11	2.39	0.50
1:A:505:PRO:CB	1:A:526:VAL:HG12	2.41	0.50
1:A:66:SER:HB3	1:A:84:ARG:HG3	1.94	0.50
1:A:489:LEU:HD11	1:A:495:PHE:CE2	2.47	0.49
1:A:541:LEU:HD13	1:A:640:VAL:HG12	1.95	0.49
1:A:202:GLY:O	1:A:203:ALA:C	2.50	0.49
1:A:631:ASN:N	1:A:631:ASN:HD22	2.10	0.49
1:A:206:PRO:HB3	1:A:212:VAL:HG23	1.94	0.49
1:A:591:PHE:HD1	1:A:598:ILE:HD11	1.78	0.49
1:A:273:ILE:O	1:A:273:ILE:HG23	2.13	0.49
1:A:61:VAL:HG22	1:A:105:LEU:HD12	1.95	0.49
1:A:621:LYS:C	1:A:622:ALA:O	2.48	0.49
1:A:591:PHE:O	1:A:595:SER:N	2.46	0.48
1:A:188:LYS:CB	1:A:190:ARG:HH11	2.16	0.48
1:A:358:LEU:HD13	1:A:377:ARG:HG3	1.96	0.48
1:A:54:PRO:HD2	1:A:109:ILE:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLN:HG2	1:A:379:ALA:H	1.79	0.48
1:A:123:LEU:HD12	1:A:143:TRP:HB3	1.96	0.48
1:A:643:VAL:HG23	1:A:643:VAL:O	2.14	0.48
1:A:481:VAL:HG11	1:A:487:VAL:HG22	1.96	0.48
1:A:504:ARG:HB3	1:A:505:PRO:CD	2.43	0.47
1:A:523:PHE:CD1	1:A:568:VAL:HG23	2.50	0.47
1:A:543:TYR:CE1	1:A:575:ILE:HG21	2.49	0.47
1:A:591:PHE:CD1	1:A:598:ILE:HD11	2.49	0.47
1:A:504:ARG:HB3	1:A:505:PRO:HD3	1.96	0.47
1:A:814:GLY:C	1:A:815:PRO:HD2	2.30	0.47
1:A:109:ILE:HG22	1:A:109:ILE:O	2.14	0.47
1:A:310:LEU:HD11	1:A:316:LEU:HD11	1.96	0.46
1:A:518:LEU:CD1	1:A:561:LEU:CD2	2.93	0.46
1:A:278:PRO:HA	1:A:305:GLU:HG2	1.98	0.46
1:A:814:GLY:CA	1:A:815:PRO:CD	2.93	0.46
1:A:12:PRO:HA	1:A:32:PRO:HB3	1.98	0.46
1:A:468:VAL:CG2	1:A:487:VAL:HG21	2.45	0.45
1:A:218:ALA:HB2	1:A:260:VAL:HG22	1.98	0.45
1:A:458:VAL:HG13	1:A:489:LEU:HB2	1.98	0.45
1:A:539:LEU:N	1:A:539:LEU:HD13	2.32	0.45
1:A:516:LEU:HD13	1:A:518:LEU:CD2	2.41	0.45
1:A:10:ILE:HD13	1:A:47:PRO:HG3	2.00	0.44
1:A:587:THR:HG23	1:A:590:ASP:HB3	2.00	0.44
1:A:802:LEU:HD12	1:A:807:ILE:HG23	1.99	0.43
1:A:67:ARG:HD3	1:A:71:SER:C	2.39	0.43
1:A:516:LEU:CD1	1:A:518:LEU:HD23	2.42	0.43
1:A:338:GLN:HB3	1:A:339:PRO:CD	2.49	0.42
1:A:541:LEU:CD1	1:A:640:VAL:HG12	2.49	0.42
1:A:378:GLN:HG2	1:A:379:ALA:N	2.35	0.42
1:A:531:THR:HG21	1:A:588:PHE:HB2	2.01	0.42
1:A:122:HIS:HB3	1:A:160:VAL:HB	2.02	0.42
1:A:457:VAL:HG13	1:A:457:VAL:O	2.20	0.41
1:A:518:LEU:CD2	1:A:561:LEU:HD22	2.51	0.41
1:A:122:HIS:HB2	1:A:163:ILE:HD11	2.02	0.41
1:A:378:GLN:CG	1:A:379:ALA:H	2.32	0.41
1:A:504:ARG:CB	1:A:505:PRO:HD3	2.50	0.41
1:A:185:ARG:HG3	1:A:204:TYR:HE1	1.86	0.41
1:A:126:LEU:HB2	1:A:127:LEU:HD13	2.03	0.41
1:A:490:ASP:HB3	1:A:491:PRO:HD2	2.02	0.40
1:A:541:LEU:N	1:A:541:LEU:HD22	2.37	0.40
1:A:392:ASP:O	1:A:396:GLY:N	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG11	1:A:308:PHE:HE2	1.87	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	776/861 (90%)	706 (91%)	62 (8%)	8 (1%)	15 54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	PRO
1	A	620	PRO
1	A	139	ALA
1	A	504	ARG
1	A	86	ALA
1	A	338	GLN
1	A	339	PRO
1	A	381	PRO

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	657/727 (90%)	603 (92%)	54 (8%)	11	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	33	LYS
1	A	53	VAL
1	A	90	ILE
1	A	95	ASP
1	A	114	VAL
1	A	127	LEU
1	A	143	TRP
1	A	144	LEU
1	A	152	ILE
1	A	162	ILE
1	A	170	GLN
1	A	186	GLU
1	A	188	LYS
1	A	253	VAL
1	A	267	VAL
1	A	303	LYS
1	A	308	PHE
1	A	316	LEU
1	A	333	LEU
1	A	337	LEU
1	A	338	GLN
1	A	340	LEU
1	A	341	GLU
1	A	342	GLU
1	A	347	GLU
1	A	382	LEU
1	A	388	ILE
1	A	426	LEU
1	A	474	ARG
1	A	482	PHE
1	A	486	LEU
1	A	488	THR
1	A	507	ARG
1	A	512	ARG
1	A	514	LEU
1	A	538	GLN
1	A	539	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	561	LEU
1	A	573	LYS
1	A	587	THR
1	A	604	PHE
1	A	631	ASN
1	A	660	LEU
1	A	662	ILE
1	A	664	ILE
1	A	669	GLN
1	A	670	GLU
1	A	723	LYS
1	A	742	LEU
1	A	770	LEU
1	A	781	VAL
1	A	787	LEU
1	A	815	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	40	ASN
1	A	80	GLN
1	A	154	GLN
1	A	170	GLN
1	A	228	HIS
1	A	311	GLN
1	A	494	GLN
1	A	538	GLN
1	A	631	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	782/861 (90%)	0.68	84 (10%) 6 6	79, 135, 221, 293	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	7.5
1	A	44	LEU	6.3
1	A	503	GLY	6.0
1	A	126	LEU	5.8
1	A	47	PRO	5.5
1	A	118	ASN	5.0
1	A	609	SER	5.0
1	A	45	PHE	5.0
1	A	43	VAL	4.8
1	A	106	GLU	4.8
1	A	153	PRO	4.6
1	A	125	ALA	4.4
1	A	10	ILE	4.4
1	A	105	LEU	4.2
1	A	127	LEU	4.1
1	A	426	LEU	4.1
1	A	139	ALA	4.1
1	A	518	LEU	4.1
1	A	575	ILE	3.9
1	A	124	LYS	3.8
1	A	102	GLY	3.8
1	A	346	GLU	3.8
1	A	527	ILE	3.7
1	A	46	ALA	3.5
1	A	19	LEU	3.5
1	A	62	ALA	3.5
1	A	17	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	537	LEU	3.3
1	A	643	VAL	3.3
1	A	553	ASN	3.3
1	A	9	ARG	3.3
1	A	11	PRO	3.2
1	A	384	GLN	3.1
1	A	529	ILE	3.0
1	A	206	PRO	3.0
1	A	56	ARG	2.9
1	A	101	PRO	2.9
1	A	634	VAL	2.9
1	A	539	LEU	2.9
1	A	85	HIS	2.9
1	A	500	LEU	2.9
1	A	390	VAL	2.9
1	A	163	ILE	2.9
1	A	42	ARG	2.8
1	A	608	MET	2.8
1	A	8	ILE	2.7
1	A	657	SER	2.7
1	A	414	LEU	2.6
1	A	385	ASN	2.6
1	A	480	VAL	2.6
1	A	51	VAL	2.6
1	A	111	PRO	2.5
1	A	164	GLN	2.5
1	A	53	VAL	2.5
1	A	419	LEU	2.5
1	A	585	SER	2.4
1	A	465	ASN	2.4
1	A	63	ASN	2.4
1	A	550	LYS	2.4
1	A	140	GLY	2.4
1	A	571	ALA	2.4
1	A	29	GLU	2.4
1	A	131	ASP	2.4
1	A	495	PHE	2.3
1	A	482	PHE	2.3
1	A	91	ARG	2.3
1	A	12	PRO	2.3
1	A	420	PRO	2.2
1	A	86	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	ASP	2.2
1	A	574	ALA	2.2
1	A	619	LEU	2.2
1	A	457	VAL	2.1
1	A	464	HIS	2.1
1	A	336	ALA	2.1
1	A	99	LEU	2.1
1	A	39	ASP	2.1
1	A	516	LEU	2.1
1	A	567	PHE	2.1
1	A	215	LEU	2.1
1	A	765	VAL	2.1
1	A	486	LEU	2.0
1	A	344	GLU	2.0
1	A	103	GLU	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 carbohydrates 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.