



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:00 PM UTC

PDB ID : 4HL8 / pdb_00004hl8
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 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

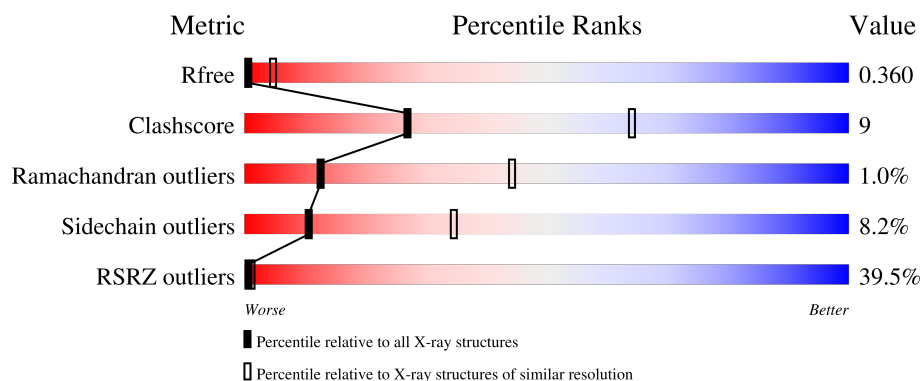
1 Overall quality at a glance

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	A	861	

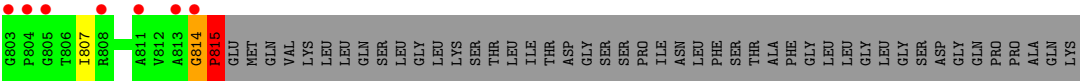
2 Entry composition

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



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 – 3.50 200.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (200.00-3.50) 92.7 (200.00-3.50)	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 0.358 , 0.360	Depositor DCC
R_{free} test set	76647 reflections (4.58%)	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)	0.33 , 45.4	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	0.49	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	0.50	1/6262 (0.0%)	1.18	83/8484 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	815	PRO	N-CD	22.67	1.79	1.47

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	606	PHE	N-CA-C	-25.34	76.52	108.45
1	A	339	PRO	CB-CA-C	-20.61	77.55	111.56
1	A	607	GLU	N-CA-C	18.04	133.60	110.33
1	A	24	ASN	CB-CA-C	-18.00	85.52	111.80
1	A	186	GLU	N-CA-CB	-16.14	87.62	111.51
1	A	339	PRO	N-CA-C	13.88	141.05	112.47
1	A	186	GLU	CB-CA-C	-13.43	88.35	111.45
1	A	512	ARG	N-CA-C	-13.29	85.27	108.13
1	A	510	ALA	N-CA-C	12.27	129.00	113.55
1	A	126	LEU	N-CA-C	-11.96	99.21	114.04
1	A	622	ALA	N-CA-C	-11.90	91.23	109.79
1	A	607	GLU	N-CA-CB	-11.88	94.13	110.29
1	A	642	SER	N-CA-C	11.60	128.61	107.73
1	A	815	PRO	CA-N-CD	-11.46	95.95	112.00
1	A	509	HIS	N-CA-C	11.42	128.50	107.60
1	A	344	GLU	CB-CA-C	-11.33	89.64	111.06
1	A	623	ARG	N-CA-CB	-11.26	92.48	110.39
1	A	185	ARG	N-CA-C	10.75	124.33	111.33
1	A	186	GLU	N-CA-C	10.66	124.53	110.88
1	A	623	ARG	N-CA-C	10.27	125.77	109.86
1	A	101	PRO	CB-CA-C	10.26	124.42	110.98
1	A	509	HIS	CB-CA-C	-10.13	96.31	111.70
1	A	85	HIS	N-CA-C	-10.01	91.96	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	PRO	N-CA-C	-9.97	95.52	111.38
1	A	513	ALA	N-CA-C	-9.67	93.81	108.99
1	A	118	ASN	N-CA-C	9.44	123.48	112.72
1	A	512	ARG	CB-CA-C	9.27	123.78	110.24
1	A	344	GLU	N-CA-C	9.10	126.20	113.56
1	A	371	VAL	N-CA-C	8.91	122.89	109.17
1	A	187	GLY	N-CA-C	8.84	128.51	114.90
1	A	345	SER	N-CA-C	-8.60	96.33	109.41
1	A	340	LEU	N-CA-CB	8.54	125.15	111.65
1	A	125	ALA	CB-CA-C	8.49	127.23	109.65
1	A	641	GLN	CB-CA-C	8.49	127.32	110.42
1	A	608	MET	N-CA-C	8.32	124.35	114.04
1	A	814	GLY	C-N-CD	-8.31	90.91	125.00
1	A	102	GLY	N-CA-C	8.24	126.75	115.30
1	A	25	VAL	N-CA-C	-8.02	96.75	108.23
1	A	125	ALA	N-CA-C	-8.02	99.92	110.43
1	A	352	GLN	N-CA-C	-8.01	97.30	109.79
1	A	510	ALA	N-CA-CB	-8.00	98.80	110.40
1	A	465	ASN	N-CA-C	7.85	122.44	113.02
1	A	476	LYS	N-CA-C	7.85	122.29	112.24
1	A	320	ILE	N-CA-C	7.83	125.62	109.34
1	A	103	GLU	N-CA-C	7.55	121.35	107.99
1	A	370	LYS	CB-CA-C	7.49	125.33	110.42
1	A	371	VAL	N-CA-CB	-7.42	97.84	112.24
1	A	93	ALA	CB-CA-C	7.35	122.31	109.89
1	A	466	ALA	N-CA-CB	-7.31	99.49	110.60
1	A	345	SER	N-CA-CB	7.25	122.95	111.43
1	A	642	SER	N-CA-CB	-7.21	94.80	110.29
1	A	25	VAL	N-CA-CB	7.16	123.51	112.06
1	A	203	ALA	CB-CA-C	7.15	120.56	109.84
1	A	466	ALA	N-CA-C	7.05	120.10	109.95
1	A	93	ALA	N-CA-C	-6.95	96.93	108.32
1	A	203	ALA	N-CA-C	-6.85	100.17	110.24
1	A	200	SER	CB-CA-C	6.79	121.53	109.65
1	A	352	GLN	CB-CA-C	6.79	128.66	113.33
1	A	608	MET	CB-CA-C	-6.71	97.20	109.15
1	A	620	PRO	N-CA-CB	6.67	110.26	103.25
1	A	636	SER	N-CA-C	6.43	121.39	112.45
1	A	513	ALA	N-CA-CB	6.42	123.45	111.52
1	A	185	ARG	CB-CA-C	6.41	121.58	110.68
1	A	321	GLN	N-CA-C	6.34	119.44	110.50
1	A	338	GLN	N-CA-CB	-6.23	99.29	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	SER	N-CA-C	6.21	120.15	112.58
1	A	337	LEU	CB-CA-C	6.11	122.83	110.38
1	A	477	ARG	N-CA-CB	-6.09	100.26	110.80
1	A	351	HIS	CB-CA-C	6.09	122.11	109.38
1	A	351	HIS	N-CA-C	-6.08	99.89	109.50
1	A	379	ALA	N-CA-C	6.00	122.21	113.40
1	A	139	ALA	CB-CA-C	5.99	122.34	110.42
1	A	814	GLY	N-CA-C	5.63	123.83	112.34
1	A	189	GLY	N-CA-C	-5.54	100.04	113.18
1	A	139	ALA	N-CA-C	5.53	122.58	110.80
1	A	107	LYS	N-CA-C	-5.53	100.87	109.72
1	A	119	THR	N-CA-CB	-5.52	102.66	111.43
1	A	106	GLU	CB-CA-C	-5.47	100.54	109.56
1	A	815	PRO	N-CA-C	5.40	125.60	112.10
1	A	609	SER	N-CA-CB	5.34	119.58	110.50
1	A	134	GLY	N-CA-C	5.30	124.77	114.16
1	A	135	ASP	N-CA-C	5.25	118.05	109.59
1	A	135	ASP	N-CA-CB	-5.21	102.31	110.69

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	113	0
All	All	6157	0	6183	113	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 (113) 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:CD	1:A:815:PRO:N	1.79	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.09
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:O	1:A:320:ILE:CG2	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
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:202:GLY:O	1:A:203:ALA:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:814:GLY:C	1:A:815:PRO:HD2	2.30	0.52
1:A:518:LEU:HD21	1:A:561:LEU:CD2	2.41	0.51
1:A:30:VAL:HG23	1:A:50:MET:HE3	1.93	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:621:LYS:C	1:A:622:ALA:O	2.48	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:631:ASN:HD22	1:A:631:ASN:N	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:61:VAL:HG22	1:A:105:LEU:HD12	1.95	0.49
1:A:273:ILE:HG23	1:A:273:ILE:O	2.13	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:67:ARG:HD3	1:A:71:SER:C	2.39	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
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:O	1:A:643:VAL:HG23	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:109:ILE:O	1:A:109:ILE:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:124:LYS:C	1:A:125:ALA:O	2.59	0.44
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: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:30:VAL:CG2	1:A:50:MET:HE3	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:O	1:A:457:VAL:HG13	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:402:ILE:HD12	1:A:402:ILE:C	2.46	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:HD22	1:A:541:LEU:N	2.37	0.40
1:A:392:ASP:O	1:A:396:GLY:N	2.52	0.40
1:A:302:VAL:HG11	1:A:308:PHE:HE2	1.87	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	
1	A	776/861 (90%)	706 (91%)	62 (8%)	8 (1%)	12	44

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 ⓘ

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%)	10	34

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

Mol	Chain	Res	Type
1	A	33	LYS
1	A	53	VAL
1	A	90	ILE
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

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Mol	Chain	Res	Type
1	A	188	LYS
1	A	251	VAL
1	A	253	VAL
1	A	260	VAL
1	A	267	VAL
1	A	270	VAL
1	A	303	LYS
1	A	316	LEU
1	A	333	LEU
1	A	337	LEU
1	A	340	LEU
1	A	341	GLU
1	A	342	GLU
1	A	347	GLU
1	A	360	ARG
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
1	A	561	LEU
1	A	573	LYS
1	A	587	THR
1	A	604	PHE
1	A	631	ASN
1	A	634	VAL
1	A	660	LEU
1	A	662	ILE
1	A	664	ILE
1	A	723	LYS
1	A	742	LEU
1	A	763	LYS
1	A	770	LEU
1	A	781	VAL
1	A	787	LEU

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Mol	Chain	Res	Type
1	A	815	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	80	GLN
1	A	88	GLN
1	A	154	GLN
1	A	228	HIS
1	A	294	ASN
1	A	298	GLN
1	A	311	GLN
1	A	330	GLN
1	A	494	GLN
1	A	538	GLN
1	A	544	ASN
1	A	631	ASN
1	A	675	HIS
1	A	776	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

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%)	1.88	309 (39%) 1 1	79, 135, 220, 293	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	MET	11.0
1	A	344	GLU	9.9
1	A	607	GLU	8.6
1	A	11	PRO	8.3
1	A	449	SER	8.0
1	A	623	ARG	7.8
1	A	465	ASN	6.5
1	A	82	ARG	6.4
1	A	164	GLN	6.3
1	A	54	PRO	6.3
1	A	328	GLU	6.1
1	A	55	PRO	6.0
1	A	147	GLY	6.0
1	A	236	ARG	5.9
1	A	659	GLN	5.7
1	A	32	PRO	5.7
1	A	530	GLU	5.7
1	A	544	ASN	5.4
1	A	609	SER	5.3
1	A	507	ARG	5.3
1	A	12	PRO	5.2
1	A	9	ARG	5.1
1	A	146	GLU	5.1
1	A	170	GLN	5.0
1	A	450	ALA	5.0
1	A	577	SER	5.0
1	A	621	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	4.9
1	A	464	HIS	4.9
1	A	49	ARG	4.8
1	A	104	VAL	4.8
1	A	222	THR	4.8
1	A	135	ASP	4.8
1	A	451	PRO	4.8
1	A	655	GLN	4.8
1	A	237	ASP	4.7
1	A	788	ALA	4.7
1	A	73	VAL	4.6
1	A	42	ARG	4.6
1	A	791	GLU	4.6
1	A	177	ARG	4.6
1	A	800	GLU	4.5
1	A	580	ARG	4.5
1	A	661	ALA	4.5
1	A	254	GLN	4.4
1	A	651	ARG	4.4
1	A	778	GLU	4.4
1	A	524	THR	4.3
1	A	606	PHE	4.3
1	A	350	SER	4.3
1	A	397	LYS	4.3
1	A	10	ILE	4.3
1	A	772	TYR	4.3
1	A	663	GLU	4.2
1	A	590	ASP	4.2
1	A	803	GLY	4.2
1	A	139	ALA	4.1
1	A	111	PRO	4.1
1	A	40	ASN	4.1
1	A	649	ARG	4.1
1	A	767	GLU	4.1
1	A	813	ALA	4.1
1	A	503	GLY	4.1
1	A	578	ARG	4.0
1	A	766	ARG	4.0
1	A	119	THR	4.0
1	A	206	PRO	4.0
1	A	504	ARG	4.0
1	A	347	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	411	ASP	3.9
1	A	53	VAL	3.9
1	A	14	HIS	3.8
1	A	682	GLN	3.8
1	A	637	SER	3.8
1	A	190	ARG	3.8
1	A	130	GLU	3.8
1	A	605	GLY	3.8
1	A	213	LEU	3.8
1	A	25	VAL	3.8
1	A	304	GLY	3.7
1	A	52	THR	3.7
1	A	342	GLU	3.7
1	A	780	GLU	3.7
1	A	636	SER	3.6
1	A	776	GLN	3.6
1	A	427	LEU	3.6
1	A	238	LEU	3.6
1	A	21	GLN	3.6
1	A	305	GLU	3.6
1	A	566	ASP	3.6
1	A	35	TYR	3.5
1	A	69	THR	3.5
1	A	277	GLY	3.5
1	A	782	SER	3.5
1	A	749	GLN	3.5
1	A	351	HIS	3.5
1	A	33	LYS	3.5
1	A	550	LYS	3.4
1	A	548	GLU	3.4
1	A	74	LEU	3.4
1	A	804	PRO	3.4
1	A	534	HIS	3.4
1	A	619	LEU	3.4
1	A	323	VAL	3.4
1	A	129	PHE	3.4
1	A	133	ASN	3.3
1	A	345	SER	3.3
1	A	101	PRO	3.3
1	A	136	LYS	3.3
1	A	626	ALA	3.3
1	A	181	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	65	VAL	3.3
1	A	39	ASP	3.3
1	A	493	GLU	3.3
1	A	171	ASN	3.2
1	A	552	ARG	3.2
1	A	736	GLU	3.2
1	A	336	ALA	3.2
1	A	796	LYS	3.2
1	A	199	ARG	3.2
1	A	528	THR	3.2
1	A	131	ASP	3.2
1	A	428	ASN	3.1
1	A	476	LYS	3.1
1	A	461	ARG	3.1
1	A	325	VAL	3.1
1	A	343	GLY	3.1
1	A	620	PRO	3.1
1	A	349	VAL	3.1
1	A	502	ALA	3.1
1	A	492	GLU	3.1
1	A	624	ASP	3.1
1	A	102	GLY	3.1
1	A	531	THR	3.1
1	A	72	SER	3.0
1	A	31	GLY	3.0
1	A	797	GLU	3.0
1	A	128	ASP	3.0
1	A	28	VAL	3.0
1	A	585	SER	3.0
1	A	792	ALA	3.0
1	A	88	GLN	3.0
1	A	790	VAL	3.0
1	A	75	PHE	3.0
1	A	469	GLN	3.0
1	A	29	GLU	2.9
1	A	66	SER	2.9
1	A	808	ARG	2.9
1	A	775	ALA	2.9
1	A	383	ASP	2.9
1	A	187	GLY	2.9
1	A	200	SER	2.9
1	A	356	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	754	GLU	2.9
1	A	653	ALA	2.9
1	A	230	ARG	2.9
1	A	113	GLN	2.9
1	A	178	ALA	2.9
1	A	398	VAL	2.8
1	A	13	TYR	2.8
1	A	789	ASN	2.8
1	A	20	ASP	2.8
1	A	625	GLN	2.8
1	A	132	LYS	2.8
1	A	399	ARG	2.8
1	A	761	ARG	2.8
1	A	234	ASN	2.8
1	A	124	LYS	2.8
1	A	783	LYS	2.8
1	A	303	LYS	2.8
1	A	165	ALA	2.8
1	A	286	ASP	2.7
1	A	306	LYS	2.7
1	A	632	GLY	2.7
1	A	96	PRO	2.7
1	A	272	PRO	2.7
1	A	248	GLU	2.7
1	A	793	LYS	2.7
1	A	404	SER	2.7
1	A	108	ASP	2.7
1	A	244	ARG	2.6
1	A	315	ARG	2.6
1	A	292	GLY	2.6
1	A	622	ALA	2.6
1	A	499	SER	2.6
1	A	346	GLU	2.6
1	A	235	PHE	2.6
1	A	574	ALA	2.6
1	A	760	GLU	2.6
1	A	484	PRO	2.6
1	A	785	GLN	2.6
1	A	151	TYR	2.6
1	A	564	VAL	2.6
1	A	565	PRO	2.6
1	A	814	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLU	2.6
1	A	635	VAL	2.6
1	A	386	GLU	2.5
1	A	794	LYS	2.5
1	A	57	HIS	2.5
1	A	543	TYR	2.5
1	A	763	LYS	2.5
1	A	639	ASP	2.5
1	A	70	GLN	2.5
1	A	352	GLN	2.5
1	A	686	GLY	2.5
1	A	56	ARG	2.5
1	A	81	VAL	2.5
1	A	355	ASP	2.5
1	A	584	ALA	2.5
1	A	811	ALA	2.5
1	A	327	SER	2.5
1	A	501	SER	2.5
1	A	364	GLU	2.5
1	A	68	ASP	2.5
1	A	773	ALA	2.5
1	A	99	LEU	2.5
1	A	665	THR	2.5
1	A	799	THR	2.5
1	A	126	LEU	2.5
1	A	145	PHE	2.4
1	A	385	ASN	2.4
1	A	41	GLU	2.4
1	A	106	GLU	2.4
1	A	83	LEU	2.4
1	A	256	THR	2.4
1	A	198	VAL	2.4
1	A	282	CYS	2.4
1	A	84	ARG	2.4
1	A	175	ARG	2.4
1	A	63	ASN	2.4
1	A	737	GLY	2.4
1	A	521	ASP	2.4
1	A	6	ALA	2.4
1	A	79	GLY	2.4
1	A	392	ASP	2.4
1	A	15	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	362	PRO	2.4
1	A	631	ASN	2.4
1	A	217	ASP	2.4
1	A	536	ARG	2.4
1	A	570	ASP	2.4
1	A	295	GLN	2.3
1	A	17	HIS	2.3
1	A	509	HIS	2.3
1	A	472	ASP	2.3
1	A	266	GLU	2.3
1	A	372	GLU	2.3
1	A	376	GLU	2.3
1	A	48	VAL	2.3
1	A	191	VAL	2.3
1	A	94	GLN	2.3
1	A	109	ILE	2.3
1	A	384	GLN	2.3
1	A	731	GLU	2.3
1	A	569	GLY	2.3
1	A	247	GLU	2.3
1	A	573	LYS	2.3
1	A	801	ALA	2.3
1	A	396	GLY	2.3
1	A	505	PRO	2.3
1	A	457	VAL	2.2
1	A	675	HIS	2.2
1	A	523	PHE	2.2
1	A	188	LYS	2.2
1	A	329	GLN	2.2
1	A	798	MET	2.2
1	A	257	GLU	2.2
1	A	805	GLY	2.2
1	A	85	HIS	2.2
1	A	264	TYR	2.2
1	A	120	ALA	2.2
1	A	391	GLN	2.2
1	A	477	ARG	2.2
1	A	226	ALA	2.1
1	A	542	ALA	2.1
1	A	59	CYS	2.1
1	A	182	CYS	2.1
1	A	184	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	690	ARG	2.1
1	A	30	VAL	2.1
1	A	324	TYR	2.1
1	A	118	ASN	2.1
1	A	163	ILE	2.1
1	A	658	VAL	2.1
1	A	173	ALA	2.1
1	A	294	ASN	2.1
1	A	335	LYS	2.1
1	A	100	TYR	2.1
1	A	24	ASN	2.1
1	A	143	TRP	2.1
1	A	204	TYR	2.1
1	A	192	THR	2.1
1	A	777	LEU	2.1
1	A	259	HIS	2.1
1	A	483	GLY	2.1
1	A	161	GLU	2.1
1	A	764	LYS	2.1
1	A	207	ALA	2.1
1	A	321	GLN	2.1
1	A	691	GLN	2.1
1	A	67	ARG	2.0
1	A	186	GLU	2.0
1	A	419	LEU	2.0
1	A	581	GLY	2.0
1	A	148	PRO	2.0
1	A	421	SER	2.0
1	A	98	PRO	2.0
1	A	510	ALA	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.