



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 AM UTC

PDB ID : 1G4M / pdb_00001g4m
Title : CRYSTAL STRUCTURE OF BOVINE BETA-ARRESTIN 1
Authors : Schubert, C.; Han, M.
Deposited on : 2000-10-27
Resolution : 1.90 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

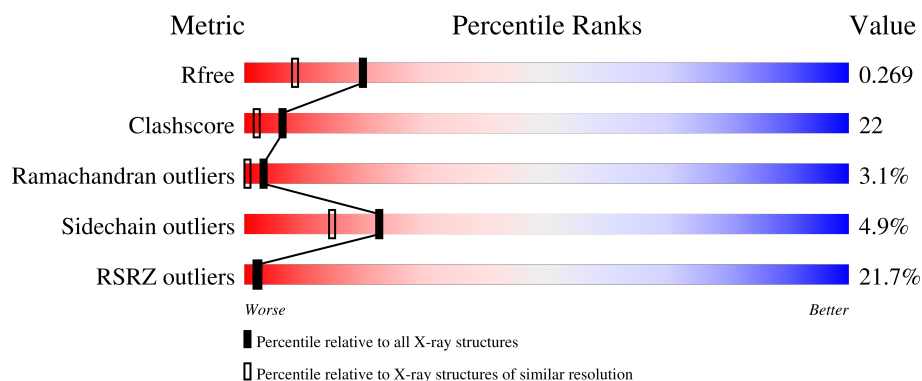
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	393	17% 65% 21% 5% 9%
1	B	393	22% 56% 27% 6% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5926 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 BETA-ARRESTIN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	72	0	0
			2821	1801	487	523	10			
1	B	357	Total	C	N	O	S	71	0	0
			2836	1809	489	528	10			

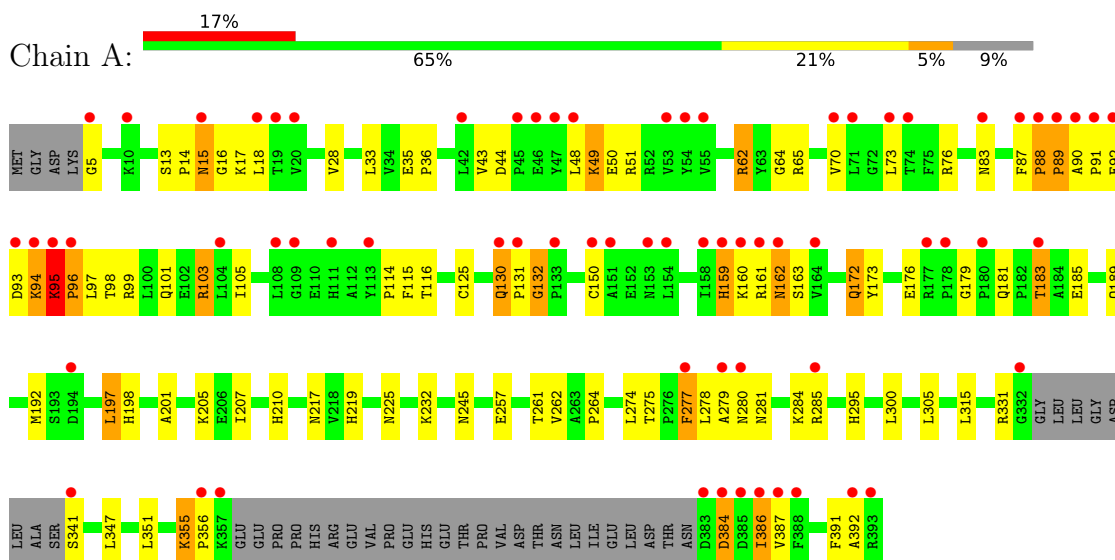
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	155	Total	O	0	0
			155	155		
2	B	114	Total	O	0	0
			114	114		

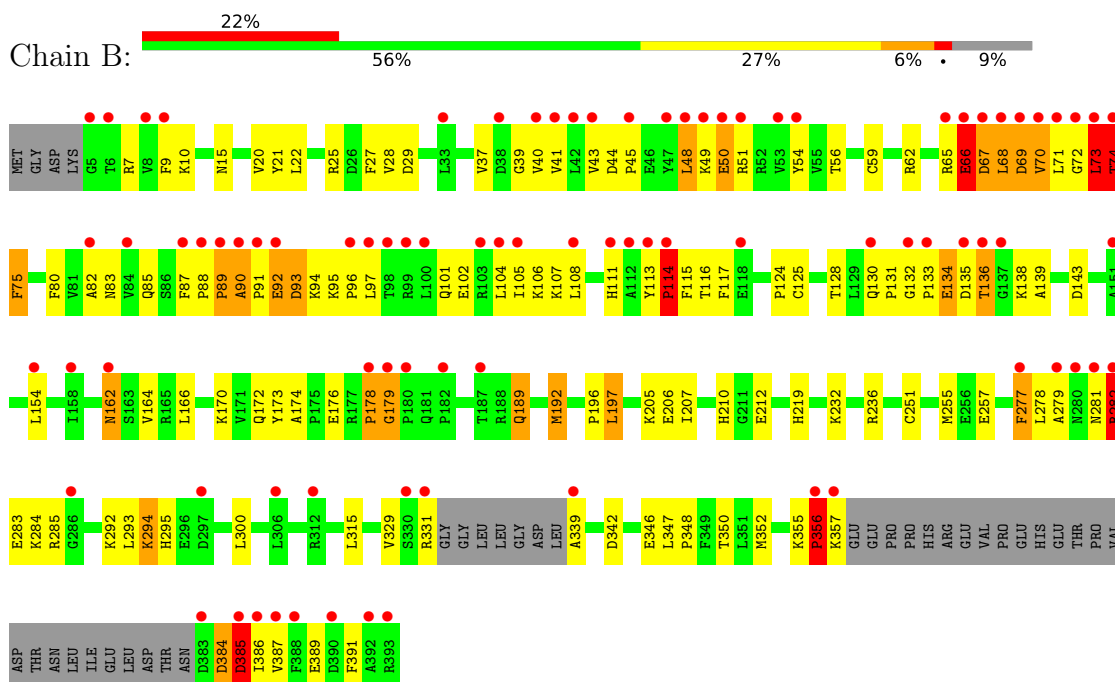
3 Residue-property plots [i](#)

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: BETA-ARRESTIN1



• Molecule 1: BETA-ARRESTIN1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.40Å 73.72Å 115.76Å 90.00° 98.73° 90.00°	Depositor
Resolution (Å)	34.54 – 1.90 34.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	86.3 (34.54-1.90) 86.4 (34.54-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.269 0.235 , 0.269	Depositor DCC
R_{free} test set	5401 reflections (7.64%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5926	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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	0.68	0/2880	1.09	25/3902 (0.6%)
1	B	0.60	0/2895	1.06	15/3921 (0.4%)
All	All	0.64	0/5775	1.07	40/7823 (0.5%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LYS	CA-C-N	8.90	130.96	119.84
1	B	95	LYS	C-N-CA	8.90	130.96	119.84
1	B	134	GLU	N-CA-C	-7.69	103.72	113.72
1	A	95	LYS	CA-C-N	-6.94	111.17	119.84
1	A	95	LYS	C-N-CA	-6.94	111.17	119.84
1	A	197	LEU	N-CA-C	-6.51	98.12	108.73
1	A	161	ARG	N-CA-C	-6.46	104.88	112.89
1	A	88	PRO	CA-C-N	6.34	127.77	119.84
1	A	88	PRO	C-N-CA	6.34	127.77	119.84
1	A	300	LEU	N-CA-C	-6.27	101.82	110.35
1	A	94	LYS	N-CA-C	-6.21	100.99	110.30
1	B	28	VAL	N-CA-C	6.18	117.05	108.89
1	A	275	THR	CA-C-N	-6.11	112.01	120.25
1	A	275	THR	C-N-CA	-6.11	112.01	120.25
1	B	342	ASP	N-CA-C	5.99	118.80	109.52
1	B	48	LEU	N-CA-C	5.96	118.27	111.11
1	A	207	ILE	N-CA-C	5.96	116.51	108.17
1	A	130	GLN	CA-C-N	5.94	125.64	119.64
1	A	130	GLN	C-N-CA	5.94	125.64	119.64
1	B	197	LEU	N-CA-C	-5.85	99.70	109.24
1	A	98	THR	N-CA-C	-5.79	101.95	110.52
1	A	28	VAL	N-CA-C	5.63	116.32	108.89
1	A	355	LYS	CA-C-N	5.62	126.87	119.84
1	A	355	LYS	C-N-CA	5.62	126.87	119.84
1	A	315	LEU	N-CA-C	-5.61	106.44	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	MET	N-CA-C	-5.59	103.68	111.39
1	B	75	PHE	N-CA-C	5.55	117.53	108.76
1	A	192	MET	N-CA-C	-5.52	103.62	111.24
1	B	59	CYS	N-CA-C	-5.50	99.94	108.90
1	B	300	LEU	N-CA-C	-5.46	102.92	110.35
1	B	329	VAL	N-CA-C	5.37	116.71	108.71
1	A	172	GLN	N-CA-C	5.36	117.98	109.24
1	A	179	GLY	CA-C-N	5.35	125.29	119.78
1	A	179	GLY	C-N-CA	5.35	125.29	119.78
1	B	73	LEU	N-CA-C	-5.25	99.62	110.80
1	B	282	ARG	N-CA-C	5.21	121.90	110.80
1	A	163	SER	N-CA-C	5.16	116.82	109.14
1	A	132	GLY	CA-C-N	5.16	125.45	119.47
1	A	132	GLY	C-N-CA	5.16	125.45	119.47
1	B	385	ASP	N-CA-C	5.14	121.74	110.80

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	2821	0	2856	99	0
1	B	2836	0	2879	148	0
2	A	155	0	0	10	0
2	B	114	0	0	25	0
All	All	5926	0	5735	246	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 22.

All (246) 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:15:ASN:ND2	1:A:17:LYS:H	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:THR:HG22	1:B:83:ASN:HB3	1.41	0.99
1:B:132:GLY:HA2	1:B:284:LYS:HB3	1.45	0.98
1:B:283:GLU:HA	1:B:293:LEU:HD21	1.47	0.96
1:A:15:ASN:C	1:A:15:ASN:HD22	1.78	0.92
1:B:131:PRO:HG2	1:B:138:LYS:HB2	1.53	0.89
1:A:48:LEU:HD12	1:A:49:LYS:N	1.88	0.88
1:B:117:PHE:O	2:B:492:HOH:O	1.91	0.88
1:A:150:CYS:HB2	1:A:162:ASN:ND2	1.89	0.87
1:A:132:GLY:HA2	1:A:285:ARG:HD3	1.57	0.87
1:B:37:VAL:O	2:B:458:HOH:O	1.91	0.86
1:B:294:LYS:HE3	1:B:294:LYS:H	1.40	0.85
1:B:232:LYS:HD3	1:B:255:MET:HE1	1.58	0.85
1:B:39:GLY:O	2:B:460:HOH:O	1.96	0.82
1:B:90:ALA:HB1	1:B:93:ASP:H	1.44	0.82
1:B:65:ARG:CZ	1:B:68:LEU:HD11	2.10	0.80
1:B:65:ARG:NH2	1:B:68:LEU:HD11	1.95	0.80
1:A:150:CYS:HB2	1:A:162:ASN:HD22	1.46	0.80
1:A:95:LYS:O	1:A:97:LEU:N	2.15	0.79
1:B:132:GLY:CA	1:B:284:LYS:HB3	2.14	0.78
1:B:115:PHE:O	2:B:459:HOH:O	2.02	0.78
1:B:90:ALA:HB1	1:B:93:ASP:N	1.99	0.77
1:B:70:VAL:HG13	1:B:71:LEU:H	1.49	0.75
1:B:124:PRO:HG3	1:B:315:LEU:HA	1.66	0.74
1:B:116:THR:HA	2:B:458:HOH:O	1.88	0.74
1:A:70:VAL:HG11	1:A:73:LEU:HD12	1.70	0.74
1:A:48:LEU:HD12	1:A:49:LYS:H	1.51	0.73
1:B:27:PHE:CE2	1:B:37:VAL:HA	2.23	0.73
1:B:114:PRO:HD2	2:B:493:HOH:O	1.86	0.73
1:B:236:ARG:HG2	1:B:236:ARG:HH11	1.53	0.72
1:A:15:ASN:HD22	1:A:17:LYS:H	1.36	0.72
1:A:15:ASN:HD22	1:A:16:GLY:N	1.88	0.71
1:A:245:ASN:OD1	1:B:192:MET:HE2	1.90	0.71
1:B:49:LYS:O	1:B:50:GLU:HB3	1.89	0.70
1:A:232:LYS:HG2	1:A:257:GLU:HG2	1.73	0.69
1:A:70:VAL:HG13	1:A:73:LEU:HB2	1.73	0.69
1:A:197:LEU:HD23	1:A:197:LEU:C	2.18	0.69
1:B:384:ASP:O	1:B:385:ASP:HB2	1.91	0.69
1:A:76:ARG:NH1	1:A:76:ARG:HB2	2.08	0.69
1:A:43:VAL:HG12	1:A:44:ASP:N	2.07	0.68
1:B:206:GLU:HB3	2:B:471:HOH:O	1.92	0.68
1:B:90:ALA:HB3	1:B:91:PRO:C	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASN:HD21	1:A:17:LYS:HB2	1.58	0.68
1:B:294:LYS:H	1:B:294:LYS:CE	2.07	0.67
1:B:70:VAL:HG13	1:B:71:LEU:HD22	1.76	0.67
1:A:15:ASN:ND2	1:A:17:LYS:HB2	2.10	0.66
1:B:210:HIS:HD2	2:B:439:HOH:O	1.76	0.66
1:B:48:LEU:O	1:B:51:ARG:HD3	1.94	0.66
1:B:132:GLY:O	1:B:134:GLU:N	2.28	0.66
1:A:70:VAL:CG1	1:A:73:LEU:HD12	2.25	0.66
1:B:7:ARG:HD2	1:B:389:GLU:OE1	1.96	0.66
1:B:10:LYS:HA	1:B:20:VAL:O	1.95	0.65
1:B:43:VAL:HG11	1:B:48:LEU:HD11	1.78	0.65
1:B:385:ASP:CG	1:B:386:ILE:H	2.03	0.65
1:B:90:ALA:HB3	1:B:92:GLU:N	2.11	0.65
1:B:45:PRO:HG2	1:B:111:HIS:ND1	2.13	0.64
1:B:56:THR:HG22	1:B:83:ASN:CB	2.21	0.64
1:B:347:LEU:N	1:B:347:LEU:HD12	2.13	0.64
1:A:295:HIS:HD2	2:A:434:HOH:O	1.78	0.64
1:B:277:PHE:O	1:B:281:ASN:ND2	2.29	0.64
1:A:90:ALA:C	1:A:92:GLU:H	2.05	0.64
1:B:88:PRO:O	1:B:89:PRO:O	2.16	0.63
1:B:87:PHE:HD2	1:B:88:PRO:HA	1.61	0.63
1:A:18:LEU:HD13	1:A:150:CYS:SG	2.39	0.63
1:B:331:ARG:HD2	1:B:339:ALA:N	2.14	0.63
1:A:90:ALA:O	1:A:92:GLU:N	2.28	0.62
1:B:107:LYS:N	2:B:463:HOH:O	2.33	0.61
1:B:219:HIS:HD2	2:B:438:HOH:O	1.82	0.61
1:A:15:ASN:ND2	1:A:15:ASN:C	2.50	0.61
1:A:185:GLU:HG3	1:A:347:LEU:HD23	1.82	0.61
1:A:130:GLN:HA	1:A:130:GLN:OE1	2.00	0.60
1:A:95:LYS:HZ1	1:A:115:PHE:HA	1.66	0.60
1:B:20:VAL:HG23	1:B:164:VAL:HG11	1.83	0.60
1:A:132:GLY:CA	1:A:285:ARG:HD3	2.30	0.60
1:B:25:ARG:HG2	1:B:391:PHE:CE1	2.37	0.60
1:B:65:ARG:HH11	1:B:65:ARG:HG2	1.67	0.60
1:B:69:ASP:O	1:B:73:LEU:N	2.35	0.59
1:B:15:ASN:HD21	1:B:162:ASN:ND2	2.00	0.59
1:A:43:VAL:HG11	1:A:87:PHE:CD1	2.38	0.59
1:A:87:PHE:HD2	1:A:88:PRO:CA	2.16	0.59
1:B:7:ARG:HD2	1:B:389:GLU:CD	2.27	0.59
1:A:95:LYS:NZ	2:A:493:HOH:O	2.34	0.58
1:A:43:VAL:CG1	1:A:44:ASP:N	2.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HB3	1:A:97:LEU:HD12	1.85	0.58
1:B:45:PRO:HG2	1:B:111:HIS:CE1	2.38	0.58
1:A:176:GLU:OE1	1:A:205:LYS:HE3	2.03	0.58
1:B:130:GLN:NE2	2:B:505:HOH:O	2.35	0.58
1:B:236:ARG:HG2	1:B:236:ARG:NH1	2.18	0.58
1:A:5:GLY:HA2	1:A:384:ASP:HB2	1.84	0.58
1:B:66:GLU:O	1:B:68:LEU:N	2.36	0.58
1:B:281:ASN:O	1:B:282:ARG:O	2.21	0.58
1:B:283:GLU:CA	1:B:293:LEU:HD21	2.29	0.58
1:B:87:PHE:HD2	1:B:88:PRO:CA	2.18	0.57
1:B:90:ALA:HB3	1:B:91:PRO:CA	2.35	0.57
1:B:101:GLN:O	1:B:105:ILE:HG22	2.04	0.57
1:B:210:HIS:CD2	2:B:439:HOH:O	2.54	0.57
1:B:70:VAL:HG13	1:B:71:LEU:N	2.19	0.57
1:B:197:LEU:C	1:B:197:LEU:HD23	2.30	0.57
1:A:189:GLN:NE2	2:A:488:HOH:O	2.37	0.56
1:A:62:ARG:NH2	2:A:514:HOH:O	2.36	0.56
1:A:15:ASN:HD21	1:A:17:LYS:H	1.52	0.56
1:B:132:GLY:HA3	1:B:284:LYS:O	2.05	0.56
1:B:43:VAL:HG12	1:B:44:ASP:N	2.21	0.56
1:A:76:ARG:HB2	1:A:76:ARG:HH11	1.70	0.56
1:B:73:LEU:O	1:B:74:THR:C	2.48	0.56
1:B:189:GLN:NE2	2:B:411:HOH:O	2.38	0.56
1:A:87:PHE:HD2	1:A:88:PRO:HA	1.71	0.56
1:A:185:GLU:CG	1:A:347:LEU:HD23	2.36	0.56
1:B:294:LYS:HE3	1:B:294:LYS:N	2.18	0.55
1:B:135:ASP:O	1:B:136:THR:CB	2.54	0.55
1:B:292:LYS:HB2	1:B:295:HIS:CD2	2.42	0.55
1:B:87:PHE:HA	1:B:88:PRO:C	2.32	0.55
1:B:251:CYS:HB2	2:B:481:HOH:O	2.07	0.55
1:B:135:ASP:O	1:B:136:THR:HB	2.08	0.54
1:B:251:CYS:SG	1:B:285:ARG:NH2	2.81	0.54
1:A:225:ASN:HA	1:A:264:PRO:HB3	1.88	0.54
1:B:69:ASP:O	1:B:70:VAL:C	2.50	0.54
1:B:91:PRO:C	1:B:93:ASP:H	2.15	0.54
1:B:131:PRO:HG2	1:B:138:LYS:CB	2.31	0.54
1:A:94:LYS:O	1:A:96:PRO:HD3	2.08	0.54
1:B:90:ALA:CB	1:B:91:PRO:C	2.81	0.53
1:B:65:ARG:NH1	1:B:68:LEU:HD11	2.22	0.53
1:B:66:GLU:O	1:B:68:LEU:HD23	2.07	0.53
1:B:117:PHE:N	2:B:458:HOH:O	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:C	1:A:285:ARG:HE	2.16	0.53
1:A:103:ARG:NH1	1:A:103:ARG:HB3	2.24	0.52
1:A:94:LYS:C	1:A:96:PRO:HD3	2.33	0.52
1:A:331:ARG:NH2	1:A:341:SER:HA	2.24	0.52
1:B:85:GLN:H	1:B:94:LYS:HE3	1.74	0.52
1:A:43:VAL:CG1	1:A:44:ASP:H	2.22	0.52
1:A:93:ASP:O	1:A:94:LYS:C	2.53	0.52
1:A:103:ARG:HB3	1:A:103:ARG:HH11	1.74	0.52
1:B:125:CYS:SG	1:B:172:GLN:HB2	2.50	0.52
1:A:48:LEU:HD13	1:A:51:ARG:O	2.10	0.51
1:B:62:ARG:NE	2:B:430:HOH:O	2.39	0.51
1:B:54:TYR:CE2	1:B:154:LEU:HD11	2.46	0.51
1:A:89:PRO:O	1:A:90:ALA:HB3	2.11	0.51
1:B:178:PRO:O	1:B:179:GLY:O	2.29	0.51
1:B:66:GLU:C	1:B:68:LEU:HD23	2.36	0.50
1:A:159:HIS:HB3	1:A:162:ASN:HB2	1.93	0.50
1:A:197:LEU:HD23	1:A:198:HIS:N	2.26	0.50
1:B:205:LYS:NZ	1:B:212:GLU:OE1	2.44	0.50
1:A:87:PHE:CD2	1:A:88:PRO:HA	2.47	0.49
1:B:7:ARG:HA	1:B:387:VAL:O	2.12	0.49
1:B:294:LYS:CE	1:B:294:LYS:N	2.74	0.49
1:A:93:ASP:O	1:A:95:LYS:HG2	2.12	0.49
1:A:355:LYS:CG	1:A:356:PRO:HD2	2.43	0.49
1:B:68:LEU:HD23	1:B:68:LEU:H	1.77	0.49
1:B:62:ARG:HH22	1:B:128:THR:HG23	1.78	0.49
1:B:73:LEU:O	1:B:75:PHE:N	2.46	0.49
1:B:91:PRO:O	1:B:93:ASP:N	2.46	0.49
1:A:277:PHE:N	1:A:277:PHE:CD2	2.78	0.49
1:A:14:PRO:HG2	1:A:160:LYS:O	2.13	0.48
1:B:356:PRO:O	1:B:357:LYS:C	2.55	0.48
1:B:43:VAL:HG12	1:B:44:ASP:H	1.79	0.48
1:A:43:VAL:CG1	1:A:48:LEU:HD21	2.43	0.48
1:B:41:VAL:O	1:B:41:VAL:HG13	2.13	0.48
1:B:62:ARG:NH1	1:B:143:ASP:OD2	2.46	0.48
1:B:22:LEU:HD23	1:B:39:GLY:HA3	1.95	0.47
1:A:391:PHE:O	1:A:392:ALA:C	2.56	0.47
1:A:50:GLU:OE1	1:A:50:GLU:N	2.47	0.47
1:A:94:LYS:O	1:A:96:PRO:CD	2.62	0.47
1:B:37:VAL:N	2:B:492:HOH:O	2.01	0.47
1:B:67:ASP:C	1:B:69:ASP:H	2.21	0.47
1:A:87:PHE:HD2	1:A:88:PRO:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:HIS:HE1	2:A:422:HOH:O	1.96	0.47
1:B:131:PRO:HD3	1:B:139:ALA:HA	1.95	0.47
1:B:355:LYS:O	1:B:356:PRO:C	2.57	0.47
1:B:210:HIS:HE1	2:B:429:HOH:O	1.98	0.47
1:B:346:GLU:C	1:B:347:LEU:HD12	2.40	0.46
1:A:95:LYS:NZ	1:A:115:PHE:CA	2.78	0.46
1:B:49:LYS:O	1:B:50:GLU:CB	2.62	0.46
1:B:29:ASP:OD2	1:B:170:LYS:HE2	2.16	0.46
1:B:115:PHE:N	2:B:460:HOH:O	2.01	0.46
1:A:15:ASN:ND2	1:A:17:LYS:N	2.44	0.45
1:B:176:GLU:OE1	1:B:205:LYS:HE3	2.17	0.45
1:A:125:CYS:SG	1:A:172:GLN:HB2	2.57	0.45
1:B:66:GLU:HG3	2:B:461:HOH:O	2.16	0.45
1:B:138:LYS:HD2	2:B:474:HOH:O	2.16	0.45
1:B:331:ARG:HD2	1:B:339:ALA:HB3	1.98	0.45
1:A:181:GLN:HA	1:A:181:GLN:NE2	2.32	0.45
1:B:15:ASN:HD21	1:B:162:ASN:HD22	1.64	0.45
1:A:95:LYS:HZ1	1:A:115:PHE:CA	2.30	0.44
1:A:101:GLN:O	1:A:105:ILE:HG13	2.18	0.44
1:B:72:GLY:O	1:B:73:LEU:C	2.58	0.44
1:B:331:ARG:HD2	1:B:339:ALA:CB	2.47	0.44
1:B:89:PRO:HD3	1:B:113:TYR:HE2	1.82	0.44
1:A:95:LYS:NZ	1:A:115:PHE:HA	2.31	0.44
1:A:173:TYR:CE1	1:A:355:LYS:HB2	2.53	0.44
1:B:173:TYR:CG	1:B:174:ALA:N	2.85	0.44
1:B:102:GLU:O	1:B:106:LYS:HG3	2.17	0.44
1:B:87:PHE:C	1:B:87:PHE:CD2	2.94	0.43
1:B:162:ASN:HD22	1:B:162:ASN:HA	1.61	0.43
1:B:205:LYS:HE2	1:B:207:ILE:O	2.18	0.43
1:B:29:ASP:HB2	1:B:170:LYS:HE2	2.00	0.43
1:B:87:PHE:CD2	1:B:88:PRO:HA	2.47	0.43
1:A:87:PHE:CD2	1:A:87:PHE:C	2.95	0.43
1:A:197:LEU:C	1:A:197:LEU:CD2	2.88	0.43
1:A:95:LYS:HE3	1:A:114:PRO:HG2	2.00	0.43
1:B:166:LEU:HD12	1:B:166:LEU:N	2.34	0.43
1:A:331:ARG:HH22	1:A:341:SER:HA	1.83	0.43
1:B:72:GLY:O	1:B:74:THR:N	2.52	0.43
1:B:232:LYS:HG2	1:B:257:GLU:HG2	2.01	0.43
1:A:284:LYS:O	1:A:285:ARG:NE	2.51	0.43
1:A:76:ARG:HH11	1:A:76:ARG:CB	2.31	0.43
1:B:236:ARG:NH1	1:B:236:ARG:CG	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HB2	1:A:14:PRO:CD	2.49	0.42
1:A:95:LYS:NZ	1:A:116:THR:N	2.67	0.42
1:A:219:HIS:HD2	2:A:424:HOH:O	2.01	0.42
1:A:62:ARG:HG2	2:A:445:HOH:O	2.19	0.42
1:B:130:GLN:CD	2:B:505:HOH:O	2.62	0.42
1:B:278:LEU:O	1:B:279:ALA:C	2.61	0.42
1:B:40:VAL:HG21	1:B:104:LEU:CB	2.49	0.42
1:A:278:LEU:O	1:A:279:ALA:C	2.63	0.42
1:B:9:PHE:O	1:B:21:TYR:HA	2.19	0.42
1:B:384:ASP:O	1:B:385:ASP:CB	2.62	0.42
1:A:183:THR:HA	2:A:446:HOH:O	2.20	0.42
1:A:43:VAL:HG11	1:A:48:LEU:HD21	2.02	0.42
1:B:70:VAL:CG1	1:B:71:LEU:HD22	2.46	0.42
1:B:108:LEU:N	2:B:463:HOH:O	2.53	0.42
1:A:392:ALA:HA	2:A:427:HOH:O	2.19	0.42
1:B:91:PRO:C	1:B:93:ASP:N	2.78	0.42
1:A:201:ALA:HA	1:A:217:ASN:O	2.20	0.41
1:A:261:THR:HG22	1:A:262:VAL:N	2.35	0.41
1:A:277:PHE:N	1:A:277:PHE:HD2	2.18	0.41
1:B:347:LEU:HA	1:B:348:PRO:HD3	1.86	0.41
1:A:95:LYS:NZ	1:A:115:PHE:C	2.78	0.41
1:B:281:ASN:HA	1:B:285:ARG:NH1	2.35	0.41
1:A:386:ILE:HG23	1:A:387:VAL:N	2.35	0.41
1:B:114:PRO:HA	2:B:460:HOH:O	2.20	0.41
1:B:350:THR:CG2	1:B:352:MET:HE3	2.50	0.41
1:B:15:ASN:OD1	1:B:15:ASN:C	2.63	0.41
1:B:80:PHE:CZ	1:B:82:ALA:HB2	2.55	0.41
1:A:99:ARG:O	1:A:103:ARG:HG3	2.21	0.41
1:B:385:ASP:CG	1:B:386:ILE:N	2.75	0.41
1:A:35:GLU:HA	1:A:36:PRO:HD3	1.93	0.41
1:B:178:PRO:HB2	1:B:179:GLY:H	1.67	0.41
1:A:181:GLN:HA	1:A:181:GLN:HE21	1.85	0.41
1:A:210:HIS:CD2	2:A:472:HOH:O	2.74	0.41
1:B:66:GLU:O	1:B:67:ASP:C	2.63	0.41
1:B:87:PHE:HD2	1:B:88:PRO:N	2.19	0.41
1:B:90:ALA:HB3	1:B:91:PRO:HA	2.03	0.41
1:A:278:LEU:O	1:A:281:ASN:N	2.46	0.41
1:A:64:GLY:O	1:A:65:ARG:C	2.65	0.40
1:B:20:VAL:CG2	1:B:164:VAL:HG11	2.51	0.40
1:B:116:THR:CA	2:B:458:HOH:O	2.59	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	350/393 (89%)	324 (93%)	21 (6%)	5 (1%)	9	3
1	B	351/393 (89%)	312 (89%)	22 (6%)	17 (5%)	2	0
All	All	701/786 (89%)	636 (91%)	43 (6%)	22 (3%)	3	0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	PRO
1	A	95	LYS
1	B	66	GLU
1	B	67	ASP
1	B	69	ASP
1	B	70	VAL
1	B	89	PRO
1	B	136	THR
1	B	178	PRO
1	B	179	GLY
1	B	282	ARG
1	B	356	PRO
1	B	74	THR
1	B	92	GLU
1	B	385	ASP
1	A	91	PRO
1	B	68	LEU
1	B	90	ALA
1	B	114	PRO
1	B	133	PRO
1	A	49	LYS
1	A	96	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	313/350 (89%)	297 (95%)	16 (5%)	21	13
1	B	317/350 (91%)	302 (95%)	15 (5%)	23	15
All	All	630/700 (90%)	599 (95%)	31 (5%)	22	14

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	33	LEU
1	A	62	ARG
1	A	83	ASN
1	A	103	ARG
1	A	131	PRO
1	A	159	HIS
1	A	162	ASN
1	A	183	THR
1	A	274	LEU
1	A	277	PHE
1	A	280	ASN
1	A	305	LEU
1	A	351	LEU
1	A	384	ASP
1	A	386	ILE
1	B	50	GLU
1	B	66	GLU
1	B	73	LEU
1	B	74	THR
1	B	93	ASP
1	B	96	PRO
1	B	97	LEU
1	B	114	PRO
1	B	162	ASN
1	B	189	GLN
1	B	196	PRO

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Mol	Chain	Res	Type
1	B	277	PHE
1	B	294	LYS
1	B	356	PRO
1	B	384	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	172	GLN
1	A	181	GLN
1	A	210	HIS
1	A	295	HIS
1	B	130	GLN
1	B	162	ASN
1	B	172	GLN
1	B	210	HIS
1	B	245	ASN
1	B	248	GLN
1	B	295	HIS
1	B	353	HIS

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	356/393 (90%)	1.03	68 (19%) 3 3	22, 46, 86, 106	17 (4%)
1	B	357/393 (90%)	1.42	87 (24%) 2 1	21, 50, 98, 117	16 (4%)
All	All	713/786 (90%)	1.22	155 (21%) 2 2	21, 48, 93, 117	33 (4%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	GLY	7.3
1	B	136	THR	5.9
1	B	68	LEU	5.6
1	B	133	PRO	5.4
1	B	100	LEU	5.2
1	A	178	PRO	5.1
1	A	386	ILE	5.0
1	A	91	PRO	4.9
1	B	112	ALA	4.8
1	B	88	PRO	4.8
1	B	91	PRO	4.7
1	B	113	TYR	4.6
1	B	392	ALA	4.5
1	B	280	ASN	4.5
1	B	97	LEU	4.5
1	A	383	ASP	4.4
1	A	277	PHE	4.4
1	A	48	LEU	4.3
1	B	339	ALA	4.3
1	B	383	ASP	4.3
1	A	87	PHE	4.2
1	A	357	LYS	4.2
1	B	73	LEU	4.2
1	A	47	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	71	LEU	4.2
1	B	72	GLY	4.1
1	B	70	VAL	4.1
1	B	386	ILE	4.1
1	B	281	ASN	4.1
1	B	130	GLN	4.0
1	B	154	LEU	4.0
1	B	92	GLU	4.0
1	A	5	GLY	3.9
1	B	67	ASP	3.9
1	B	43	VAL	3.9
1	B	277	PHE	3.9
1	B	89	PRO	3.9
1	A	332	GLY	3.9
1	B	357	LYS	3.8
1	A	285	ARG	3.8
1	B	48	LEU	3.8
1	B	279	ALA	3.7
1	B	178	PRO	3.7
1	A	93	ASP	3.6
1	A	133	PRO	3.5
1	A	356	PRO	3.5
1	A	90	ALA	3.4
1	B	5	GLY	3.4
1	A	388	PHE	3.4
1	B	387	VAL	3.3
1	B	96	PRO	3.3
1	B	393	ARG	3.2
1	A	180	PRO	3.2
1	A	384	ASP	3.2
1	A	92	GLU	3.2
1	B	108	LEU	3.1
1	A	183	THR	3.1
1	B	90	ALA	3.1
1	B	282	ARG	3.1
1	A	46	GLU	3.1
1	B	38	ASP	3.1
1	B	49	LYS	3.1
1	B	114	PRO	3.1
1	B	104	LEU	3.0
1	A	280	ASN	3.0
1	B	158	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	111	HIS	3.0
1	A	130	GLN	3.0
1	A	18	LEU	2.9
1	A	73	LEU	2.9
1	A	151	ALA	2.9
1	A	42	LEU	2.9
1	B	50	GLU	2.9
1	B	45	PRO	2.9
1	B	66	GLU	2.9
1	A	162	ASN	2.8
1	B	74	THR	2.8
1	B	8	VAL	2.8
1	A	159	HIS	2.8
1	B	33	LEU	2.8
1	B	180	PRO	2.8
1	A	95	LYS	2.7
1	B	135	ASP	2.7
1	A	341	SER	2.7
1	A	387	VAL	2.7
1	B	82	ALA	2.7
1	B	286	GLY	2.7
1	B	297	ASP	2.7
1	B	388	PHE	2.7
1	B	103	ARG	2.6
1	A	74	THR	2.6
1	B	87	PHE	2.6
1	A	109	GLY	2.6
1	A	161	ARG	2.6
1	B	385	ASP	2.6
1	A	392	ALA	2.6
1	A	96	PRO	2.5
1	A	113	TYR	2.5
1	B	54	TYR	2.5
1	A	71	LEU	2.5
1	B	356	PRO	2.5
1	A	45	PRO	2.5
1	B	390	ASP	2.4
1	A	55	VAL	2.4
1	B	42	LEU	2.4
1	B	105	ILE	2.4
1	A	89	PRO	2.4
1	A	111	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	TYR	2.4
1	A	15	ASN	2.4
1	B	41	VAL	2.4
1	B	47	TYR	2.3
1	B	6	THR	2.3
1	A	154	LEU	2.3
1	A	131	PRO	2.3
1	A	10	LYS	2.3
1	A	19	THR	2.3
1	A	160	LYS	2.3
1	B	65	ARG	2.3
1	A	150	CYS	2.3
1	B	9	PHE	2.2
1	B	151	ALA	2.2
1	A	164	VAL	2.2
1	A	385	ASP	2.2
1	A	177	ARG	2.2
1	B	312	ARG	2.2
1	B	331	ARG	2.2
1	A	104	LEU	2.2
1	B	69	ASP	2.2
1	B	51	ARG	2.2
1	A	53	VAL	2.2
1	B	84	VAL	2.2
1	B	98	THR	2.2
1	A	158	ILE	2.1
1	A	70	VAL	2.1
1	B	187	THR	2.1
1	A	108	LEU	2.1
1	A	393	ARG	2.1
1	B	118	GLU	2.1
1	A	279	ALA	2.1
1	A	20	VAL	2.1
1	B	53	VAL	2.1
1	A	94	LYS	2.1
1	A	88	PRO	2.1
1	B	306	LEU	2.1
1	A	194	ASP	2.1
1	B	330	SER	2.0
1	B	179	GLY	2.0
1	A	83	ASN	2.0
1	B	162	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	40	VAL	2.0
1	B	182	PRO	2.0
1	A	153	ASN	2.0
1	B	132	GLY	2.0
1	B	99	ARG	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 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.