



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:20 PM UTC

PDB ID : 8HST / pdb_00008hst
Title : The structure of rat beta-arrestin1
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Deposited on : 2022-12-20
Resolution : 2.66 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

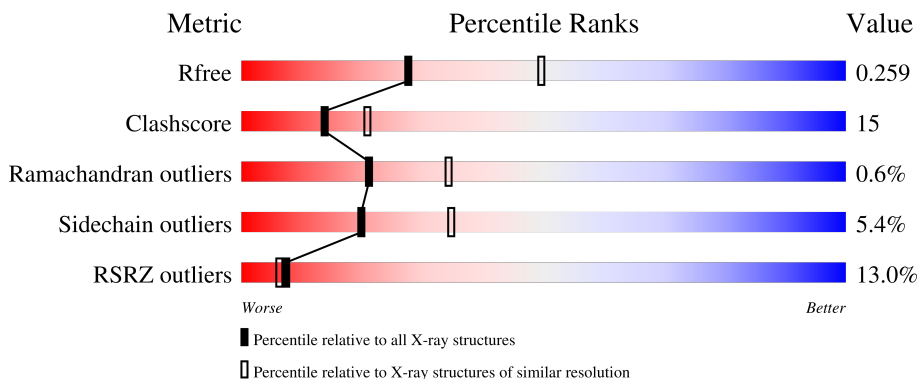
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	414	12% 62% 24% • 13%
1	B	414	11% 59% 26% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5904 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-arrestin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2879	1841	495	540	3			
1	B	361	Total	C	N	O	S	0	0	0
			2879	1841	495	540	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P29066
A	-18	GLY	-	expression tag	UNP P29066
A	-17	SER	-	expression tag	UNP P29066
A	-16	SER	-	expression tag	UNP P29066
A	-15	HIS	-	expression tag	UNP P29066
A	-14	HIS	-	expression tag	UNP P29066
A	-13	HIS	-	expression tag	UNP P29066
A	-12	HIS	-	expression tag	UNP P29066
A	-11	HIS	-	expression tag	UNP P29066
A	-10	HIS	-	expression tag	UNP P29066
A	-9	SER	-	expression tag	UNP P29066
A	-8	SER	-	expression tag	UNP P29066
A	-7	GLY	-	expression tag	UNP P29066
A	-6	LEU	-	expression tag	UNP P29066
A	-5	VAL	-	expression tag	UNP P29066
A	-4	PRO	-	expression tag	UNP P29066
A	-3	ARG	-	expression tag	UNP P29066
A	-2	GLY	-	expression tag	UNP P29066
A	-1	SER	-	expression tag	UNP P29066
A	0	HIS	-	expression tag	UNP P29066
A	59	VAL	CYS	engineered mutation	UNP P29066
A	125	SER	CYS	engineered mutation	UNP P29066
A	140	LEU	CYS	engineered mutation	UNP P29066
A	150	VAL	CYS	engineered mutation	UNP P29066
A	242	VAL	CYS	engineered mutation	UNP P29066

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Chain	Residue	Modelled	Actual	Comment	Reference
A	251	VAL	CYS	engineered mutation	UNP P29066
A	269	SER	CYS	engineered mutation	UNP P29066
B	-19	MET	-	initiating methionine	UNP P29066
B	-18	GLY	-	expression tag	UNP P29066
B	-17	SER	-	expression tag	UNP P29066
B	-16	SER	-	expression tag	UNP P29066
B	-15	HIS	-	expression tag	UNP P29066
B	-14	HIS	-	expression tag	UNP P29066
B	-13	HIS	-	expression tag	UNP P29066
B	-12	HIS	-	expression tag	UNP P29066
B	-11	HIS	-	expression tag	UNP P29066
B	-10	HIS	-	expression tag	UNP P29066
B	-9	SER	-	expression tag	UNP P29066
B	-8	SER	-	expression tag	UNP P29066
B	-7	GLY	-	expression tag	UNP P29066
B	-6	LEU	-	expression tag	UNP P29066
B	-5	VAL	-	expression tag	UNP P29066
B	-4	PRO	-	expression tag	UNP P29066
B	-3	ARG	-	expression tag	UNP P29066
B	-2	GLY	-	expression tag	UNP P29066
B	-1	SER	-	expression tag	UNP P29066
B	0	HIS	-	expression tag	UNP P29066
B	59	VAL	CYS	engineered mutation	UNP P29066
B	125	SER	CYS	engineered mutation	UNP P29066
B	140	LEU	CYS	engineered mutation	UNP P29066
B	150	VAL	CYS	engineered mutation	UNP P29066
B	242	VAL	CYS	engineered mutation	UNP P29066
B	251	VAL	CYS	engineered mutation	UNP P29066
B	269	SER	CYS	engineered mutation	UNP P29066

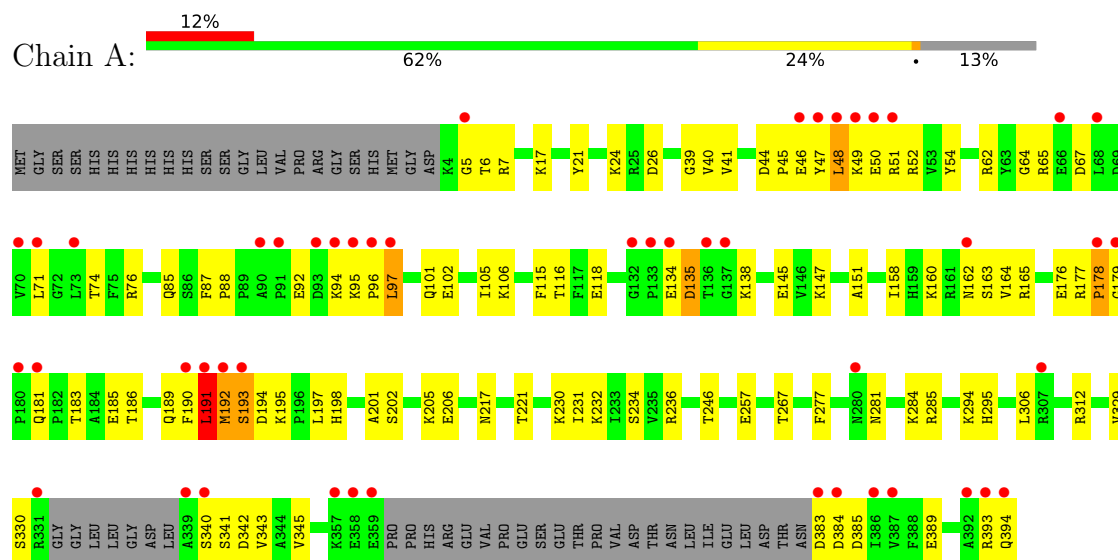
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	70	Total O 70 70	0	0
2	B	76	Total O 76 76	0	0

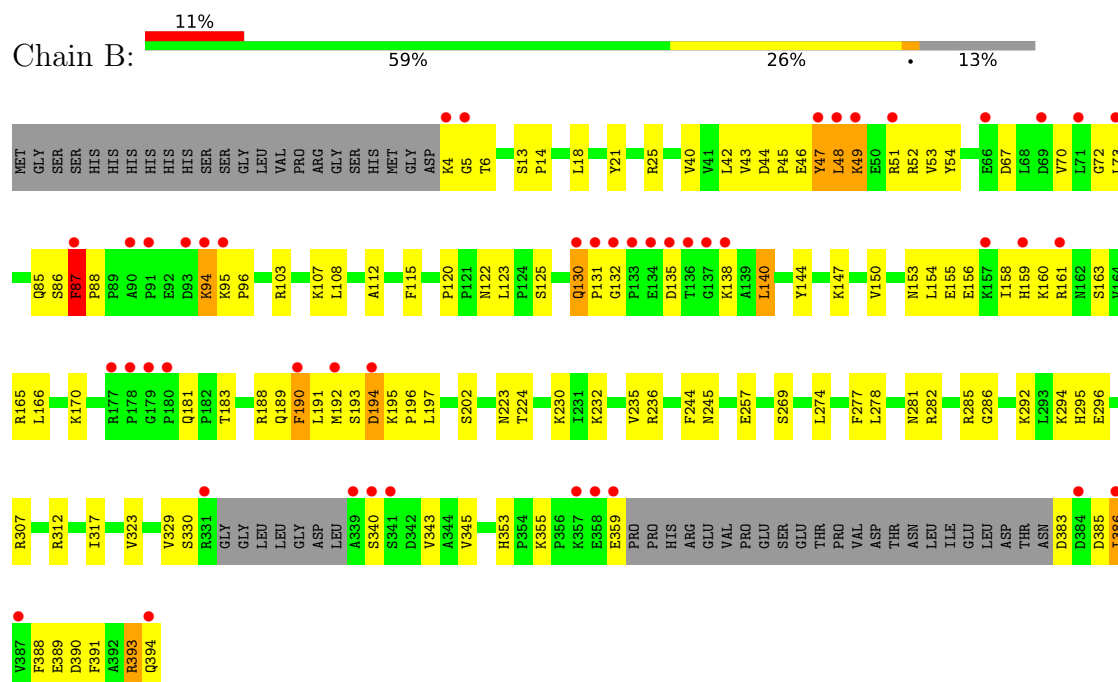
3 Residue-property plots [i](#)

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

• Molecule 1: Beta-arrestin-1



• Molecule 1: Beta-arrestin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.28Å 72.48Å 116.39Å 90.00° 98.78° 90.00°	Depositor
Resolution (Å)	38.62 – 2.66 38.62 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.62-2.66) 99.7 (38.62-2.66)	Depositor EDS
R_{merge}	0.98	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.46 (at 2.65Å)	Xtriage
Refinement program	PHENIX v1.19.2	Depositor
R, R_{free}	0.184 , 0.248 0.196 , 0.259	Depositor DCC
R_{free} test set	1455 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5904	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/2938	0.67	2/3982 (0.1%)
1	B	0.42	0/2938	0.65	1/3982 (0.0%)
All	All	0.41	0/5876	0.66	3/7964 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	47	TYR	CA-CB-CG	-10.14	95.66	113.90
1	A	118	GLU	CA-C-N	-5.89	118.35	122.59
1	A	118	GLU	C-N-CA	-5.89	118.35	122.59

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	PRO	Peptide
1	A	179	GLY	Peptide
1	A	50	GLU	Peptide
1	B	340	SER	Peptide
1	B	87	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2879	0	2934	77	1
1	B	2879	0	2934	95	1
2	A	70	0	0	5	0
2	B	76	0	0	5	0
All	All	5904	0	5868	169	1

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 15.

All (169) 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:160:LYS:H	1:A:160:LYS:HD2	1.31	0.92
1:B:160:LYS:HG2	1:B:163:SER:HB2	1.55	0.88
1:B:188:ARG:HH11	1:B:188:ARG:HB2	1.37	0.87
1:A:183:THR:HG22	1:A:202:SER:HB3	1.61	0.82
1:A:190:PHE:H	1:A:193:SER:HB2	1.47	0.80
1:A:48:LEU:O	1:A:51:ARG:HG2	1.82	0.79
1:B:188:ARG:HD2	1:B:343:VAL:HG22	1.65	0.79
1:B:181:GLN:N	1:B:181:GLN:OE1	2.19	0.76
1:B:193:SER:O	1:B:195:LYS:N	2.19	0.75
1:A:51:ARG:CZ	1:A:51:ARG:HB3	2.15	0.74
1:B:70:VAL:HG12	1:B:72:GLY:H	1.53	0.72
1:A:230:LYS:NZ	1:A:257:GLU:OE1	2.20	0.72
1:B:277:PHE:O	1:B:281:ASN:ND2	2.23	0.71
1:B:188:ARG:HB2	1:B:188:ARG:NH1	2.05	0.70
1:B:53:VAL:HG22	1:B:150:VAL:HG22	1.73	0.69
1:B:294:LYS:HD2	1:B:294:LYS:H	1.57	0.69
1:B:140:LEU:HD13	1:B:317:ILE:HD11	1.76	0.68
1:B:130:GLN:O	1:B:132:GLY:N	2.27	0.67
1:B:52:ARG:HG2	1:B:88:PRO:HG3	1.78	0.65
1:A:97:LEU:HD13	1:A:101:GLN:HB3	1.79	0.65
1:A:51:ARG:O	1:A:51:ARG:NH1	2.30	0.65
1:B:46:GLU:HB3	1:B:47:TYR:CE2	2.32	0.64
1:A:134:GLU:N	1:A:134:GLU:OE1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HE3	1:A:116:THR:HG23	1.79	0.63
1:B:188:ARG:NH2	2:B:405:HOH:O	2.31	0.62
1:B:86:SER:O	1:B:88:PRO:HD2	2.00	0.62
1:A:134:GLU:HG3	1:A:285:ARG:HG3	1.82	0.62
1:B:95:LYS:HB2	1:B:96:PRO:HD2	1.81	0.62
1:A:190:PHE:N	1:A:193:SER:HB2	2.14	0.61
1:B:48:LEU:O	1:B:51:ARG:N	2.34	0.61
1:A:393:ARG:NH1	2:A:404:HOH:O	2.34	0.61
1:A:295:HIS:HB3	1:A:394:GLN:HB3	1.83	0.60
1:A:221:THR:HG23	1:A:267:THR:HG22	1.83	0.60
1:A:192:MET:HA	1:B:244:PHE:CZ	2.36	0.60
1:A:342:ASP:O	2:A:401:HOH:O	2.16	0.60
1:B:192:MET:HE2	1:B:223:ASN:O	2.02	0.60
1:A:92:GLU:OE1	1:A:95:LYS:N	2.26	0.59
1:B:193:SER:OG	1:B:194:ASP:N	2.22	0.59
1:A:183:THR:CG2	1:A:202:SER:HB3	2.30	0.59
1:A:145:GLU:OE2	1:A:165:ARG:HD2	2.02	0.58
1:A:191:LEU:O	1:A:191:LEU:HG	2.04	0.58
1:B:45:PRO:HA	1:B:48:LEU:HD12	1.86	0.57
1:A:5:GLY:H	1:A:385:ASP:HB3	1.67	0.57
1:A:393:ARG:CZ	1:A:393:ARG:HA	2.34	0.57
1:B:13:SER:HB2	1:B:18:LEU:HB2	1.86	0.57
1:A:158:ILE:HD11	1:A:162:ASN:HB2	1.86	0.57
1:A:181:GLN:HG3	1:A:206:GLU:HG2	1.86	0.57
1:B:42:LEU:HD12	1:B:108:LEU:HB3	1.87	0.56
1:A:277:PHE:O	1:A:281:ASN:ND2	2.39	0.56
1:B:194:ASP:OD2	2:B:401:HOH:O	2.17	0.56
1:A:45:PRO:HA	1:A:48:LEU:HG	1.88	0.56
1:A:44:ASP:OD1	1:A:46:GLU:HG2	2.06	0.56
1:A:94:LYS:HG2	1:A:96:PRO:HD3	1.88	0.55
1:A:52:ARG:HB2	1:A:151:ALA:O	2.06	0.55
1:A:21:TYR:HB2	1:A:40:VAL:HG23	1.88	0.55
1:B:25:ARG:HG2	1:B:391:PHE:CE1	2.41	0.55
1:B:45:PRO:HA	1:B:48:LEU:CD1	2.37	0.55
1:A:7:ARG:HD2	1:A:389:GLU:CD	2.31	0.55
1:B:72:GLY:O	1:B:73:LEU:HD23	2.07	0.55
1:A:393:ARG:HA	1:A:393:ARG:NE	2.24	0.53
1:A:193:SER:O	1:A:194:ASP:HB3	2.08	0.53
1:B:295:HIS:CD2	1:B:393:ARG:HB2	2.44	0.53
1:A:87:PHE:CD1	1:A:88:PRO:HA	2.44	0.52
1:B:183:THR:HG22	1:B:202:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:PHE:H	1:A:193:SER:CB	2.20	0.52
1:B:107:LYS:HD2	1:B:386:ILE:HG21	1.91	0.52
1:A:134:GLU:HG3	1:A:285:ARG:CG	2.40	0.52
1:B:4:LYS:N	1:B:385:ASP:OD1	2.42	0.52
1:A:190:PHE:O	1:A:192:MET:N	2.43	0.52
1:B:94:LYS:HZ2	1:B:115:PHE:HA	1.75	0.51
1:A:181:GLN:HG3	1:A:206:GLU:OE1	2.11	0.51
1:A:190:PHE:HZ	1:A:343:VAL:HG21	1.76	0.50
1:B:190:PHE:HZ	1:B:197:LEU:HD23	1.76	0.50
1:B:193:SER:O	1:B:194:ASP:C	2.55	0.50
1:B:144:TYR:OH	1:B:170:LYS:HE2	2.12	0.50
1:B:21:TYR:CE2	1:B:388:PHE:HE2	2.30	0.50
1:A:94:LYS:HZ3	1:A:96:PRO:HG3	1.76	0.50
1:B:135:ASP:CG	1:B:285:ARG:HE	2.20	0.50
1:A:185:GLU:OE1	1:A:198:HIS:NE2	2.44	0.50
1:B:296:GLU:OE2	1:B:394:GLN:NE2	2.40	0.50
1:A:186:THR:HG22	1:A:345:VAL:HG13	1.94	0.49
1:B:155:GLU:HG2	1:B:155:GLU:O	2.12	0.49
1:A:306:LEU:HD11	1:A:312:ARG:HG3	1.93	0.49
1:A:246:THR:HB	1:B:188:ARG:HG3	1.95	0.49
1:A:97:LEU:HB3	1:A:102:GLU:HG3	1.94	0.49
1:B:166:LEU:HD23	1:B:391:PHE:CG	2.47	0.49
1:B:120:PRO:HG2	1:B:123:LEU:HD11	1.95	0.49
1:A:193:SER:C	1:A:195:LYS:H	2.21	0.48
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.60	0.48
1:B:159:HIS:ND1	1:B:161:ARG:HG2	2.29	0.48
1:A:65:ARG:HH21	1:A:71:LEU:HD23	1.79	0.47
1:A:284:LYS:O	2:A:402:HOH:O	2.20	0.47
1:A:94:LYS:NZ	1:A:96:PRO:HG3	2.29	0.47
1:B:87:PHE:CD2	1:B:88:PRO:HD3	2.50	0.47
1:B:131:PRO:HA	1:B:286:GLY:H	1.78	0.47
1:B:6:THR:OG1	1:B:386:ILE:HD12	2.15	0.47
1:B:94:LYS:NZ	1:B:115:PHE:HA	2.30	0.47
1:A:39:GLY:HA3	1:A:115:PHE:CZ	2.50	0.46
1:B:6:THR:HG21	1:B:103:ARG:HH22	1.79	0.46
1:A:62:ARG:NH1	1:A:76:ARG:HE	2.14	0.46
1:B:131:PRO:O	1:B:135:ASP:HB2	2.15	0.46
1:B:353:HIS:HD2	2:B:429:HOH:O	1.98	0.46
1:B:192:MET:SD	1:B:224:THR:HA	2.56	0.46
1:B:292:LYS:HB2	1:B:295:HIS:ND1	2.31	0.46
1:A:135:ASP:HB2	2:A:417:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ILE:HG23	1:B:386:ILE:O	2.16	0.46
1:B:193:SER:C	1:B:195:LYS:H	2.24	0.46
1:A:191:LEU:HA	1:A:192:MET:HA	1.67	0.46
1:B:85:GLN:NE2	1:B:88:PRO:HG2	2.31	0.46
1:A:17:LYS:HG3	1:A:47:TYR:CE1	2.51	0.45
1:A:96:PRO:O	1:A:97:LEU:C	2.59	0.45
1:A:294:LYS:HB3	1:A:294:LYS:HE3	1.65	0.45
1:B:355:LYS:NZ	2:B:404:HOH:O	2.43	0.45
1:A:64:GLY:HA2	1:A:138:LYS:HD3	1.98	0.45
1:B:44:ASP:C	1:B:46:GLU:H	2.24	0.45
1:B:192:MET:HG3	1:B:195:LYS:O	2.17	0.45
1:B:232:LYS:NZ	1:B:257:GLU:OE2	2.28	0.45
1:B:329:VAL:HG12	1:B:330:SER:O	2.17	0.45
1:B:43:VAL:CG1	1:B:48:LEU:HD11	2.46	0.45
1:A:94:LYS:HB3	1:A:94:LYS:HE3	1.57	0.45
1:A:201:ALA:HA	1:A:217:ASN:O	2.17	0.45
1:B:125:SER:HA	1:B:170:LYS:HE3	1.97	0.45
1:B:154:LEU:HA	1:B:154:LEU:HD12	1.69	0.45
1:A:145:GLU:CD	1:A:165:ARG:HD2	2.40	0.44
1:B:5:GLY:N	1:B:385:ASP:OD2	2.50	0.44
1:B:292:LYS:C	1:B:294:LYS:H	2.25	0.44
1:A:191:LEU:HB3	1:B:245:ASN:CG	2.41	0.44
1:B:147:LYS:HG3	1:B:165:ARG:HG2	1.98	0.44
1:B:292:LYS:HB3	1:B:294:LYS:CD	2.48	0.44
1:B:48:LEU:O	1:B:49:LYS:C	2.59	0.44
1:A:54:TYR:CE1	1:A:85:GLN:HG3	2.53	0.44
1:B:385:ASP:OD1	1:B:385:ASP:N	2.50	0.44
1:A:147:LYS:HG3	1:A:165:ARG:HG2	1.99	0.44
1:B:131:PRO:HB2	1:B:135:ASP:HB3	1.99	0.44
1:A:383:ASP:HB3	1:A:384:ASP:H	1.46	0.43
1:B:292:LYS:C	1:B:294:LYS:N	2.77	0.43
1:A:197:LEU:HD23	1:A:197:LEU:C	2.43	0.43
1:B:85:GLN:HE21	1:B:88:PRO:HG2	1.83	0.43
1:B:194:ASP:HB3	1:B:195:LYS:HG3	2.00	0.43
1:B:312:ARG:NH2	2:B:402:HOH:O	2.24	0.43
1:A:236:ARG:NH1	2:A:420:HOH:O	2.52	0.42
1:A:329:VAL:O	1:A:340:SER:HA	2.19	0.42
1:B:190:PHE:O	1:B:191:LEU:C	2.61	0.42
1:B:193:SER:C	1:B:195:LYS:N	2.77	0.42
1:A:145:GLU:OE2	1:A:165:ARG:NH1	2.47	0.42
1:B:235:VAL:HG22	1:B:323:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:HD3	1:A:26:ASP:O	2.20	0.42
1:A:21:TYR:HB2	1:A:40:VAL:CG2	2.50	0.42
1:B:192:MET:HG2	1:B:224:THR:HG22	2.01	0.42
1:B:359:GLU:H	1:B:359:GLU:HG3	1.64	0.42
1:A:177:ARG:NH1	1:A:178:PRO:O	2.51	0.42
1:B:54:TYR:CE1	1:B:85:GLN:HB2	2.54	0.42
1:B:14:PRO:HG2	1:B:161:ARG:HA	2.02	0.42
1:B:278:LEU:O	1:B:282:ARG:NH1	2.51	0.41
1:B:236:ARG:NH1	1:B:236:ARG:HG2	2.35	0.41
1:B:389:GLU:HG3	1:B:390:ASP:N	2.36	0.41
1:A:160:LYS:H	1:A:160:LYS:CD	2.08	0.41
1:B:122:ASN:OD1	1:B:307:ARG:HD3	2.21	0.41
1:B:195:LYS:HA	1:B:196:PRO:HD3	1.98	0.41
1:A:97:LEU:HD11	1:A:105:ILE:HD12	2.03	0.41
1:B:6:THR:HG21	1:B:103:ARG:NH2	2.36	0.41
1:B:153:ASN:CG	1:B:154:LEU:N	2.79	0.41
1:A:232:LYS:HG2	1:A:257:GLU:HG2	2.02	0.41
1:B:67:ASP:OD1	1:B:67:ASP:N	2.52	0.40
1:B:230:LYS:NZ	1:B:257:GLU:HB3	2.36	0.40
1:B:138:LYS:HD2	1:B:138:LYS:HA	1.96	0.40
1:B:355:LYS:H	1:B:355:LYS:HG3	1.65	0.40
1:A:92:GLU:HG2	1:A:95:LYS:HB2	2.04	0.40
1:B:40:VAL:HG11	1:B:112:ALA:HB1	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:NH1	1:B:47:TYR:OH[1_656]	1.97	0.23

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	355/414 (86%)	325 (92%)	29 (8%)	1 (0%)	36	52
1	B	355/414 (86%)	325 (92%)	27 (8%)	3 (1%)	16	27
All	All	710/828 (86%)	650 (92%)	56 (8%)	4 (1%)	21	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	PHE
1	B	194	ASP
1	A	191	LEU
1	B	49	LYS

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	322/368 (88%)	301 (94%)	21 (6%)	15	27
1	B	322/368 (88%)	308 (96%)	14 (4%)	26	44
All	All	644/736 (88%)	609 (95%)	35 (5%)	20	35

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	41	VAL
1	A	48	LEU
1	A	49	LYS
1	A	67	ASP
1	A	74	THR
1	A	97	LEU
1	A	106	LYS
1	A	135	ASP
1	A	163	SER
1	A	164	VAL
1	A	176	GLU

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Mol	Chain	Res	Type
1	A	189	GLN
1	A	191	LEU
1	A	192	MET
1	A	193	SER
1	A	205	LYS
1	A	231	ILE
1	A	234	SER
1	A	330	SER
1	A	341	SER
1	B	48	LEU
1	B	94	LYS
1	B	130	GLN
1	B	140	LEU
1	B	156	GLU
1	B	158	ILE
1	B	189	GLN
1	B	190	PHE
1	B	269	SER
1	B	274	LEU
1	B	345	VAL
1	B	383	ASP
1	B	386	ILE
1	B	393	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	217	ASN
1	A	219	HIS
1	B	111	HIS
1	B	353	HIS

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 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	361/414 (87%)	0.36	48 (13%) 7 6	6, 30, 79, 105	0
1	B	361/414 (87%)	0.38	46 (12%) 8 6	6, 29, 83, 105	0
All	All	722/828 (87%)	0.37	94 (13%) 7 6	6, 30, 82, 105	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	GLY	6.4
1	B	91	PRO	6.2
1	A	48	LEU	5.6
1	A	178	PRO	5.6
1	B	133	PRO	5.4
1	A	91	PRO	5.3
1	B	339	ALA	5.0
1	A	133	PRO	5.0
1	B	137	GLY	5.0
1	A	192	MET	4.7
1	B	87	PHE	4.6
1	B	194	ASP	4.5
1	A	191	LEU	4.5
1	B	136	THR	4.3
1	A	132	GLY	4.3
1	A	190	PHE	4.2
1	A	179	GLY	4.1
1	B	340	SER	4.1
1	B	131	PRO	4.0
1	B	47	TYR	4.0
1	A	90	ALA	3.9
1	A	70	VAL	3.9
1	A	137	GLY	3.8
1	B	357	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	138	LYS	3.7
1	A	97	LEU	3.6
1	B	135	ASP	3.5
1	B	180	PRO	3.4
1	B	49	LYS	3.3
1	B	73	LEU	3.3
1	B	134	GLU	3.3
1	A	193	SER	3.3
1	A	359	GLU	3.3
1	A	392	ALA	3.3
1	B	90	ALA	3.3
1	A	96	PRO	3.2
1	B	159	HIS	3.2
1	A	393	ARG	3.2
1	A	339	ALA	3.2
1	B	179	GLY	3.2
1	A	47	TYR	3.2
1	B	4	LYS	3.1
1	A	5	GLY	3.1
1	A	93	ASP	3.1
1	A	95	LYS	3.1
1	B	384	ASP	3.0
1	A	49	LYS	3.0
1	B	358	GLU	3.0
1	B	359	GLU	2.9
1	A	331	ARG	2.9
1	A	357	LYS	2.9
1	A	180	PRO	2.9
1	A	51	ARG	2.9
1	B	69	ASP	2.8
1	B	71	LEU	2.8
1	B	95	LYS	2.8
1	B	93	ASP	2.7
1	A	94	LYS	2.7
1	B	130	GLN	2.7
1	B	394	GLN	2.7
1	A	68	LEU	2.7
1	A	383	ASP	2.7
1	A	386	ILE	2.6
1	B	190	PHE	2.6
1	B	48	LEU	2.6
1	A	181	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	177	ARG	2.5
1	A	134	GLU	2.5
1	A	280	ASN	2.5
1	B	51	ARG	2.5
1	B	341	SER	2.4
1	A	66	GLU	2.4
1	A	358	GLU	2.4
1	B	66	GLU	2.4
1	A	387	VAL	2.4
1	A	73	LEU	2.4
1	B	386	ILE	2.4
1	A	162	ASN	2.4
1	A	46	GLU	2.3
1	B	192	MET	2.3
1	A	50	GLU	2.3
1	B	178	PRO	2.2
1	A	71	LEU	2.2
1	A	136	THR	2.2
1	A	394	GLN	2.2
1	A	340	SER	2.2
1	B	387	VAL	2.2
1	A	384	ASP	2.2
1	A	307	ARG	2.1
1	B	161	ARG	2.1
1	B	94	LYS	2.1
1	B	5	GLY	2.1
1	B	157	LYS	2.1
1	B	331	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.