



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:02 am GMT

PDB ID : 1G4M  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

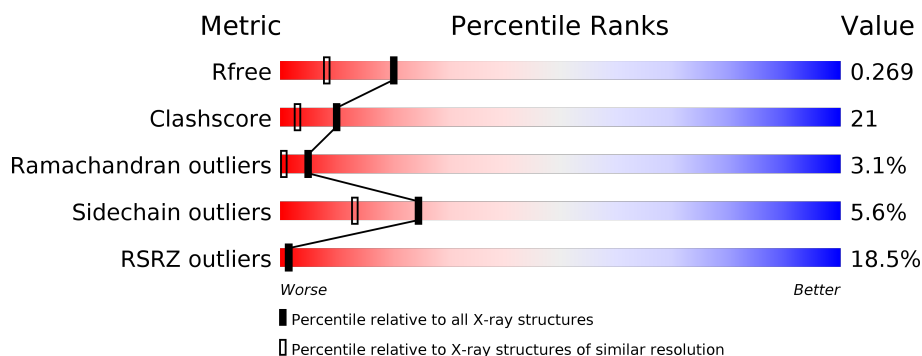
# 1 Overall quality at a glance

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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>11%</div> <div>68%</div> <div>19%</div> <div>•</div> <div>9%</div> </div>
1	B	393	<div> <div>22%</div> <div>59%</div> <div>26%</div> <div>6%</div> <div>•</div> <div>9%</div> </div>

## 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			

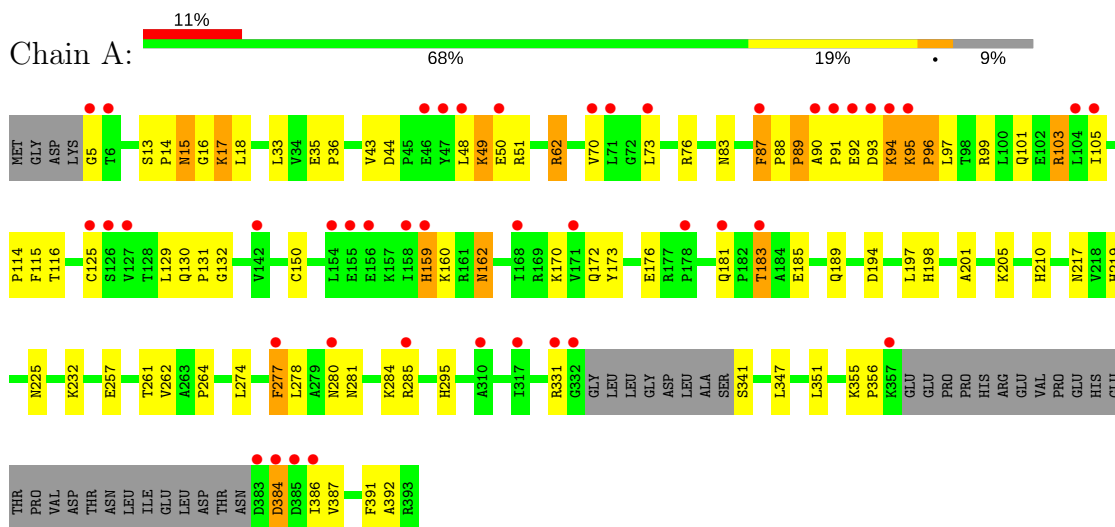
- Molecule 2 is water.

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

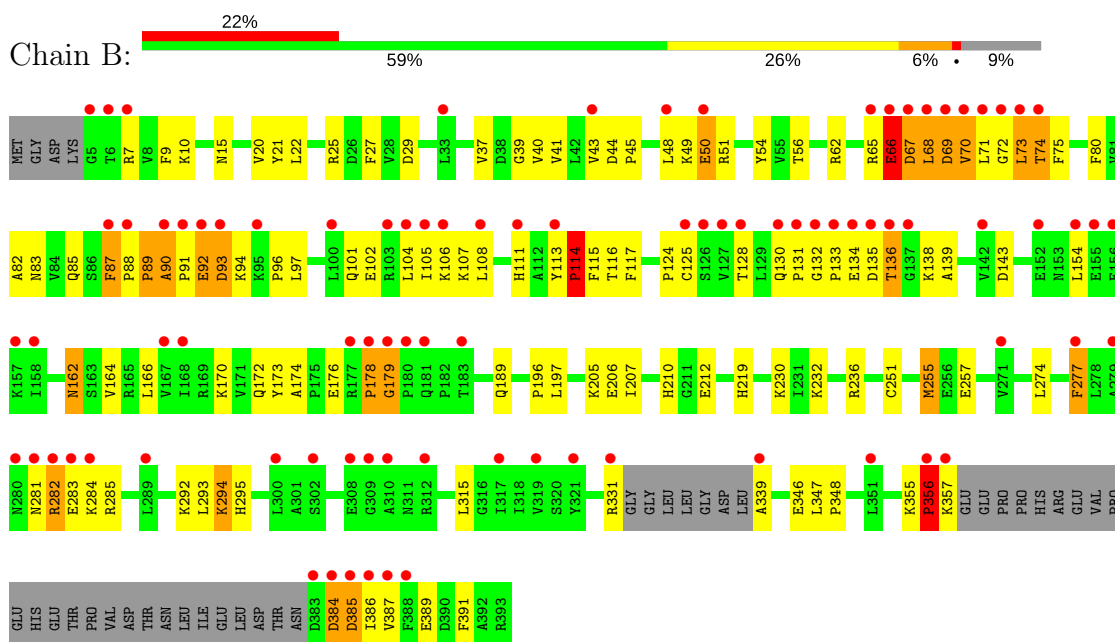
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	62.40Å 73.72Å 115.76Å 90.00° 98.73° 90.00°	Depositor
Resolution (Å)	34.54 – 1.90 34.53 – 1.90	Depositor EDS
% Data completeness (in resolution range)	86.3 (34.54-1.90) 86.4 (34.53-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 1.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.235 , 0.269 0.235 , 0.269	Depositor DCC
$R_{free}$ test set	5397 reflections (7.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.57	0/2880	0.78	1/3902 (0.0%)
1	B	0.52	0/2895	0.75	0/3921
All	All	0.55	0/5775	0.76	1/7823 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	LYS	CD-CE-NZ	-5.45	99.17	111.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	93	0
1	B	2836	0	2879	141	0
2	A	155	0	0	11	0
2	B	114	0	0	24	0
All	All	5926	0	5735	234	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 21.

All (234) 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
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: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:15:ASN:C	1:A:15:ASN:HD22	1.78	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:H	1:B:294:LYS:HE3	1.40	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:114:PRO:HD2	2:B:493:HOH:O	1.86	0.73
1:B:27:PHE:CE2	1:B:37:VAL:HA	2.23	0.73
1:B:236:ARG:HH11	1:B:236:ARG:HG2	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:197:LEU:C	1:A:197:LEU:HD23	2.18	0.64
1:B:347:LEU:N	1:B:347:LEU:HD12	2.13	0.64
1:B:56:THR:HG22	1:B:83:ASN:CB	2.21	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:B:88:PRO:O	1:B:89:PRO:O	2.16	0.63
1:B:90:ALA:HB3	1:B:91:PRO:C	2.19	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:185:GLU:HG3	1:A:347:LEU:HD23	1.82	0.61
1:B:385:ASP:CG	1:B:386:ILE:H	2.03	0.61
1:A:130:GLN:OE1	1:A:130:GLN:HA	2.00	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:HG2	1:B:65:ARG:HH11	1.67	0.60
1:B:69:ASP:O	1:B:73:LEU:N	2.35	0.59
1:A:90:ALA:C	1:A:92:GLU:H	2.05	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:A:43:VAL:CG1	1:A:44:ASP:N	2.65	0.58
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:NH1	1:B:236:ARG:HG2	2.18	0.58
1:A:5:GLY:HA2	1:A:384:ASP:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASN:O	1:B:282:ARG:O	2.21	0.58
1:B:66:GLU:O	1:B:68:LEU:N	2.36	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:A:15:ASN:C	1:A:15:ASN:ND2	2.50	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:189:GLN:NE2	2:B:411:HOH:O	2.38	0.56
1:A:185:GLU:CG	1:A:347:LEU:HD23	2.36	0.56
1:A:87:PHE:HD2	1:A:88:PRO:HA	1.71	0.56
1:A:95:LYS:NZ	2:A:493:HOH:O	2.34	0.56
1:B:294:LYS:N	1:B:294:LYS:HE3	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:251:CYS:HB2	2:B:481:HOH:O	2.07	0.55
1:A:95:LYS:HZ1	1:A:115:PHE:HA	1.72	0.54
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: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:66:GLU:O	1:B:68:LEU:HD23	2.07	0.53
1:B:65:ARG:NH1	1:B:68:LEU:HD11	2.22	0.53
1:B:7:ARG:HD2	1:B:389:GLU:CD	2.27	0.53
1:B:117:PHE:N	2:B:458:HOH:O	2.06	0.53
1:B:197:LEU:C	1:B:197:LEU:HD23	2.30	0.53
1:A:103:ARG:HB3	1:A:103:ARG:NH1	2.24	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:103:ARG:HB3	1:A:103:ARG:HH11	1.74	0.52
1:A:43:VAL:CG1	1:A:44:ASP:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:NE	2:B:430:HOH:O	2.39	0.51
1:A:89:PRO:O	1:A:90:ALA:HB3	2.11	0.51
1:B:73:LEU:O	1:B:74:THR:C	2.48	0.51
1:A:170:LYS:NZ	2:A:497:HOH:O	2.43	0.51
1:B:54:TYR:CE2	1:B:154:LEU:HD11	2.46	0.51
1:B:178:PRO:O	1:B:179:GLY:O	2.29	0.51
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:87:PHE:HA	1:B:88:PRO:C	2.32	0.50
1:A:87:PHE:CD2	1:A:88:PRO:HA	2.47	0.49
1:B:294:LYS:N	1:B:294:LYS:CE	2.74	0.49
1:B:7:ARG:HA	1:B:387:VAL:O	2.12	0.49
1:A:355:LYS:CG	1:A:356:PRO:HD2	2.43	0.49
1:A:93:ASP:O	1:A:95:LYS:HG2	2.12	0.49
1:B:68:LEU:HD23	1:B:68:LEU:H	1.77	0.49
1:B:69:ASP:O	1:B:70:VAL:C	2.50	0.49
1:B:91:PRO:C	1:B:93:ASP:H	2.15	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:90:ALA:CB	1:B:91:PRO:C	2.81	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: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:HG13	1:B:41:VAL:O	2.13	0.48
1:B:62:ARG:NH1	1:B:143:ASP:OD2	2.46	0.48
1:A:284:LYS:C	1:A:285:ARG:HE	2.16	0.48
1:B:22:LEU:HD23	1:B:39:GLY:HA3	1.95	0.47
1:A:94:LYS:C	1:A:96:PRO:HD3	2.33	0.47
1:A:50:GLU:N	1:A:50:GLU:OE1	2.47	0.47
1:A:93:ASP:O	1:A:94:LYS:C	2.53	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:A:87:PHE:HD2	1:A:88:PRO:N	2.11	0.47
1:B:131:PRO:HD3	1:B:139:ALA:HA	1.95	0.47
1:A:210:HIS:HE1	2:A:422:HOH:O	1.96	0.47
1:B:232:LYS:HD3	1:B:255:MET:HE1	1.96	0.47
1:B:210:HIS:HE1	2:B:429:HOH:O	1.98	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:OD2	1:B:170:LYS:HE2	2.16	0.46
1:B:66:GLU:C	1:B:68:LEU:HD23	2.36	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:138:LYS:HD2	2:B:474:HOH:O	2.16	0.45
1:B:66:GLU:HG3	2:B:461:HOH:O	2.16	0.45
1:B:331:ARG:HD2	1:B:339:ALA:HB3	1.98	0.45
1:A:181:GLN:NE2	1:A:181:GLN:HA	2.32	0.45
1:B:15:ASN:HD21	1:B:162:ASN:HD22	1.64	0.45
1:A:101:GLN:O	1:A:105:ILE:HG13	2.18	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:356:PRO:O	1:B:357:LYS:C	2.55	0.44
1:B:102:GLU:O	1:B:106:LYS:HG3	2.17	0.44
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:95:LYS:HE3	1:A:114:PRO:HG2	2.00	0.43
1:B:166:LEU:N	1:B:166:LEU:HD12	2.34	0.43
1:A:331:ARG:HH22	1:A:341:SER:HA	1.83	0.43
1:B:232:LYS:HG2	1:B:257:GLU:HG2	2.01	0.43
1:B:355:LYS:O	1:B:356:PRO:C	2.57	0.43
1:B:72:GLY:O	1:B:74:THR:N	2.52	0.43
1:A:284:LYS:O	1:A:285:ARG:NE	2.51	0.43
1:A:391:PHE:O	1:A:392:ALA:C	2.56	0.43
1:A:76:ARG:CB	1:A:76:ARG:HH11	2.31	0.43
1:B:236:ARG:CG	1:B:236:ARG:NH1	2.82	0.43
1:A:13:SER:HB2	1:A:14:PRO:CD	2.49	0.42
1:A:219:HIS:HD2	2:A:424:HOH:O	2.01	0.42
1:A:95:LYS:NZ	1:A:116:THR:N	2.67	0.42
1:A:62:ARG:HG2	2:A:445:HOH:O	2.19	0.42
1:B:67:ASP:C	1:B:69:ASP:H	2.21	0.42
1:B:40:VAL:HG21	1:B:104:LEU:CB	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:LEU:N	2:B:463:HOH:O	2.53	0.42
1:B:70:VAL:CG1	1:B:71:LEU:HD22	2.46	0.42
1:A:392:ALA:HA	2:A:427:HOH:O	2.19	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:HD2	1:A:277:PHE:N	2.18	0.41
1:B:347:LEU:HA	1:B:348:PRO:HD3	1.86	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:87:PHE:CD2	1:B:87:PHE:C	2.94	0.41
1:B:72:GLY:O	1:B:73:LEU:C	2.58	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: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:HE21	1:A:181:GLN:HA	1.85	0.41
1:A:210:HIS:CD2	2:A:472:HOH:O	2.74	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:B:205:LYS:NZ	1:B:212:GLU:OE1	2.44	0.41
1:B:232:LYS:HD3	1:B:255:MET:CE	2.51	0.41
1:B:346:GLU:C	1:B:347:LEU:HD12	2.40	0.41
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 [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	350/393 (89%)	324 (93%)	21 (6%)	5 (1%)	13	4
1	B	351/393 (89%)	312 (89%)	22 (6%)	17 (5%)	2	0
All	All	701/786 (89%)	636 (91%)	43 (6%)	22 (3%)	5	1

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%)	295 (94%)	18 (6%)	23	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	317/350 (91%)	300 (95%)	17 (5%)	26	14
All	All	630/700 (90%)	595 (94%)	35 (6%)	25	13

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

Mol	Chain	Res	Type
1	A	15	ASN
1	A	17	LYS
1	A	33	LEU
1	A	62	ARG
1	A	83	ASN
1	A	87	PHE
1	A	103	ARG
1	A	129	LEU
1	A	131	PRO
1	A	159	HIS
1	A	162	ASN
1	A	183	THR
1	A	194	ASP
1	A	274	LEU
1	A	277	PHE
1	A	280	ASN
1	A	351	LEU
1	A	384	ASP
1	B	50	GLU
1	B	66	GLU
1	B	73	LEU
1	B	87	PHE
1	B	93	ASP
1	B	96	PRO
1	B	97	LEU
1	B	114	PRO
1	B	162	ASN
1	B	196	PRO
1	B	230	LYS
1	B	255	MET
1	B	274	LEU
1	B	277	PHE
1	B	294	LYS
1	B	356	PRO
1	B	384	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	181	GLN
1	A	210	HIS
1	B	130	GLN
1	B	162	ASN
1	B	210	HIS
1	B	245	ASN
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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	356/393 (90%)	0.73	44 (12%) 4 5	25, 47, 87, 106	17 (4%)
1	B	357/393 (90%)	1.40	88 (24%) 1 1	30, 52, 98, 117	16 (4%)
All	All	713/786 (90%)	1.07	132 (18%) 1 1	25, 49, 93, 117	33 (4%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	LEU	14.1
1	B	71	LEU	11.4
1	B	136	THR	11.2
1	B	137	GLY	10.6
1	A	383	ASP	9.5
1	B	67	ASP	8.9
1	A	384	ASP	8.6
1	B	91	PRO	8.5
1	B	72	GLY	8.5
1	B	70	VAL	8.2
1	B	339	ALA	7.9
1	B	280	ASN	7.5
1	B	134	GLU	7.3
1	B	133	PRO	6.9
1	B	282	ARG	6.7
1	B	387	VAL	6.7
1	A	5	GLY	6.6
1	B	384	ASP	6.5
1	A	92	GLU	6.4
1	B	385	ASP	6.2
1	B	69	ASP	6.1
1	A	154	LEU	6.0
1	B	65	ARG	6.0
1	B	180	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	331	ARG	5.8
1	B	132	GLY	5.7
1	A	71	LEU	5.7
1	A	386	ILE	5.5
1	B	90	ALA	5.4
1	A	332	GLY	5.2
1	B	6	THR	5.2
1	B	357	LYS	5.2
1	B	178	PRO	5.1
1	A	385	ASP	5.0
1	B	154	LEU	5.0
1	B	5	GLY	4.7
1	A	158	ILE	4.7
1	B	177	ARG	4.6
1	A	357	LYS	4.6
1	B	100	LEU	4.5
1	B	309	GLY	4.4
1	A	178	PRO	4.4
1	B	279	ALA	4.3
1	B	50	GLU	4.3
1	B	383	ASP	4.3
1	B	281	ASN	4.2
1	B	73	LEU	4.2
1	B	158	ILE	4.2
1	A	94	LYS	4.1
1	B	179	GLY	4.0
1	B	104	LEU	4.0
1	A	93	ASP	3.9
1	B	317	ILE	3.9
1	B	310	ALA	3.8
1	A	73	LEU	3.8
1	B	92	GLU	3.8
1	A	47	TYR	3.6
1	B	135	ASP	3.5
1	B	66	GLU	3.5
1	A	183	THR	3.5
1	A	285	ARG	3.5
1	B	283	GLU	3.4
1	A	48	LEU	3.4
1	B	106	LYS	3.3
1	A	277	PHE	3.2
1	B	142	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	3.1
1	A	46	GLU	3.1
1	A	142	VAL	3.1
1	B	386	ILE	3.1
1	B	48	LEU	3.0
1	A	70	VAL	3.0
1	A	90	ALA	3.0
1	A	280	ASN	3.0
1	A	159	HIS	2.9
1	B	181	GLN	2.9
1	B	131	PRO	2.9
1	B	319	VAL	2.8
1	B	7	ARG	2.8
1	B	168	ILE	2.8
1	A	168	ILE	2.8
1	A	95	LYS	2.8
1	B	284	LYS	2.8
1	B	157	LYS	2.7
1	B	105	ILE	2.7
1	A	87	PHE	2.7
1	B	321	TYR	2.7
1	B	152	GLU	2.7
1	A	6	THR	2.7
1	B	128	THR	2.7
1	B	88	PRO	2.7
1	B	183	THR	2.6
1	A	331	ARG	2.6
1	B	125	CYS	2.6
1	B	127	VAL	2.6
1	A	181	GLN	2.6
1	A	155	GLU	2.6
1	A	317	ILE	2.5
1	B	87	PHE	2.5
1	B	113	TYR	2.5
1	B	155	GLU	2.5
1	B	156	GLU	2.5
1	B	108	LEU	2.5
1	B	167	VAL	2.5
1	A	91	PRO	2.4
1	B	103	ARG	2.4
1	A	104	LEU	2.4
1	A	127	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	356	PRO	2.3
1	B	126	SER	2.3
1	B	130	GLN	2.2
1	A	156	GLU	2.2
1	A	105	ILE	2.2
1	B	111	HIS	2.2
1	B	95	LYS	2.2
1	B	300	LEU	2.2
1	B	277	PHE	2.2
1	A	171	VAL	2.2
1	A	126	SER	2.2
1	A	50	GLU	2.2
1	B	271	VAL	2.2
1	B	302	SER	2.1
1	B	93	ASP	2.1
1	B	289	LEU	2.1
1	B	312	ARG	2.1
1	B	308	GLU	2.1
1	B	74	THR	2.1
1	B	388	PHE	2.1
1	A	310	ALA	2.1
1	A	125	CYS	2.0
1	B	43	VAL	2.0
1	B	351	LEU	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.