



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:05 AM UTC

PDB ID : 1JSY / pdb_00001jsy
Title : Crystal structure of bovine arrestin-2
Authors : Milano, S.K.; Pace, H.C.; Kim, Y.M.; Brenner, C.; Benovic, J.L.
Deposited on : 2001-08-19
Resolution : 2.90 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

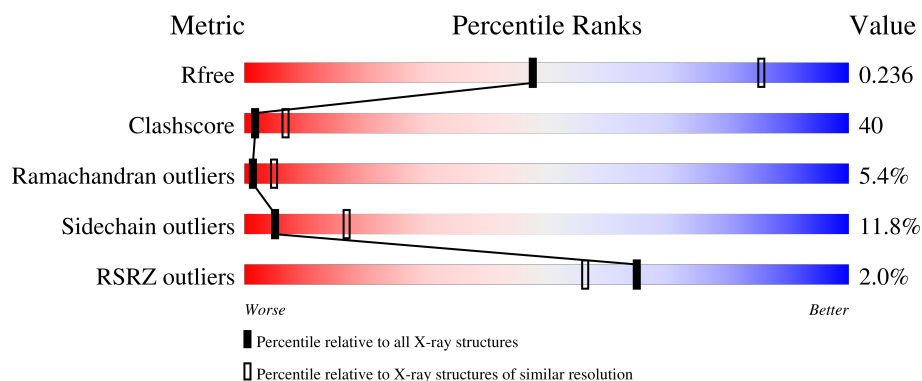
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	418	2% 36% 39% 9% 14%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2905 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 Bovine arrestin-2 (full length).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2829	1809	485	524	11			

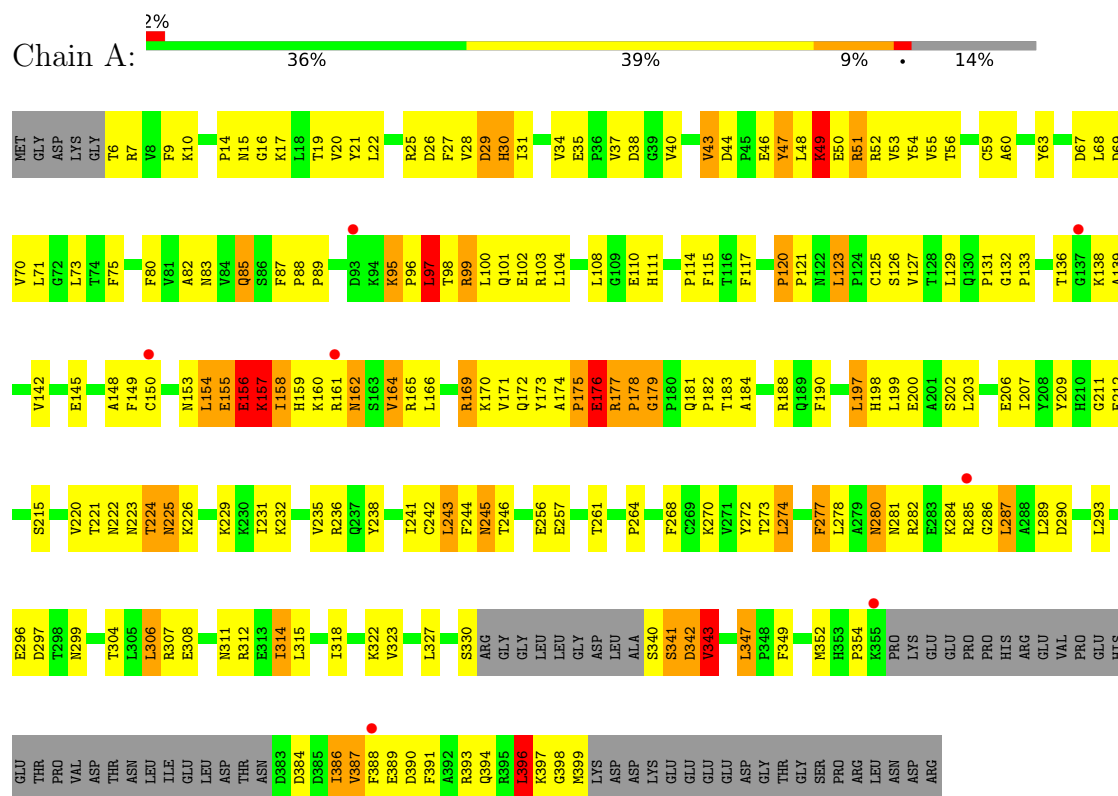
- Molecule 2 is water.

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

3 Residue-property plots

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: Bovine arrestin-2 (full length)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	78.95Å 78.95Å 158.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.00 – 2.90 19.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.00-2.90) 98.6 (19.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	7.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.79Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.230 , 0.238 0.230 , 0.236	Depositor DCC
R_{free} test set	1347 reflections (9.11%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2905	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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	0.64	2/2887 (0.1%)	1.11	19/3912 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	MET	SD-CE	7.01	1.97	1.79
1	A	157	LYS	N-CA	-5.28	1.39	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLU	N-CA-C	10.92	123.19	111.28
1	A	286	GLY	N-CA-C	-8.42	104.46	114.48
1	A	95	LYS	CA-C-N	8.07	127.63	119.24
1	A	95	LYS	C-N-CA	8.07	127.63	119.24
1	A	120	PRO	CA-C-N	7.93	128.67	119.47
1	A	120	PRO	C-N-CA	7.93	128.67	119.47
1	A	156	GLU	CA-C-N	-7.22	111.25	121.72
1	A	156	GLU	C-N-CA	-7.22	111.25	121.72
1	A	30	HIS	N-CA-C	-6.26	103.64	108.78
1	A	30	HIS	CA-C-O	6.06	121.45	117.94
1	A	307	ARG	N-CA-C	6.02	118.25	108.26
1	A	157	LYS	CB-CG-CD	-5.78	98.00	111.30
1	A	158	ILE	N-CA-C	-5.78	102.13	109.58
1	A	43	VAL	N-CA-C	5.73	118.08	109.20
1	A	155	GLU	CA-C-O	-5.59	114.62	120.55
1	A	30	HIS	CB-CA-C	-5.55	109.08	117.07
1	A	175	PRO	N-CA-C	5.50	123.81	112.47
1	A	343	VAL	N-CA-C	-5.10	101.14	108.53
1	A	223	ASN	N-CA-C	-5.09	107.07	113.28

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	2829	0	2866	230	0
2	A	76	0	0	8	0
All	All	2905	0	2866	230	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 40.

All (230) 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:285:ARG:HH22	1:A:293:LEU:HD12	1.16	1.10
1:A:285:ARG:NH2	1:A:293:LEU:HD12	1.66	1.09
1:A:29:ASP:HB2	1:A:34:VAL:HG13	1.42	1.00
1:A:129:LEU:HD13	1:A:241:ILE:HD11	1.45	0.98
1:A:154:LEU:HD22	1:A:154:LEU:H	1.27	0.98
1:A:98:THR:HG22	1:A:101:GLN:HG3	1.44	0.97
1:A:155:GLU:O	1:A:156:GLU:O	1.82	0.96
1:A:177:ARG:HB3	1:A:178:PRO:HD2	1.47	0.96
1:A:280:ASN:H	1:A:280:ASN:HD22	1.15	0.94
1:A:224:THR:CG2	1:A:226:LYS:H	1.80	0.94
1:A:224:THR:HG23	1:A:226:LYS:H	1.35	0.91
1:A:153:ASN:HD22	1:A:155:GLU:HG2	1.39	0.88
1:A:177:ARG:HB3	1:A:178:PRO:CD	2.04	0.87
1:A:285:ARG:NH2	1:A:293:LEU:CD1	2.38	0.86
1:A:153:ASN:ND2	1:A:155:GLU:HG2	1.91	0.85
1:A:87:PHE:HB3	1:A:88:PRO:HD3	1.59	0.83
1:A:96:PRO:O	1:A:97:LEU:HB2	1.82	0.79
1:A:222:ASN:HD21	1:A:224:THR:HB	1.47	0.79
1:A:162:ASN:C	1:A:162:ASN:HD22	1.92	0.78
1:A:63:TYR:HE1	1:A:138:LYS:HG2	1.49	0.78
1:A:340:SER:O	1:A:341:SER:O	2.03	0.77
1:A:120:PRO:HG2	1:A:123:LEU:HD22	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:ND2	1:A:224:THR:HB	2.00	0.76
1:A:63:TYR:CE1	1:A:138:LYS:HG2	2.22	0.75
1:A:176:GLU:HA	1:A:207:ILE:HD12	1.68	0.75
1:A:280:ASN:H	1:A:280:ASN:ND2	1.85	0.74
1:A:104:LEU:O	1:A:108:LEU:HD23	1.87	0.74
1:A:172:GLN:HG2	1:A:352:MET:HE1	1.69	0.74
1:A:98:THR:HG22	1:A:101:GLN:CG	2.16	0.73
1:A:30:HIS:C	1:A:31:ILE:HD12	2.13	0.72
1:A:178:PRO:HG2	1:A:179:GLY:H	1.54	0.72
1:A:314:ILE:HG23	2:A:445:HOH:O	1.90	0.71
1:A:285:ARG:CZ	1:A:293:LEU:HD12	2.20	0.70
1:A:48:LEU:HB2	1:A:51:ARG:HB3	1.75	0.68
1:A:59:CYS:HB3	1:A:80:PHE:HB3	1.74	0.68
1:A:27:PHE:CE2	1:A:37:VAL:HA	2.29	0.67
1:A:38:ASP:OD2	1:A:98:THR:HG21	1.95	0.67
1:A:17:LYS:NZ	1:A:47:TYR:HB2	2.11	0.66
1:A:98:THR:CG2	1:A:101:GLN:HG3	2.22	0.66
1:A:197:LEU:HD13	1:A:343:VAL:HG21	1.77	0.66
1:A:182:PRO:HA	2:A:444:HOH:O	1.96	0.65
1:A:285:ARG:CZ	1:A:293:LEU:CD1	2.74	0.65
1:A:280:ASN:ND2	1:A:280:ASN:N	2.43	0.64
1:A:245:ASN:C	1:A:245:ASN:HD22	2.03	0.64
1:A:229:LYS:CD	1:A:330:SER:HB2	2.28	0.64
1:A:87:PHE:O	1:A:89:PRO:HD3	1.98	0.64
1:A:44:ASP:O	1:A:48:LEU:HD23	1.98	0.64
1:A:131:PRO:HG2	1:A:138:LYS:C	2.22	0.63
1:A:235:VAL:HG23	1:A:274:LEU:HD12	1.81	0.62
1:A:226:LYS:O	1:A:264:PRO:HG3	2.01	0.61
1:A:49:LYS:HA	1:A:49:LYS:HZ3	1.64	0.61
1:A:17:LYS:HZ2	1:A:47:TYR:HB2	1.65	0.61
1:A:220:VAL:HB	1:A:268:PHE:HB3	1.82	0.61
1:A:40:VAL:HG12	1:A:114:PRO:HA	1.83	0.61
1:A:17:LYS:HE3	1:A:47:TYR:CD1	2.36	0.60
1:A:155:GLU:O	1:A:156:GLU:C	2.42	0.60
1:A:178:PRO:O	1:A:179:GLY:O	2.20	0.60
1:A:242:CYS:HA	1:A:246:THR:HG22	1.84	0.60
1:A:224:THR:HG22	1:A:226:LYS:H	1.65	0.60
1:A:15:ASN:O	1:A:17:LYS:N	2.35	0.59
1:A:43:VAL:HG12	1:A:44:ASP:N	2.17	0.59
1:A:56:THR:HA	1:A:82:ALA:O	2.02	0.59
1:A:154:LEU:HD22	1:A:154:LEU:N	2.08	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:HB	1:A:87:PHE:HB2	1.84	0.58
1:A:25:ARG:HB3	1:A:391:PHE:CE1	2.38	0.58
1:A:188:ARG:HH22	1:A:341:SER:CB	2.16	0.58
1:A:222:ASN:HD21	1:A:224:THR:CB	2.17	0.58
1:A:25:ARG:NH1	1:A:391:PHE:O	2.37	0.57
1:A:177:ARG:HB2	2:A:434:HOH:O	2.03	0.57
1:A:87:PHE:O	1:A:89:PRO:CD	2.53	0.57
1:A:188:ARG:HH22	1:A:341:SER:HB2	1.70	0.56
1:A:280:ASN:HD22	1:A:280:ASN:N	1.91	0.56
1:A:245:ASN:C	1:A:245:ASN:ND2	2.60	0.56
1:A:6:THR:O	1:A:386:ILE:O	2.24	0.56
1:A:162:ASN:C	1:A:162:ASN:ND2	2.63	0.56
1:A:224:THR:HG23	1:A:225:ASN:N	2.21	0.56
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.70	0.56
1:A:53:VAL:HB	1:A:87:PHE:CB	2.37	0.55
1:A:273:THR:C	1:A:274:LEU:HD23	2.32	0.55
1:A:28:VAL:O	1:A:35:GLU:HG3	2.06	0.55
1:A:49:LYS:HA	1:A:49:LYS:NZ	2.21	0.55
1:A:85:GLN:OE1	1:A:88:PRO:HB2	2.07	0.55
1:A:15:ASN:ND2	1:A:17:LYS:HB2	2.21	0.55
1:A:125:CYS:HB3	1:A:170:LYS:O	2.06	0.55
1:A:306:LEU:HD23	1:A:306:LEU:N	2.22	0.55
1:A:149:PHE:CD2	1:A:158:ILE:HG12	2.42	0.54
1:A:277:PHE:HB3	1:A:280:ASN:ND2	2.22	0.54
1:A:311:ASN:C	1:A:311:ASN:HD22	2.15	0.54
1:A:56:THR:HG22	1:A:83:ASN:HA	1.90	0.54
1:A:211:GLY:HA2	1:A:277:PHE:CE2	2.43	0.54
1:A:60:ALA:HB3	1:A:68:LEU:HD21	1.90	0.53
1:A:132:GLY:HA2	1:A:285:ARG:CB	2.38	0.53
1:A:171:VAL:HA	2:A:449:HOH:O	2.09	0.53
1:A:98:THR:HG23	1:A:100:LEU:N	2.24	0.53
1:A:131:PRO:HD3	1:A:139:ALA:HA	1.91	0.52
1:A:211:GLY:HA2	1:A:277:PHE:CZ	2.43	0.52
1:A:34:VAL:O	1:A:35:GLU:C	2.52	0.52
1:A:231:ILE:HG12	1:A:327:LEU:HD23	1.91	0.52
1:A:178:PRO:HG2	1:A:179:GLY:N	2.24	0.52
1:A:281:ASN:ND2	1:A:284:LYS:NZ	2.57	0.52
1:A:145:GLU:HG3	1:A:165:ARG:HE	1.74	0.52
1:A:224:THR:CG2	1:A:225:ASN:N	2.73	0.52
1:A:154:LEU:H	1:A:154:LEU:CD2	2.06	0.51
1:A:225:ASN:HD22	1:A:225:ASN:H	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HG23	1:A:164:VAL:HG21	1.91	0.51
1:A:229:LYS:HD2	1:A:330:SER:HB2	1.91	0.51
1:A:296:GLU:OE1	1:A:394:GLN:CD	2.53	0.51
1:A:14:PRO:HG2	1:A:160:LYS:O	2.11	0.51
1:A:224:THR:CG2	1:A:226:LYS:N	2.63	0.51
1:A:136:THR:HG22	2:A:466:HOH:O	2.12	0.50
1:A:343:VAL:HG13	2:A:437:HOH:O	2.10	0.50
1:A:235:VAL:HG22	1:A:323:VAL:HG22	1.94	0.50
1:A:174:ALA:HB2	1:A:352:MET:SD	2.51	0.50
1:A:287:LEU:HD12	1:A:287:LEU:O	2.11	0.50
1:A:297:ASP:OD2	1:A:393:ARG:NH1	2.45	0.50
1:A:278:LEU:HD22	1:A:289:LEU:HD22	1.93	0.50
1:A:98:THR:HG23	1:A:99:ARG:N	2.26	0.49
1:A:232:LYS:NZ	1:A:232:LYS:HB3	2.26	0.49
1:A:129:LEU:O	1:A:131:PRO:HD3	2.12	0.49
1:A:311:ASN:HD22	1:A:312:ARG:N	2.10	0.49
1:A:284:LYS:O	1:A:285:ARG:HD3	2.13	0.49
1:A:340:SER:O	1:A:341:SER:C	2.55	0.49
1:A:15:ASN:HD22	1:A:17:LYS:CG	2.26	0.49
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.26	0.49
1:A:103:ARG:NH2	1:A:384:ASP:CB	2.76	0.49
1:A:175:PRO:O	1:A:176:GLU:CD	2.56	0.49
1:A:327:LEU:O	1:A:342:ASP:HB3	2.13	0.49
1:A:287:LEU:HD12	1:A:287:LEU:C	2.38	0.49
1:A:56:THR:HG22	1:A:83:ASN:CG	2.39	0.48
1:A:323:VAL:HG23	1:A:349:PHE:CE1	2.49	0.48
1:A:236:ARG:HG3	1:A:236:ARG:HH11	1.79	0.48
1:A:282:ARG:NH1	1:A:396:LEU:HD11	2.28	0.48
1:A:157:LYS:O	1:A:159:HIS:CD2	2.67	0.48
1:A:48:LEU:HG	1:A:48:LEU:O	2.13	0.48
1:A:54:TYR:O	1:A:148:ALA:HA	2.14	0.47
1:A:173:TYR:C	1:A:173:TYR:CD2	2.92	0.47
1:A:225:ASN:N	1:A:225:ASN:HD22	2.10	0.47
1:A:396:LEU:HB3	1:A:397:LYS:H	1.50	0.47
1:A:285:ARG:CZ	1:A:293:LEU:HD11	2.45	0.47
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.77	0.47
1:A:98:THR:HG23	1:A:101:GLN:H	1.80	0.47
1:A:131:PRO:CD	1:A:139:ALA:HA	2.45	0.47
1:A:129:LEU:C	1:A:129:LEU:HD23	2.40	0.46
1:A:290:ASP:OD1	1:A:299:ASN:N	2.39	0.46
1:A:9:PHE:HA	1:A:389:GLU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:CD2	1:A:289:LEU:HD22	2.46	0.46
1:A:87:PHE:O	1:A:89:PRO:N	2.49	0.46
1:A:190:PHE:CG	1:A:226:LYS:HE3	2.51	0.46
1:A:198:HIS:HB3	1:A:221:THR:HB	1.97	0.46
1:A:225:ASN:C	1:A:225:ASN:ND2	2.74	0.46
1:A:48:LEU:HD23	1:A:48:LEU:H	1.81	0.46
1:A:87:PHE:HB3	1:A:88:PRO:CD	2.39	0.45
1:A:178:PRO:CG	1:A:179:GLY:H	2.24	0.45
1:A:155:GLU:C	1:A:156:GLU:O	2.58	0.45
1:A:49:LYS:HB3	1:A:50:GLU:H	1.54	0.45
1:A:241:ILE:N	1:A:241:ILE:HD12	2.32	0.45
1:A:285:ARG:NH1	1:A:293:LEU:CD1	2.79	0.45
1:A:386:ILE:O	1:A:387:VAL:HB	2.16	0.45
1:A:52:ARG:O	1:A:150:CYS:HA	2.17	0.45
1:A:393:ARG:HG2	1:A:393:ARG:NH1	2.31	0.45
1:A:14:PRO:HD2	1:A:161:ARG:O	2.16	0.44
1:A:142:VAL:HG23	1:A:142:VAL:O	2.17	0.44
1:A:34:VAL:CG2	1:A:121:PRO:HA	2.47	0.44
1:A:70:VAL:CG1	2:A:486:HOH:O	2.65	0.44
1:A:99:ARG:C	1:A:101:GLN:N	2.73	0.44
1:A:98:THR:CG2	1:A:101:GLN:H	2.31	0.44
1:A:159:HIS:C	1:A:161:ARG:H	2.26	0.44
1:A:243:LEU:HD12	1:A:243:LEU:HA	1.84	0.44
1:A:287:LEU:C	1:A:287:LEU:CD1	2.91	0.44
1:A:282:ARG:C	1:A:284:LYS:H	2.25	0.44
1:A:43:VAL:HG12	1:A:44:ASP:H	1.82	0.44
1:A:199:LEU:HD13	1:A:327:LEU:HD11	2.00	0.44
1:A:304:THR:HG21	1:A:318:ILE:HG13	1.99	0.44
1:A:342:ASP:OD1	1:A:342:ASP:N	2.41	0.44
1:A:154:LEU:N	1:A:154:LEU:HD13	2.33	0.43
1:A:87:PHE:CB	1:A:88:PRO:HD3	2.38	0.43
1:A:166:LEU:O	1:A:166:LEU:HD12	2.18	0.43
1:A:174:ALA:CB	1:A:352:MET:SD	3.07	0.43
1:A:224:THR:HG22	1:A:226:LYS:N	2.32	0.43
1:A:132:GLY:HA2	1:A:285:ARG:HB3	2.00	0.43
1:A:159:HIS:C	1:A:161:ARG:N	2.76	0.43
1:A:224:THR:HG21	1:A:226:LYS:HB2	2.01	0.43
1:A:44:ASP:O	1:A:48:LEU:CD2	2.67	0.43
1:A:69:ASP:OD1	1:A:69:ASP:O	2.37	0.43
1:A:120:PRO:HA	1:A:121:PRO:HD3	1.66	0.43
1:A:87:PHE:HD1	1:A:88:PRO:HG3	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLN:HB3	1:A:203:LEU:O	2.18	0.43
1:A:80:PHE:HB2	1:A:123:LEU:HD21	2.01	0.42
1:A:115:PHE:CD1	1:A:115:PHE:C	2.96	0.42
1:A:238:TYR:CE1	1:A:322:LYS:HE3	2.54	0.42
1:A:30:HIS:O	1:A:172:GLN:NE2	2.51	0.42
1:A:182:PRO:O	1:A:202:SER:HA	2.19	0.42
1:A:202:SER:HA	1:A:347:LEU:CD2	2.50	0.42
1:A:55:VAL:HG22	1:A:148:ALA:CB	2.49	0.42
1:A:75:PHE:CD2	1:A:244:PHE:HB2	2.54	0.42
1:A:17:LYS:HG3	1:A:47:TYR:CE1	2.54	0.42
1:A:285:ARG:NH1	1:A:293:LEU:HD12	2.33	0.42
1:A:17:LYS:HZ3	1:A:44:ASP:CG	2.26	0.42
1:A:108:LEU:N	1:A:108:LEU:HD22	2.35	0.42
1:A:52:ARG:HD2	1:A:54:TYR:OH	2.20	0.42
1:A:127:VAL:HG12	1:A:142:VAL:HG22	2.01	0.42
1:A:175:PRO:C	1:A:176:GLU:CG	2.93	0.42
1:A:270:LYS:HD3	1:A:272:TYR:CZ	2.55	0.42
1:A:278:LEU:O	1:A:282:ARG:N	2.53	0.42
1:A:6:THR:HG22	1:A:7:ARG:H	1.84	0.42
1:A:241:ILE:O	1:A:246:THR:HA	2.20	0.42
1:A:19:THR:HG22	1:A:21:TYR:CE1	2.55	0.41
1:A:232:LYS:HE2	1:A:257:GLU:HB3	2.02	0.41
1:A:281:ASN:O	1:A:282:ARG:C	2.64	0.41
1:A:284:LYS:HE3	1:A:284:LYS:HB2	1.66	0.41
1:A:9:PHE:N	1:A:22:LEU:O	2.47	0.41
1:A:15:ASN:HD21	1:A:17:LYS:HB2	1.85	0.41
1:A:26:ASP:OD1	1:A:169:ARG:NH2	2.47	0.41
1:A:101:GLN:O	1:A:102:GLU:C	2.62	0.41
1:A:184:ALA:O	1:A:200:GLU:HA	2.20	0.41
1:A:10:LYS:HG2	1:A:388:PHE:HB3	2.02	0.41
1:A:37:VAL:HB	1:A:117:PHE:HB2	2.02	0.41
1:A:315:LEU:HB2	1:A:318:ILE:HD11	2.02	0.41
1:A:55:VAL:HA	1:A:148:ALA:HA	2.03	0.41
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.71	0.41
1:A:98:THR:HG22	1:A:101:GLN:CB	2.50	0.41
1:A:46:GLU:O	1:A:47:TYR:C	2.64	0.41
1:A:153:ASN:ND2	1:A:155:GLU:H	2.19	0.41
1:A:70:VAL:HG11	2:A:486:HOH:O	2.21	0.40
1:A:176:GLU:HG3	1:A:209:TYR:OH	2.22	0.40
1:A:274:LEU:HD23	1:A:274:LEU:N	2.35	0.40
1:A:110:GLU:HG3	1:A:111:HIS:ND1	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HB2	1:A:391:PHE:CE2	2.56	0.40
1:A:209:TYR:O	1:A:212:GLU:HB3	2.22	0.40
1:A:229:LYS:HD3	1:A:330:SER:HB2	2.01	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	352/418 (84%)	285 (81%)	48 (14%)	19 (5%)	1 5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLY
1	A	49	LYS
1	A	156	GLU
1	A	179	GLY
1	A	341	SER
1	A	354	PRO
1	A	308	GLU
1	A	398	GLY
1	A	177	ARG
1	A	178	PRO
1	A	386	ILE
1	A	97	LEU
1	A	126	SER
1	A	133	PRO
1	A	176	GLU
1	A	390	ASP
1	A	396	LEU
1	A	47	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	387	VAL

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	314/372 (84%)	277 (88%)	37 (12%)	5 17

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	49	LYS
1	A	51	ARG
1	A	67	ASP
1	A	71	LEU
1	A	73	LEU
1	A	85	GLN
1	A	95	LYS
1	A	97	LEU
1	A	99	ARG
1	A	123	LEU
1	A	154	LEU
1	A	157	LYS
1	A	162	ASN
1	A	164	VAL
1	A	169	ARG
1	A	176	GLU
1	A	183	THR
1	A	197	LEU
1	A	206	GLU
1	A	215	SER
1	A	224	THR
1	A	225	ASN
1	A	243	LEU
1	A	245	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	GLU
1	A	261	THR
1	A	274	LEU
1	A	277	PHE
1	A	280	ASN
1	A	287	LEU
1	A	306	LEU
1	A	314	ILE
1	A	342	ASP
1	A	343	VAL
1	A	347	LEU
1	A	396	LEU

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	83	ASN
1	A	153	ASN
1	A	159	HIS
1	A	162	ASN
1	A	172	GLN
1	A	181	GLN
1	A	189	GLN
1	A	222	ASN
1	A	225	ASN
1	A	245	ASN
1	A	280	ASN
1	A	281	ASN
1	A	299	ASN
1	A	311	ASN
1	A	394	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	358/418 (85%)	0.03	7 (1%) 65 56	21, 50, 99, 141	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	ASP	3.8
1	A	285	ARG	3.1
1	A	355	LYS	2.6
1	A	137	GLY	2.4
1	A	161	ARG	2.3
1	A	388	PHE	2.2
1	A	150	CYS	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.