Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 02:17 pm GMT

PDB ID	:	2WTR
Title	:	Full length Arrestin2
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Deposited on	:	2009-09-21
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:

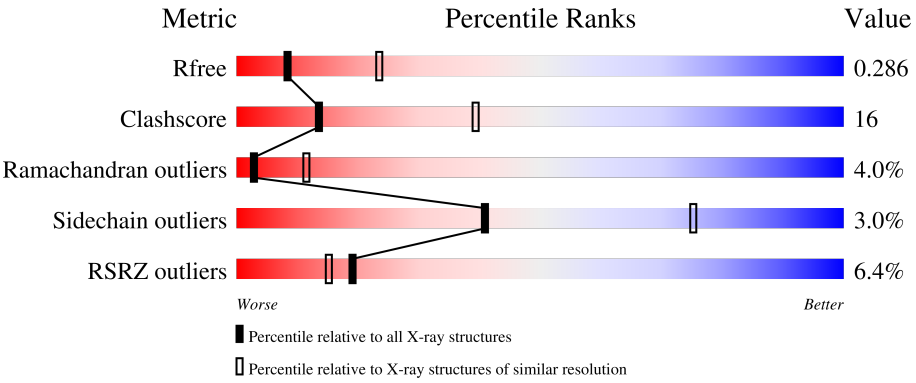
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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% 57% 26% · 15%
2	B	418	9% 57% 27% · 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5826 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	356	Total	C	N	O	S	121	0	0
			2821	1802	487	522	10			

- Molecule 2 is a protein called BETA-ARRESTIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	367	Total	C	N	O	S	204	0	0
			2906	1851	504	540	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	VAL	LEU	conflict	UNP P17870

- Molecule 3 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ba	0	0
			2	2		
3	B	2	Total	Ba	0	0
			2	2		

- Molecule 4 is water.

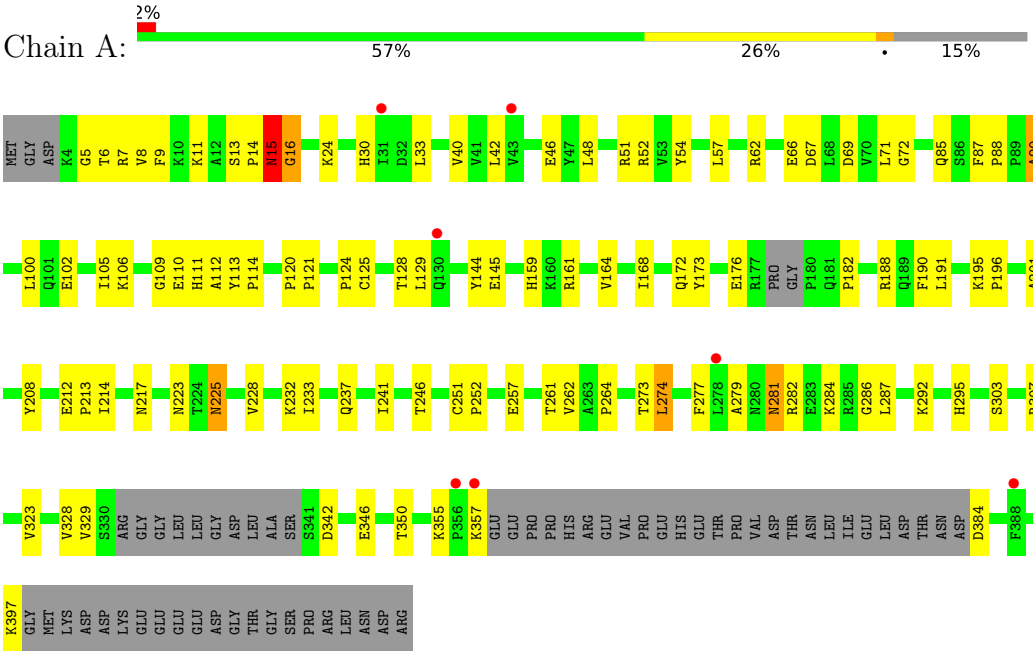
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		
4	B	40	Total	O	0	0
			40	40		

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.

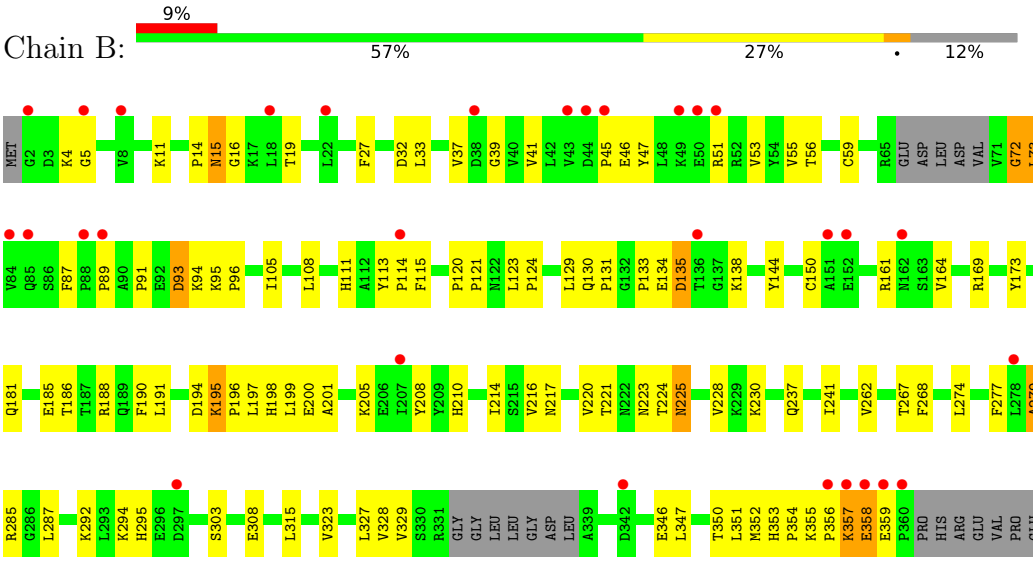
• Molecule 1: BETA-ARRESTIN-1

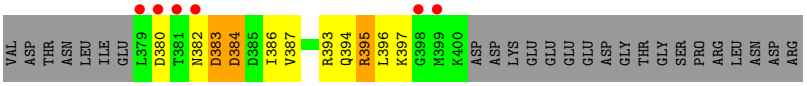
Chain A:



• Molecule 2: BETA-ARRESTIN-1

Chain B:




VAL
ASP
THR
ASN
LEU
ILE
GLU
L379
D380
T381
N382
D383
D384
D385
I386
V387
R393
Q394
R395
L396
K397
G398
M399
K400
ASP
ASP
LYS
GLU
GLU
GLU
GLU
ASP
GLY
THR
GLY
SER
PRO
ARG
LEU
ASN
ASP
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.29Å 72.93Å 115.36Å 90.00° 98.33° 90.00°	Depositor
Resolution (Å)	47.07 – 2.90 47.07 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.07-2.90) 97.1 (47.07-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.248 , 0.295 0.242 , 0.286	Depositor DCC
R_{free} test set	1144 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5826	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: BA

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	0.21	0/2877	0.39	0/3895
2	B	0.21	0/2963	0.39	0/4007
All	All	0.21	0/5840	0.39	0/7902

There are no bond length outliers.

There are no bond angle outliers.

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	2862	87	0
2	B	2906	0	2941	85	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	55	0	0	0	0
4	B	40	0	0	0	0
All	All	5826	0	5803	172	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 16.

All (172) 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)
2:B:394:GLN:HB2	2:B:395:ARG:HB2	1.19	1.11
1:A:92:GLU:H	1:A:93:ASP:HA	1.18	1.00
1:A:91:PRO:HB2	1:A:92:GLU:HA	1.02	0.99
1:A:91:PRO:CB	1:A:92:GLU:HA	1.92	0.99
2:B:282:ARG:HH21	2:B:282:ARG:HG2	1.31	0.96
1:A:91:PRO:HB2	1:A:92:GLU:CA	1.95	0.95
2:B:357:LYS:HA	2:B:358:GLU:C	1.91	0.89
2:B:394:GLN:CB	2:B:395:ARG:HB2	2.08	0.81
2:B:133:PRO:HD3	2:B:285:ARG:HG3	1.62	0.79
1:A:188:ARG:HH21	1:A:196:PRO:HG2	1.49	0.76
1:A:307:ARG:HB2	1:A:310:ALA:HB2	1.72	0.71
1:A:105:ILE:HD11	1:A:114:PRO:HG3	1.73	0.69
1:A:292:LYS:HB2	1:A:295:HIS:CD2	2.28	0.69
2:B:191:LEU:HD13	2:B:329:VAL:HG11	1.74	0.68
1:A:92:GLU:N	1:A:93:ASP:HA	1.92	0.68
2:B:4:LYS:HD2	2:B:387:VAL:HG21	1.77	0.67
2:B:282:ARG:HH21	2:B:282:ARG:CG	2.07	0.66
2:B:188:ARG:HH21	2:B:196:PRO:HG2	1.60	0.66
1:A:277:PHE:HD1	1:A:279:ALA:HB3	1.61	0.65
1:A:92:GLU:HB2	1:A:93:ASP:O	1.97	0.64
1:A:90:ALA:HB1	1:A:91:PRO:HD2	1.79	0.64
2:B:45:PRO:HG3	2:B:111:HIS:CE1	2.33	0.64
2:B:4:LYS:HG2	2:B:5:GLY:H	1.63	0.63
2:B:225:ASN:ND2	2:B:225:ASN:H	1.95	0.63
2:B:73:LEU:HD22	2:B:73:LEU:H	1.64	0.63
2:B:357:LYS:HA	2:B:358:GLU:O	1.99	0.62
1:A:225:ASN:H	1:A:225:ASN:HD22	1.47	0.62
1:A:15:ASN:ND2	1:A:16:GLY:H	1.97	0.62
1:A:92:GLU:HB2	1:A:93:ASP:C	2.20	0.62
2:B:292:LYS:HB2	2:B:295:HIS:CD2	2.35	0.62
2:B:190:PHE:CZ	2:B:196:PRO:HG3	2.34	0.62
2:B:53:VAL:HG22	2:B:150:CYS:HA	1.81	0.61
2:B:15:ASN:HD22	2:B:16:GLY:N	1.98	0.61
2:B:73:LEU:HB2	2:B:74:THR:CA	2.31	0.61
1:A:85:GLN:NE2	1:A:88:PRO:HD2	2.17	0.60
1:A:62:ARG:HH22	1:A:128:THR:HG23	1.65	0.60
1:A:225:ASN:H	1:A:225:ASN:ND2	2.00	0.59
2:B:93:ASP:CG	2:B:94:LYS:HA	2.22	0.59
2:B:73:LEU:HB2	2:B:74:THR:HA	1.84	0.59
2:B:282:ARG:HG2	2:B:282:ARG:NH2	2.10	0.59
1:A:173:TYR:CE1	1:A:355:LYS:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD13	1:A:329:VAL:HG11	1.83	0.58
2:B:225:ASN:H	2:B:225:ASN:HD22	1.50	0.57
1:A:190:PHE:CZ	1:A:196:PRO:HG3	2.39	0.57
2:B:129:LEU:HD13	2:B:241:ILE:HD11	1.87	0.56
1:A:277:PHE:CD1	1:A:279:ALA:HB3	2.39	0.56
1:A:85:GLN:HE21	1:A:88:PRO:HD2	1.72	0.55
2:B:124:PRO:HG3	2:B:315:LEU:HA	1.87	0.54
2:B:33:LEU:H	2:B:33:LEU:HD23	1.72	0.54
2:B:73:LEU:HB2	2:B:74:THR:C	2.28	0.54
2:B:11:LYS:O	2:B:164:VAL:HG21	2.08	0.54
1:A:237:GLN:OE1	1:A:287:LEU:HD12	2.08	0.53
1:A:93:ASP:HB2	1:A:94:LYS:HA	1.91	0.52
2:B:277:PHE:HE1	2:B:280:ASN:HB2	1.73	0.52
1:A:90:ALA:HB1	1:A:91:PRO:CD	2.39	0.52
2:B:185:GLU:HG2	2:B:347:LEU:HD23	1.92	0.52
1:A:87:PHE:HA	1:A:88:PRO:C	2.30	0.52
1:A:159:HIS:CE1	1:A:161:ARG:HG3	2.46	0.51
1:A:228:VAL:HB	1:A:262:VAL:HB	1.91	0.51
1:A:261:THR:HG22	1:A:262:VAL:N	2.26	0.51
2:B:282:ARG:CG	2:B:282:ARG:NH2	2.70	0.51
2:B:131:PRO:HG2	2:B:138:LYS:CA	2.41	0.51
2:B:15:ASN:HD22	2:B:15:ASN:C	2.14	0.50
1:A:52:ARG:HD3	1:A:54:TYR:OH	2.10	0.50
1:A:92:GLU:H	1:A:93:ASP:CA	2.08	0.50
1:A:125:CYS:SG	1:A:172:GLN:HB2	2.52	0.50
1:A:15:ASN:HD22	1:A:16:GLY:N	2.10	0.49
1:A:15:ASN:ND2	1:A:15:ASN:H	2.10	0.49
1:A:9:PHE:CE1	1:A:24:LYS:HA	2.47	0.49
2:B:396:LEU:O	2:B:397:LYS:HB2	2.13	0.49
1:A:71:LEU:HD23	1:A:72:GLY:N	2.28	0.48
2:B:395:ARG:O	2:B:396:LEU:HB2	2.12	0.48
1:A:295:HIS:CE1	1:A:393:ARG:HG3	2.49	0.48
1:A:15:ASN:HD22	1:A:16:GLY:H	1.61	0.48
1:A:40:VAL:HG11	1:A:112:ALA:HB1	1.96	0.48
2:B:131:PRO:HG2	2:B:138:LYS:HA	1.96	0.47
1:A:48:LEU:O	1:A:51:ARG:HG2	2.15	0.47
1:A:5:GLY:HA2	1:A:384:ASP:HB3	1.97	0.47
1:A:225:ASN:HA	1:A:264:PRO:HB3	1.96	0.47
1:A:196:PRO:O	1:A:223:ASN:HB2	2.14	0.47
2:B:208:TYR:CZ	2:B:214:ILE:HG23	2.50	0.47
2:B:323:VAL:O	2:B:346:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:GLN:OE1	2:B:287:LEU:HD12	2.14	0.47
1:A:195:LYS:HB3	1:A:223:ASN:HB3	1.96	0.46
2:B:113:TYR:HA	2:B:114:PRO:HD3	1.80	0.46
1:A:173:TYR:CZ	1:A:355:LYS:HD3	2.50	0.46
1:A:281:ASN:HA	1:A:284:LYS:HG2	1.97	0.46
1:A:52:ARG:HG2	1:A:85:GLN:NE2	2.31	0.46
1:A:129:LEU:HD13	1:A:241:ILE:HD11	1.97	0.46
1:A:120:PRO:HA	1:A:121:PRO:HD3	1.78	0.46
2:B:228:VAL:HB	2:B:262:VAL:HB	1.97	0.46
1:A:8:VAL:HG11	1:A:100:LEU:HD11	1.98	0.46
2:B:173:TYR:HD1	2:B:353:HIS:O	1.98	0.46
1:A:396:LEU:HA	1:A:397:LYS:HA	1.52	0.46
1:A:128:THR:HG22	1:A:129:LEU:N	2.31	0.45
2:B:195:LYS:O	2:B:224:THR:HG22	2.16	0.45
1:A:251:CYS:HA	1:A:252:PRO:HD3	1.83	0.45
2:B:27:PHE:CE2	2:B:37:VAL:HA	2.52	0.45
2:B:72:GLY:O	2:B:73:LEU:C	2.54	0.45
2:B:73:LEU:CB	2:B:74:THR:CA	2.93	0.45
2:B:130:GLN:HB2	2:B:285:ARG:HH12	1.81	0.45
1:A:57:LEU:HD12	1:A:145:GLU:O	2.16	0.45
1:A:15:ASN:ND2	1:A:15:ASN:N	2.64	0.45
2:B:198:HIS:HB3	2:B:221:THR:HB	1.99	0.45
2:B:95:LYS:HA	2:B:96:PRO:HD3	1.84	0.45
1:A:303:SER:HB2	1:A:350:THR:HG23	1.99	0.45
2:B:277:PHE:HD1	2:B:279:ALA:HB3	1.82	0.45
1:A:233:ILE:HG22	1:A:274:LEU:HD21	1.98	0.44
2:B:59:CYS:HB2	2:B:144:TYR:CE2	2.52	0.44
1:A:144:TYR:HB2	1:A:168:ILE:O	2.18	0.44
1:A:212:GLU:HA	1:A:213:PRO:HD3	1.81	0.44
2:B:134:GLU:HA	2:B:135:ASP:HA	1.80	0.44
2:B:201:ALA:HA	2:B:217:ASN:O	2.17	0.44
2:B:277:PHE:CE1	2:B:280:ASN:HB2	2.52	0.44
1:A:6:THR:OG1	1:A:384:ASP:HB2	2.18	0.43
1:A:124:PRO:HG3	1:A:315:LEU:HA	2.00	0.43
1:A:9:PHE:HE1	1:A:24:LYS:HA	1.84	0.43
2:B:39:GLY:HA3	2:B:115:PHE:CZ	2.53	0.43
2:B:350:THR:HG22	2:B:352:MET:HG2	2.01	0.43
2:B:386:ILE:HG23	2:B:386:ILE:O	2.17	0.43
1:A:93:ASP:N	1:A:94:LYS:HA	2.32	0.43
2:B:56:THR:HG23	2:B:82:ALA:O	2.19	0.43
1:A:13:SER:HB2	1:A:14:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HE3	1:A:357:LYS:HA	1.99	0.43
2:B:199:LEU:HD12	2:B:200:GLU:H	1.82	0.43
1:A:124:PRO:HG3	1:A:315:LEU:HD23	2.00	0.43
1:A:182:PRO:HG2	1:A:203:LEU:O	2.19	0.43
2:B:93:ASP:CB	2:B:94:LYS:HA	2.49	0.43
2:B:120:PRO:HA	2:B:121:PRO:HD3	1.88	0.43
1:A:7:ARG:HG2	1:A:8:VAL:N	2.34	0.42
1:A:323:VAL:O	1:A:346:GLU:HA	2.18	0.42
2:B:220:VAL:HG12	2:B:221:THR:N	2.34	0.42
1:A:30:HIS:HB2	1:A:33:LEU:HD23	2.02	0.42
1:A:102:GLU:O	1:A:106:LYS:HG3	2.20	0.42
2:B:199:LEU:HD13	2:B:327:LEU:HD11	2.01	0.42
1:A:113:TYR:HA	1:A:114:PRO:HD3	1.79	0.42
1:A:214:ILE:O	1:A:273:THR:HA	2.19	0.42
2:B:51:ARG:HH11	2:B:150:CYS:HB3	1.85	0.42
2:B:267:THR:HG22	2:B:268:PHE:N	2.34	0.41
1:A:232:LYS:HG2	1:A:257:GLU:HG2	2.02	0.41
2:B:123:LEU:HA	2:B:124:PRO:HD3	1.91	0.41
1:A:109:GLY:O	1:A:111:HIS:N	2.53	0.41
2:B:55:VAL:HG11	2:B:115:PHE:CE1	2.55	0.41
2:B:282:ARG:HD2	2:B:282:ARG:H	1.85	0.41
2:B:355:LYS:HA	2:B:356:PRO:HD3	1.84	0.41
2:B:19:THR:O	2:B:41:VAL:HG23	2.21	0.41
1:A:11:LYS:O	1:A:164:VAL:HG21	2.20	0.41
2:B:230:LYS:HG3	2:B:328:VAL:HB	2.02	0.41
2:B:169:ARG:HG3	2:B:393:ARG:HH22	1.86	0.41
2:B:292:LYS:HB3	2:B:294:LYS:HG2	2.03	0.41
1:A:48:LEU:O	1:A:48:LEU:HD13	2.21	0.41
1:A:201:ALA:HA	1:A:217:ASN:O	2.21	0.41
2:B:93:ASP:OD1	2:B:93:ASP:N	2.41	0.41
2:B:216:VAL:HG21	2:B:323:VAL:HG11	2.02	0.41
1:A:93:ASP:H	1:A:94:LYS:HA	1.85	0.41
1:A:328:VAL:HA	1:A:342:ASP:OD1	2.21	0.41
2:B:303:SER:HB2	2:B:350:THR:HG23	2.02	0.41
1:A:241:ILE:O	1:A:246:THR:HA	2.20	0.41
2:B:14:PRO:HG2	2:B:161:ARG:HA	2.03	0.41
2:B:210:HIS:ND1	2:B:354:PRO:HD3	2.35	0.41
1:A:14:PRO:HG2	1:A:161:ARG:HA	2.02	0.40
1:A:67:ASP:OD1	1:A:67:ASP:N	2.52	0.40
2:B:195:LYS:HB2	2:B:223:ASN:O	2.21	0.40
1:A:393:ARG:HB2	1:A:394:GLN:H	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:LEU:C	2:B:197:LEU:HD23	2.41	0.40
1:A:205:LYS:HB2	1:A:208:TYR:CZ	2.56	0.40
1:A:228:VAL:O	1:A:261:THR:HG23	2.22	0.40
2:B:205:LYS:HB3	2:B:205:LYS:HE2	1.88	0.40
2:B:383:ASP:O	2:B:384:ASP:O	2.38	0.40
2:B:393:ARG:H	2:B:393:ARG:HG2	1.71	0.40
2:B:46:GLU:O	2:B:47:TYR:HB2	2.21	0.40
2:B:353:HIS:CD2	2:B:354:PRO:HD2	2.57	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	348/418 (83%)	314 (90%)	22 (6%)	12 (3%)	3 15
2	B	357/418 (85%)	294 (82%)	47 (13%)	16 (4%)	2 9
All	All	705/836 (84%)	608 (86%)	69 (10%)	28 (4%)	3 11

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
2	B	73	LEU
2	B	89	PRO
2	B	279	ALA
2	B	357	LYS
2	B	384	ASP
1	A	110	GLU
1	A	281	ASN
1	A	286	GLY
1	A	393	ARG

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Mol	Chain	Res	Type
2	B	32	ASP
2	B	72	GLY
2	B	358	GLU
2	B	383	ASP
1	A	46	GLU
1	A	69	ASP
1	A	90	ALA
2	B	380	ASP
2	B	181	GLN
2	B	359	GLU
2	B	382	ASN
2	B	395	ARG
2	B	308	GLU
1	A	15	ASN
1	A	176	GLU
1	A	395	ARG
1	A	16	GLY
2	B	91	PRO

5.3.2 Protein sidechains (i)

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	313/372 (84%)	307 (98%)	6 (2%)	57 84
2	B	322/372 (87%)	309 (96%)	13 (4%)	31 65
All	All	635/744 (85%)	616 (97%)	19 (3%)	41 75

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	42	LEU
1	A	66	GLU
1	A	225	ASN
1	A	274	LEU

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Mol	Chain	Res	Type
1	A	282	ARG
2	B	15	ASN
2	B	87	PHE
2	B	93	ASP
2	B	105	ILE
2	B	108	LEU
2	B	135	ASP
2	B	186	THR
2	B	194	ASP
2	B	195	LYS
2	B	225	ASN
2	B	274	LEU
2	B	282	ARG
2	B	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	83	ASN
1	A	85	GLN
1	A	198	HIS
1	A	225	ASN
1	A	245	ASN
1	A	353	HIS
2	B	15	ASN
2	B	83	ASN
2	B	85	GLN
2	B	111	HIS
2	B	245	ASN
2	B	295	HIS
2	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	356/418 (85%)	0.31	7 (1%) 65 63	37, 64, 106, 128	30 (8%)
2	B	367/418 (87%)	0.69	39 (10%) 6 4	36, 73, 136, 178	49 (13%)
All	All	723/836 (86%)	0.50	46 (6%) 19 15	36, 68, 119, 178	79 (10%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	359	GLU	9.6
2	B	360	PRO	9.0
2	B	358	GLU	6.2
2	B	357	LYS	5.8
2	B	280	ASN	5.2
2	B	18	LEU	5.2
2	B	381	THR	4.8
1	A	43	VAL	4.7
2	B	356	PRO	4.3
2	B	44	ASP	3.9
2	B	51	ARG	3.9
2	B	162	ASN	3.8
2	B	180	PRO	3.7
2	B	50	GLU	3.7
2	B	398	GLY	3.7
2	B	151	ALA	3.5
2	B	152	GLU	3.3
2	B	379	LEU	3.3
1	A	130	GLN	3.3
2	B	49	LYS	3.2
2	B	38	ASP	3.1
1	A	278	LEU	2.9
2	B	2	GLY	2.8
2	B	88	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	8	VAL	2.8
2	B	207	ILE	2.7
2	B	382	ASN	2.6
2	B	45	PRO	2.5
2	B	278	LEU	2.5
2	B	281	ASN	2.4
2	B	114	PRO	2.4
2	B	89	PRO	2.4
2	B	297	ASP	2.4
1	A	356	PRO	2.3
2	B	85	GLN	2.3
2	B	342	ASP	2.2
2	B	380	ASP	2.2
2	B	5	GLY	2.2
1	A	31	ILE	2.2
1	A	388	PHE	2.1
2	B	43	VAL	2.1
1	A	357	LYS	2.1
2	B	22	LEU	2.0
2	B	136	THR	2.0
2	B	399	MET	2.0
2	B	84	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BA	A	1399	1/1	0.57	0.27	142,142,142,142	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BA	B	1401	1/1	0.77	0.18	122,122,122,122	1
3	BA	B	1402	1/1	0.83	0.16	119,119,119,119	1
3	BA	A	1398	1/1	0.90	0.14	122,122,122,122	1

6.5 Other polymers (i)

There are no such residues in this entry.