



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:20 am BST

PDB ID : 1G6Y
Title : CRYSTAL STRUCTURE OF THE GLOBULAR REGION OF THE PRION PROTEIN URE2 FROM YEAST SACCHAROMYCES CEREVISIAE
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Deposited on : 2000-11-08
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

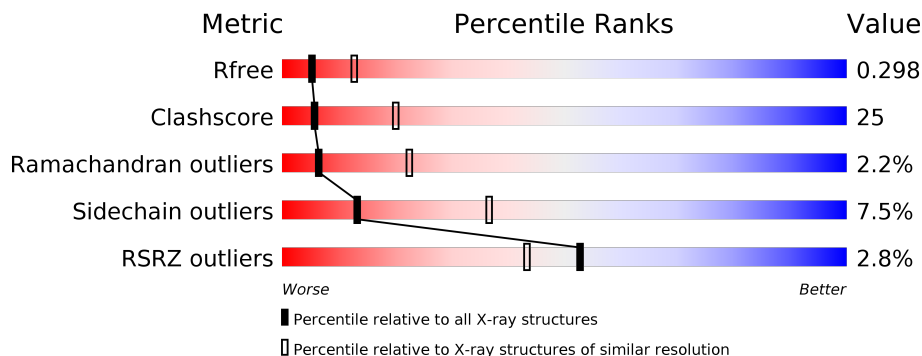
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 ≥ 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	261	
1	B	261	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4072 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 URE2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	1965	1270	337	351	7	0	0	0
1	B	257	2086	1347	357	375	7	0	0	0

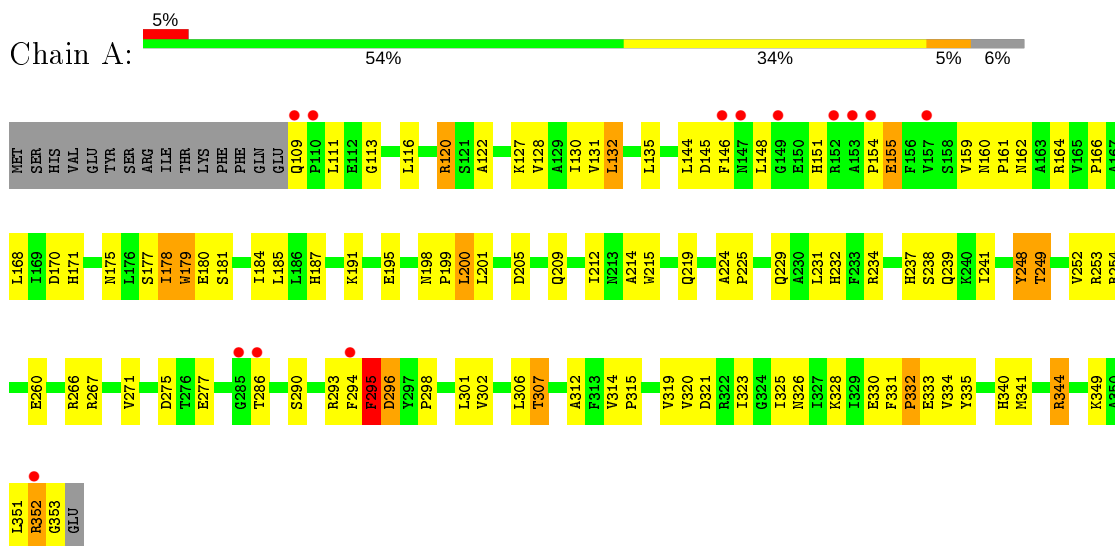
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total 9	O 9	0	0
2	B	12	Total 12	O 12	0	0

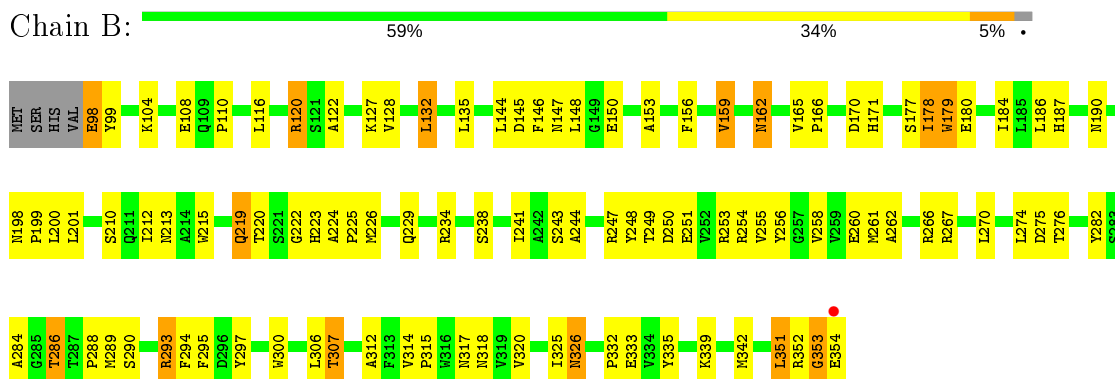
3 Residue-property plots

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: URE2 PROTEIN



• Molecule 1: URE2 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.49Å 73.70Å 130.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.80) 99.5 (19.93-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.79Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.293 0.227 , 0.298	Depositor DCC
R_{free} test set	684 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtrriage
Anisotropy	0.687	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4072	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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	0.42	0/2021	0.64	0/2750
1	B	0.43	0/2145	0.64	0/2914
All	All	0.43	0/4166	0.64	0/5664

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	TYR	Sidechain

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	1965	0	1916	111	0
1	B	2086	0	2033	104	0
2	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	0	0	0
All	All	4072	0	3949	203	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 25.

All (203) 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:239:GLN:HE21	1:A:241:ILE:HD11	1.30	0.97
1:A:205:ASP:O	1:A:209:GLN:HG3	1.83	0.79
1:A:290:SER:HA	1:A:295:PHE:CE1	2.19	0.78
1:B:159:VAL:HG22	1:B:177:SER:HB2	1.63	0.77
1:B:186:LEU:HD21	1:B:213:ASN:HD21	1.49	0.77
1:B:200:LEU:HG	1:B:201:LEU:HD13	1.66	0.76
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.51	0.76
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.50	0.76
1:B:282:TYR:HB3	1:B:289:MET:HE3	1.67	0.76
1:B:282:TYR:HB3	1:B:289:MET:CE	2.18	0.74
1:B:339:LYS:HA	1:B:339:LYS:HE2	1.69	0.73
1:A:254:ARG:HH22	1:B:162:ASN:ND2	1.88	0.71
1:A:239:GLN:HE21	1:A:241:ILE:CD1	2.03	0.71
1:B:104:LYS:HG2	1:B:108:GLU:OE2	1.91	0.70
1:B:200:LEU:HG	1:B:201:LEU:CD1	2.21	0.70
1:A:130:ILE:HD11	1:A:351:LEU:HD21	1.73	0.69
1:B:159:VAL:HG22	1:B:177:SER:CB	2.22	0.69
1:A:253:ARG:NH1	1:A:330:GLU:OE1	2.25	0.69
1:A:349:LYS:HA	1:A:352:ARG:HH11	1.59	0.68
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.59	0.68
1:A:293:ARG:HG2	1:A:294:PHE:CE1	2.29	0.68
1:B:178:ILE:HD12	1:B:178:ILE:N	2.09	0.68
1:A:239:GLN:NE2	1:A:241:ILE:HD11	2.07	0.66
1:B:198:ASN:HD22	1:B:199:PRO:HD2	1.60	0.65
1:A:200:LEU:HD22	1:A:201:LEU:HG	1.81	0.63
1:B:145:ASP:OD2	1:B:148:LEU:HG	1.99	0.63
1:B:267:ARG:HH11	1:B:267:ARG:HG3	1.64	0.63
1:A:254:ARG:HH22	1:B:162:ASN:HD21	1.46	0.61
1:A:179:TRP:O	1:A:180:GLU:HB2	1.98	0.61
1:B:256:TYR:HE1	1:B:320:VAL:HG11	1.65	0.61
1:A:241:ILE:HG21	1:B:241:ILE:HD13	1.83	0.61
1:A:249:THR:O	1:A:253:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:O	1:A:195:GLU:HG3	2.00	0.60
1:B:314:VAL:HB	1:B:315:PRO:HD3	1.81	0.60
1:B:186:LEU:HD21	1:B:213:ASN:ND2	2.16	0.60
1:A:111:LEU:HD23	1:A:111:LEU:H	1.66	0.60
1:A:127:LYS:HD2	1:A:312:ALA:HA	1.82	0.60
1:B:253:ARG:NH1	1:B:325:ILE:HD13	2.17	0.60
1:A:352:ARG:HG3	1:A:353:GLY:H	1.65	0.60
1:A:178:ILE:HD12	1:A:178:ILE:N	2.17	0.60
1:A:352:ARG:HG3	1:A:352:ARG:HH21	1.67	0.59
1:A:328:LYS:HD3	1:A:335:TYR:CZ	2.37	0.59
1:B:146:PHE:H	1:B:146:PHE:HD1	1.49	0.59
1:B:275:ASP:HB2	1:B:294:PHE:CD1	2.39	0.58
1:B:135:LEU:HD23	1:B:200:LEU:HD23	1.84	0.58
1:B:256:TYR:OH	1:B:317:ASN:ND2	2.34	0.57
1:A:187:HIS:HD2	1:B:210:SER:OG	1.88	0.57
1:A:120:ARG:H	1:A:120:ARG:HD2	1.69	0.56
1:B:110:PRO:HD2	1:B:171:HIS:CE1	2.40	0.56
1:A:160:ASN:HD22	1:A:161:PRO:HD2	1.69	0.56
1:B:275:ASP:OD1	1:B:293:ARG:HD3	2.06	0.56
1:B:120:ARG:HD2	1:B:120:ARG:H	1.69	0.55
1:A:290:SER:HA	1:A:295:PHE:CD1	2.41	0.55
1:A:155:GLU:N	1:A:155:GLU:OE1	2.40	0.55
1:A:253:ARG:NH1	1:A:325:ILE:HG12	2.22	0.55
1:B:120:ARG:CD	1:B:120:ARG:H	2.21	0.54
1:B:222:GLY:O	1:B:226:MET:HG2	2.07	0.54
1:B:342:MET:CE	1:B:351:LEU:HD21	2.37	0.54
1:B:226:MET:HE3	1:B:251:GLU:HG3	1.90	0.54
1:B:275:ASP:HB2	1:B:294:PHE:CE1	2.43	0.54
1:A:159:VAL:HG13	1:A:177:SER:OG	2.07	0.53
1:A:179:TRP:N	1:A:179:TRP:CD1	2.76	0.53
1:A:248:TYR:O	1:A:252:VAL:HG23	2.08	0.53
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.23	0.53
1:A:254:ARG:NH2	1:B:162:ASN:ND2	2.56	0.53
1:A:120:ARG:CD	1:A:120:ARG:H	2.21	0.53
1:A:267:ARG:HD3	1:A:295:PHE:CE2	2.43	0.53
1:B:326:ASN:HD22	1:B:326:ASN:C	2.11	0.53
1:B:352:ARG:O	1:B:353:GLY:O	2.27	0.53
1:A:314:VAL:HB	1:A:315:PRO:HD3	1.91	0.53
1:B:146:PHE:N	1:B:146:PHE:CD1	2.77	0.52
1:B:282:TYR:CE2	1:B:289:MET:HA	2.45	0.52
1:A:120:ARG:HG3	1:A:120:ARG:NH1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:O	1:A:323:ILE:HG22	2.10	0.52
1:A:146:PHE:CD2	1:A:151:HIS:HB3	2.45	0.52
1:A:294:PHE:CD1	1:A:294:PHE:N	2.77	0.52
1:B:256:TYR:CE1	1:B:320:VAL:HG11	2.44	0.52
1:B:262:ALA:O	1:B:266:ARG:HG2	2.10	0.52
1:B:244:ALA:O	1:B:247:ARG:HG2	2.10	0.52
1:A:326:ASN:O	1:A:330:GLU:HG2	2.10	0.51
1:B:234:ARG:HG3	1:B:234:ARG:O	2.09	0.51
1:A:260:GLU:OE1	1:A:333:GLU:HB2	2.11	0.51
1:A:214:ALA:O	1:B:180:GLU:HG3	2.10	0.51
1:A:306:LEU:HD22	1:A:344:ARG:HE	1.76	0.51
1:A:231:LEU:HG	1:A:323:ILE:HD11	1.93	0.51
1:A:171:HIS:HA	1:A:175:ASN:HD22	1.75	0.51
1:A:332:PRO:O	1:A:335:TYR:HB3	2.12	0.50
1:A:238:SER:O	1:A:239:GLN:HB3	2.11	0.50
1:A:351:LEU:O	1:A:352:ARG:HG2	2.11	0.50
1:A:349:LYS:HA	1:A:352:ARG:NH1	2.25	0.50
1:B:120:ARG:HG3	1:B:120:ARG:NH1	2.23	0.50
1:B:224:ALA:N	1:B:225:PRO:HD2	2.26	0.50
1:A:179:TRP:HH2	1:B:215:TRP:CE3	2.29	0.50
1:B:145:ASP:CG	1:B:145:ASP:O	2.50	0.50
1:B:201:LEU:N	1:B:201:LEU:HD12	2.27	0.49
1:A:351:LEU:O	1:A:352:ARG:CB	2.60	0.49
1:B:179:TRP:CD1	1:B:179:TRP:N	2.76	0.49
1:A:170:ASP:OD2	1:A:187:HIS:HE1	1.95	0.49
1:A:135:LEU:HD23	1:A:200:LEU:HD13	1.93	0.49
1:A:306:LEU:HD22	1:A:344:ARG:NE	2.27	0.49
1:A:349:LYS:O	1:A:352:ARG:NH1	2.45	0.49
1:B:267:ARG:HG3	1:B:267:ARG:NH1	2.26	0.49
1:B:219:GLN:NE2	1:B:220:THR:HG22	2.27	0.49
1:A:275:ASP:C	1:A:277:GLU:H	2.15	0.49
1:A:298:PRO:HD3	1:A:340:HIS:CE1	2.48	0.48
1:A:232:HIS:NE2	1:A:237:HIS:HD2	2.12	0.48
1:A:352:ARG:HG3	1:A:353:GLY:N	2.29	0.48
1:A:145:ASP:OD2	1:A:148:LEU:HD12	2.13	0.48
1:A:314:VAL:CG2	1:A:341:MET:SD	3.02	0.48
1:B:251:GLU:OE2	1:B:254:ARG:HD3	2.13	0.48
1:A:162:ASN:HD22	1:A:164:ARG:HG2	1.79	0.48
1:B:270:LEU:HD12	1:B:270:LEU:O	2.14	0.48
1:B:98:GLU:HB2	1:B:99:TYR:H	1.57	0.48
1:A:201:LEU:HA	1:A:307:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:HD11	1:B:156:PHE:CZ	2.49	0.47
1:B:198:ASN:HD22	1:B:199:PRO:CD	2.26	0.47
1:B:99:TYR:HB3	1:B:150:GLU:HA	1.96	0.47
1:A:215:TRP:CD2	1:A:301:LEU:HD13	2.50	0.47
1:A:352:ARG:CG	1:A:353:GLY:H	2.26	0.47
1:B:332:PRO:O	1:B:335:TYR:HB3	2.13	0.47
1:B:120:ARG:HH11	1:B:120:ARG:CG	2.23	0.46
1:A:351:LEU:O	1:A:352:ARG:CG	2.63	0.46
1:A:351:LEU:C	1:A:352:ARG:HG2	2.36	0.46
1:B:226:MET:CE	1:B:251:GLU:HG3	2.46	0.46
1:B:127:LYS:HD2	1:B:312:ALA:HA	1.98	0.46
1:A:212:ILE:HG12	1:A:302:VAL:HG11	1.96	0.46
1:B:219:GLN:HE21	1:B:220:THR:CG2	2.29	0.46
1:A:331:PHE:HB3	1:A:334:VAL:HB	1.98	0.46
1:A:161:PRO:HB2	1:B:258:VAL:HG13	1.98	0.46
1:B:270:LEU:HD11	1:B:274:LEU:CD1	2.46	0.46
1:A:229:GLN:NE2	1:B:247:ARG:HH12	2.14	0.46
1:B:253:ARG:CZ	1:B:325:ILE:HD13	2.46	0.46
1:A:231:LEU:HD23	1:A:323:ILE:HD11	1.98	0.45
1:B:219:GLN:HE21	1:B:220:THR:HG22	1.81	0.45
1:A:161:PRO:HB2	1:B:258:VAL:CG1	2.47	0.45
1:A:231:LEU:CD2	1:A:323:ILE:HD11	2.46	0.45
1:B:300:TRP:CZ3	1:B:306:LEU:HD13	2.52	0.45
1:B:339:LYS:CE	1:B:339:LYS:HA	2.43	0.45
1:B:290:SER:HA	1:B:295:PHE:CE1	2.52	0.45
1:B:128:VAL:O	1:B:132:LEU:HB2	2.16	0.44
1:A:162:ASN:ND2	1:A:164:ARG:HG2	2.32	0.44
1:B:282:TYR:HB3	1:B:289:MET:HE2	1.94	0.44
1:A:131:VAL:HG21	1:A:185:LEU:HD22	1.99	0.44
1:A:331:PHE:N	1:A:332:PRO:HD3	2.33	0.44
1:B:260:GLU:OE2	1:B:333:GLU:HB2	2.18	0.44
1:A:146:PHE:N	1:A:146:PHE:CD2	2.85	0.44
1:A:113:GLY:O	1:A:171:HIS:HB2	2.18	0.44
1:A:237:HIS:HE1	1:B:243:SER:OG	2.00	0.44
1:A:293:ARG:HG2	1:A:294:PHE:CD1	2.52	0.44
1:B:219:GLN:HG2	1:B:312:ALA:HB1	1.98	0.44
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.82	0.44
1:A:166:PRO:HG3	1:A:181:SER:HB3	1.99	0.43
1:A:212:ILE:CG1	1:A:302:VAL:HG11	2.48	0.43
1:A:144:LEU:HB2	1:A:146:PHE:HE2	1.83	0.43
1:A:198:ASN:HA	1:A:199:PRO:HD2	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PRO:O	1:B:229:GLN:HG2	2.18	0.43
1:B:288:PRO:C	1:B:290:SER:H	2.22	0.43
1:A:145:ASP:O	1:A:145:ASP:CG	2.56	0.43
1:A:231:LEU:CG	1:A:323:ILE:HD11	2.48	0.43
1:A:319:VAL:C	1:A:321:ASP:H	2.22	0.43
1:B:219:GLN:HA	1:B:223:HIS:HB3	2.00	0.43
1:A:241:ILE:HG21	1:B:241:ILE:CD1	2.47	0.43
1:B:318:ASN:HD21	1:B:342:MET:HG3	1.84	0.42
1:A:171:HIS:HA	1:A:175:ASN:ND2	2.35	0.42
1:B:180:GLU:O	1:B:184:ILE:HG13	2.19	0.42
1:B:353:GLY:O	1:B:354:GLU:OE1	2.38	0.42
1:B:120:ARG:CG	1:B:120:ARG:NH1	2.81	0.42
1:B:156:PHE:O	1:B:159:VAL:HG12	2.20	0.42
1:A:160:ASN:ND2	1:A:162:ASN:H	2.18	0.42
1:A:271:VAL:O	1:A:271:VAL:CG1	2.67	0.42
1:B:223:HIS:HD2	1:B:255:VAL:HG11	1.85	0.42
1:A:160:ASN:HD22	1:A:161:PRO:CD	2.33	0.41
1:B:314:VAL:CB	1:B:315:PRO:HD3	2.49	0.41
1:A:120:ARG:N	1:A:120:ARG:HD2	2.34	0.41
1:A:224:ALA:HB3	1:A:225:PRO:HD3	2.02	0.41
1:A:128:VAL:O	1:A:132:LEU:HB2	2.20	0.41
1:A:271:VAL:O	1:A:271:VAL:HG12	2.19	0.41
1:B:170:ASP:OD2	1:B:187:HIS:HE1	2.02	0.41
1:B:284:ALA:HB3	1:B:286:THR:HG23	2.01	0.41
1:A:146:PHE:C	1:A:148:LEU:H	2.24	0.41
1:A:168:LEU:HD22	1:A:184:ILE:HG23	2.03	0.41
1:B:165:VAL:HB	1:B:166:PRO:HA	2.03	0.41
1:B:135:LEU:CD2	1:B:200:LEU:HD23	2.50	0.41
1:B:270:LEU:HD11	1:B:274:LEU:HD12	2.02	0.41
1:A:109:GLN:NE2	1:A:171:HIS:HE1	2.19	0.41
1:B:352:ARG:O	1:B:353:GLY:C	2.59	0.41
1:A:159:VAL:HG13	1:A:177:SER:CB	2.50	0.41
1:B:294:PHE:HA	1:B:297:TYR:CD1	2.56	0.41
1:A:275:ASP:C	1:A:277:GLU:N	2.73	0.41
1:A:253:ARG:CZ	1:A:325:ILE:HG12	2.51	0.41
1:A:352:ARG:NH2	1:A:353:GLY:O	2.54	0.41
1:B:178:ILE:HD12	1:B:178:ILE:H	1.83	0.41
1:B:229:GLN:HB2	1:B:248:TYR:CG	2.56	0.41
1:B:99:TYR:CG	1:B:153:ALA:HB2	2.56	0.41
1:A:127:LYS:CD	1:A:312:ALA:HA	2.50	0.40
1:B:229:GLN:HB2	1:B:248:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:O	1:A:201:LEU:HB2	2.20	0.40
1:B:145:ASP:C	1:B:147:ASN:H	2.25	0.40
1:B:212:ILE:HD11	1:B:307:THR:HG21	2.04	0.40
1:B:247:ARG:NH1	1:B:248:TYR:CZ	2.88	0.40
1:A:351:LEU:O	1:A:352:ARG:HB3	2.21	0.40
1:B:120:ARG:HD2	1:B:120:ARG:N	2.35	0.40
1:B:288:PRO:O	1:B:289:MET:HB3	2.21	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	243/261 (93%)	216 (89%)	20 (8%)	7 (3%)	4	15
1	B	255/261 (98%)	231 (91%)	20 (8%)	4 (2%)	9	31
All	All	498/522 (95%)	447 (90%)	40 (8%)	11 (2%)	6	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	ARG
1	B	353	GLY
1	A	296	ASP
1	B	238	SER
1	B	351	LEU
1	A	295	PHE
1	A	122	ALA
1	B	122	ALA
1	A	154	PRO
1	A	320	VAL
1	A	332	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	206/224 (92%)	192 (93%)	14 (7%)	16	42
1	B	220/224 (98%)	202 (92%)	18 (8%)	11	33
All	All	426/448 (95%)	394 (92%)	32 (8%)	13	37

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	120	ARG
1	A	132	LEU
1	A	155	GLU
1	A	178	ILE
1	A	179	TRP
1	A	200	LEU
1	A	219	GLN
1	A	249	THR
1	A	286	THR
1	A	295	PHE
1	A	296	ASP
1	A	307	THR
1	A	344	ARG
1	B	98	GLU
1	B	116	LEU
1	B	120	ARG
1	B	132	LEU
1	B	159	VAL
1	B	162	ASN
1	B	178	ILE
1	B	179	TRP
1	B	190	ASN
1	B	219	GLN
1	B	249	THR
1	B	250	ASP
1	B	261	MET

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Mol	Chain	Res	Type
1	B	276	THR
1	B	286	THR
1	B	293	ARG
1	B	307	THR
1	B	326	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	160	ASN
1	A	175	ASN
1	A	187	HIS
1	A	213	ASN
1	A	219	GLN
1	A	229	GLN
1	A	237	HIS
1	A	239	GLN
1	A	291	GLN
1	B	107	GLN
1	B	162	ASN
1	B	187	HIS
1	B	190	ASN
1	B	198	ASN
1	B	209	GLN
1	B	213	ASN
1	B	219	GLN
1	B	237	HIS
1	B	291	GLN
1	B	317	ASN
1	B	318	ASN
1	B	326	ASN

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 [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	245/261 (93%)	-0.05	13 (5%) 26 17	10, 35, 77, 80	0
1	B	257/261 (98%)	-0.35	1 (0%) 92 91	16, 37, 58, 70	0
All	All	502/522 (96%)	-0.21	14 (2%) 53 43	10, 36, 71, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLY	4.6
1	A	147	ASN	4.5
1	A	154	PRO	3.9
1	A	146	PHE	3.5
1	A	109	GLN	3.4
1	A	153	ALA	2.5
1	A	286	THR	2.5
1	A	110	PRO	2.4
1	A	157	VAL	2.2
1	A	352	ARG	2.2
1	B	354	GLU	2.2
1	A	285	GLY	2.1
1	A	152	ARG	2.1
1	A	294	PHE	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.