



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:32 PM UTC

PDB ID : 1G6W / pdb_00001g6w
Title : CRYSTAL STRUCTURE OF THE GLOBULAR REGION OF THE PRION
PROTEIN URE2 FROM THE YEAST SACCAROMYCES CEREVISIAE
Authors : Bousset, L.; Belrhali, H.; Janin, J.; Melki, R.; Morera, S.
Deposited on : 2000-11-08
Resolution : 2.50 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

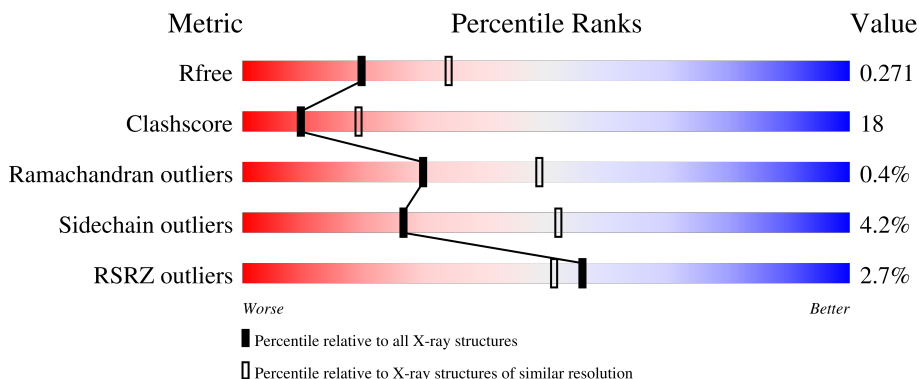
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	261	 4% 56% 30% 10%
1	B	261	 4% 57% 32% 7%
1	C	261	 % 57% 36% 5%
1	D	261	 % 69% 28% 3%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8343 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
1	A	234	Total	C	N	O	S	0	0	0
			1907	1236	329	336	6			
1	B	242	Total	C	N	O	S	0	0	0
			1981	1286	340	349	6			
1	C	255	Total	C	N	O	S	0	0	0
			2065	1333	355	370	7			
1	D	259	Total	C	N	O	S	0	0	0
			2104	1358	361	378	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	68	Total	O	0	0
			68	68		
2	C	69	Total	O	0	0
			69	69		
2	D	85	Total	O	0	0
			85	85		

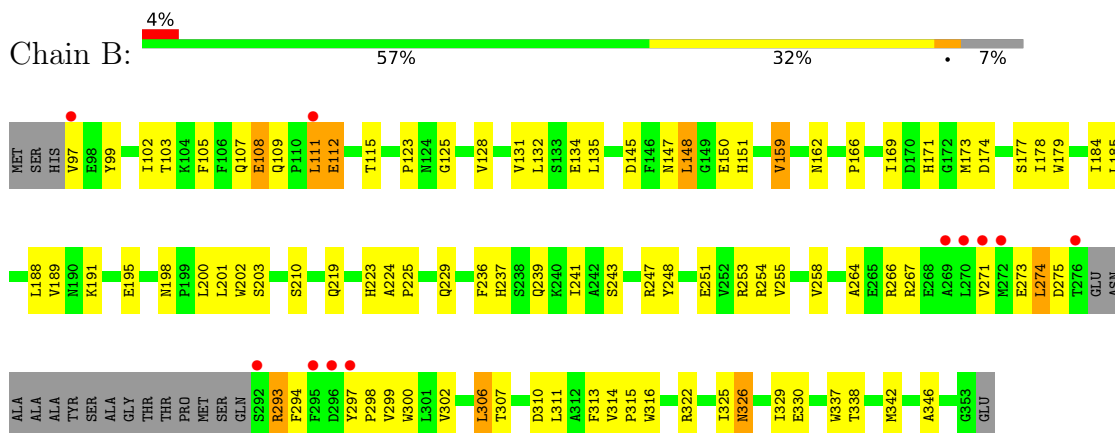
3 Residue-property plots

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.

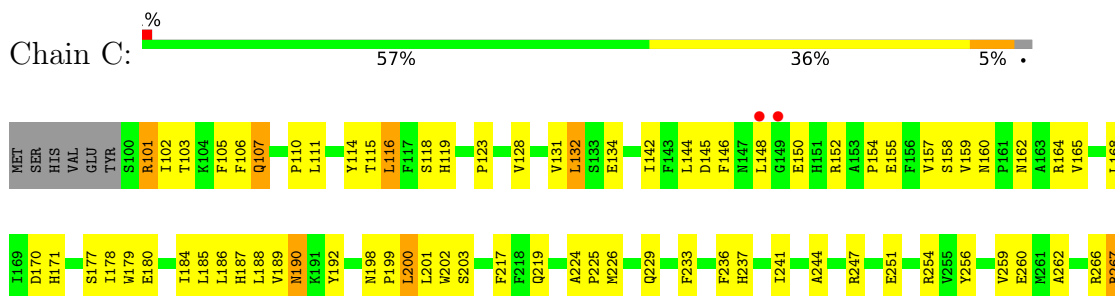
• Molecule 1: URE2 PROTEIN

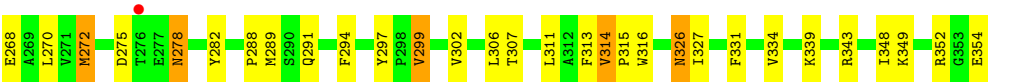


• Molecule 1: URE2 PROTEIN

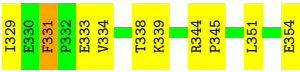
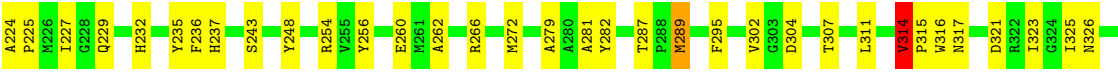


• Molecule 1: URE2 PROTEIN





● 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	54.68Å 125.02Å 159.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 95.9 (20.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.270 0.212 , 0.271	Depositor DCC
R_{free} test set	1861 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8343	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.57% 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	0.41	0/1960	0.92	7/2661 (0.3%)
1	B	0.40	0/2037	0.89	2/2765 (0.1%)
1	C	0.44	0/2123	0.92	6/2884 (0.2%)
1	D	0.48	1/2164 (0.0%)	0.91	5/2939 (0.2%)
All	All	0.43	1/8284 (0.0%)	0.91	20/11249 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	314	VAL	CA-CB	6.65	1.57	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	TRP	N-CA-C	8.72	123.23	112.59
1	D	179	TRP	N-CA-C	8.31	122.72	112.59
1	A	179	TRP	N-CA-C	6.73	123.71	113.61
1	C	236	PHE	N-CA-C	6.02	122.64	113.61
1	A	125	GLY	N-CA-C	-5.83	105.56	113.37
1	C	101	ARG	N-CA-C	-5.74	106.32	113.55
1	A	158	SER	N-CA-C	-5.69	106.17	113.23
1	A	139	TYR	N-CA-C	5.56	117.71	108.99
1	A	302	VAL	N-CA-C	5.51	116.67	108.46
1	D	331	PHE	CA-C-N	5.50	126.72	119.84
1	D	331	PHE	C-N-CA	5.50	126.72	119.84
1	D	321	ASP	N-CA-C	-5.46	105.87	112.54
1	A	178	ILE	N-CA-C	-5.46	100.56	108.36
1	C	314	VAL	N-CA-C	5.39	118.82	112.35
1	C	302	VAL	N-CA-C	5.34	116.42	108.46
1	B	236	PHE	N-CA-C	5.28	121.46	114.12
1	C	327	ILE	N-CA-C	5.19	115.40	110.42
1	D	302	VAL	N-CA-C	5.12	116.03	108.45
1	C	107	GLN	N-CA-C	-5.07	107.07	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASN	N-CA-C	-5.05	102.59	110.42

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	1907	0	1876	84	0
1	B	1981	0	1943	77	0
1	C	2065	0	2018	86	0
1	D	2104	0	2049	59	0
2	A	64	0	0	4	0
2	B	68	0	0	1	0
2	C	69	0	0	1	0
2	D	85	0	0	2	0
All	All	8343	0	7886	284	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 18.

All (284) 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:B:111:LEU:HD13	1:B:112:GLU:HG2	1.41	1.01
1:C:314:VAL:HG23	1:C:315:PRO:HD3	1.45	0.97
1:C:226:MET:HE3	1:C:251:GLU:HG2	1.51	0.92
1:A:131:VAL:HG21	1:A:185:LEU:HD22	1.54	0.90
1:D:323:ILE:HG13	1:D:325:ILE:HD13	1.52	0.90
1:D:314:VAL:HG13	1:D:315:PRO:HD3	1.54	0.89
1:A:109:GLN:HG2	1:A:175:ASN:ND2	1.91	0.85
1:C:314:VAL:CG2	1:C:315:PRO:HD3	2.07	0.85
1:C:288:PRO:HG2	1:C:291:GLN:HG3	1.61	0.81
1:C:247:ARG:HH21	1:D:229:GLN:HE22	1.29	0.80
1:C:311:LEU:O	1:C:314:VAL:HG22	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:VAL:HG21	1:C:185:LEU:HD22	1.70	0.74
1:C:226:MET:CE	1:C:251:GLU:HG2	2.18	0.74
1:B:159:VAL:HG22	1:B:177:SER:CB	2.18	0.73
1:B:131:VAL:HG21	1:B:185:LEU:HD22	1.70	0.73
1:D:282:TYR:HB3	1:D:289:MET:HE1	1.70	0.73
1:C:314:VAL:HG23	1:C:315:PRO:CD	2.18	0.73
1:B:326:ASN:O	1:B:330:GLU:HG3	1.89	0.72
1:C:186:LEU:O	1:C:190:ASN:HB2	1.90	0.72
1:B:159:VAL:HG22	1:B:177:SER:HB3	1.72	0.71
1:C:270:LEU:HD22	1:C:299:VAL:HG23	1.73	0.71
1:B:264:ALA:O	1:B:267:ARG:HB3	1.92	0.70
1:A:198:ASN:HD22	1:A:199:PRO:HD2	1.57	0.70
1:C:254:ARG:HH12	1:D:162:ASN:ND2	1.90	0.68
1:A:266:ARG:HB3	1:A:299:VAL:HG13	1.75	0.68
1:B:111:LEU:HD12	1:B:112:GLU:H	1.57	0.68
1:B:314:VAL:HG22	1:B:315:PRO:HD3	1.74	0.68
1:A:104:LYS:HD3	1:A:107:GLN:OE1	1.94	0.68
1:C:114:TYR:HB3	1:C:168:LEU:HD11	1.75	0.68
1:A:254:ARG:HH12	1:B:162:ASN:ND2	1.92	0.67
1:C:198:ASN:HD22	1:C:199:PRO:HD2	1.58	0.67
1:B:326:ASN:C	1:B:326:ASN:HD22	2.01	0.66
1:B:111:LEU:CD1	1:B:112:GLU:H	2.08	0.66
1:D:232:HIS:NE2	1:D:237:HIS:HD2	1.94	0.65
1:C:224:ALA:HB3	1:C:225:PRO:HD3	1.80	0.64
1:D:256:TYR:OH	1:D:317:ASN:ND2	2.29	0.64
1:A:162:ASN:ND2	1:B:254:ARG:HH22	1.95	0.64
1:A:186:LEU:HD21	1:A:213:ASN:HD21	1.63	0.64
1:A:253:ARG:HD3	1:A:330:GLU:OE1	1.98	0.64
1:D:314:VAL:CG1	1:D:315:PRO:HD3	2.29	0.63
1:C:326:ASN:C	1:C:326:ASN:HD22	2.07	0.63
1:D:178:ILE:N	1:D:178:ILE:HD12	2.13	0.62
1:D:289:MET:HB3	1:D:295:PHE:CE1	2.34	0.62
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.64	0.62
1:D:132:LEU:HD13	1:D:188:LEU:HD11	1.81	0.62
1:A:202:TRP:CG	1:A:203:SER:H	2.17	0.62
1:C:103:THR:O	1:C:107:GLN:HG2	2.00	0.61
1:C:145:ASP:CG	1:C:148:LEU:HD13	2.25	0.61
1:D:326:ASN:HD22	1:D:329:ILE:H	1.49	0.61
1:B:103:THR:O	1:B:107:GLN:HG2	2.00	0.61
1:D:266:ARG:NH2	1:D:304:ASP:H	1.98	0.60
1:A:154:PRO:HA	1:A:157:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HB3	1:A:241:ILE:HD11	1.82	0.60
1:C:159:VAL:HG13	1:C:177:SER:OG	2.00	0.60
1:D:104:LYS:O	1:D:108:GLU:HG2	2.01	0.60
1:B:314:VAL:CG2	1:B:315:PRO:HD3	2.32	0.60
1:C:268:GLU:HA	1:C:289:MET:HE1	1.84	0.60
1:B:151:HIS:H	1:B:151:HIS:CD2	2.20	0.60
1:C:179:TRP:O	1:C:180:GLU:HB2	2.02	0.59
1:C:247:ARG:HH21	1:D:229:GLN:NE2	1.98	0.59
1:D:201:LEU:HA	1:D:307:THR:HA	1.85	0.59
1:D:207:ALA:O	1:D:211:GLN:HG2	2.02	0.59
1:B:123:PRO:HB2	1:B:316:TRP:CE2	2.38	0.59
1:B:224:ALA:HB3	1:B:225:PRO:HD3	1.84	0.58
1:B:99:TYR:HB3	1:B:150:GLU:HA	1.85	0.58
1:D:131:VAL:HG21	1:D:185:LEU:HD22	1.86	0.58
1:C:198:ASN:HD22	1:C:199:PRO:CD	2.16	0.57
1:B:178:ILE:N	1:B:178:ILE:HD12	2.19	0.57
1:A:102:ILE:HG22	1:A:106:PHE:HE1	1.69	0.57
1:A:178:ILE:N	1:A:178:ILE:HD12	2.18	0.57
1:B:293:ARG:HH11	1:B:294:PHE:HE1	1.51	0.57
1:B:202:TRP:CG	1:B:203:SER:H	2.23	0.57
1:A:198:ASN:HD22	1:A:199:PRO:CD	2.17	0.56
1:A:229:GLN:HE22	1:B:247:ARG:HH21	1.53	0.56
1:B:189:VAL:HB	1:B:202:TRP:HB2	1.88	0.56
1:D:112:GLU:HB3	2:D:413:HOH:O	2.04	0.56
1:A:102:ILE:HB	1:A:155:GLU:HG3	1.88	0.56
1:A:271:VAL:C	1:A:273:GLU:H	2.13	0.56
1:C:233:PHE:HE1	1:D:248:TYR:HH	1.53	0.56
1:A:109:GLN:HG2	1:A:175:ASN:CG	2.30	0.56
1:A:225:PRO:O	1:A:229:GLN:HG2	2.05	0.56
1:A:349:LYS:HD3	1:A:349:LYS:C	2.31	0.56
1:B:266:ARG:HB2	1:B:299:VAL:HG11	1.87	0.56
1:C:202:TRP:CG	1:C:203:SER:H	2.24	0.56
1:A:232:HIS:NE2	1:A:237:HIS:HD2	2.04	0.56
1:D:202:TRP:CG	1:D:203:SER:H	2.23	0.55
1:C:189:VAL:HB	1:C:202:TRP:HB2	1.87	0.55
1:A:241:ILE:N	1:A:241:ILE:HD12	2.22	0.55
1:A:296:ASP:N	2:A:359:HOH:O	2.40	0.55
1:C:339:LYS:O	1:C:343:ARG:HG3	2.07	0.55
1:B:338:THR:O	1:B:342:MET:HG2	2.06	0.55
1:A:319:VAL:HG21	1:A:322:ARG:HH21	1.71	0.55
1:D:266:ARG:HH22	1:D:304:ASP:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:THR:O	1:C:168:LEU:HD12	2.07	0.54
1:C:162:ASN:HD21	1:D:254:ARG:HH22	1.55	0.54
1:A:254:ARG:HH22	1:B:162:ASN:HD21	1.54	0.54
1:C:101:ARG:HH11	1:C:101:ARG:HG3	1.73	0.53
1:C:179:TRP:H	1:C:179:TRP:CD1	2.26	0.53
1:A:237:HIS:HE1	1:B:243:SER:OG	1.91	0.53
1:D:118:SER:O	1:D:143:PHE:HA	2.08	0.53
1:D:325:ILE:HD12	1:D:325:ILE:N	2.24	0.53
1:B:109:GLN:HE21	1:B:171:HIS:HE1	1.55	0.52
1:C:259:VAL:HG23	1:C:334:VAL:CG2	2.39	0.52
1:A:314:VAL:HB	1:A:315:PRO:HD3	1.91	0.52
1:C:260:GLU:OE1	1:C:331:PHE:HB3	2.10	0.52
1:B:306:LEU:HD21	1:B:311:LEU:HG	1.91	0.52
1:B:184:ILE:O	1:B:188:LEU:HG	2.09	0.52
1:A:319:VAL:CG2	1:A:322:ARG:HH21	2.23	0.51
1:A:105:PHE:CZ	1:A:115:THR:HG21	2.46	0.51
1:D:170:ASP:OD2	1:D:187:HIS:HE1	1.93	0.51
1:A:273:GLU:OE2	1:A:273:GLU:HA	2.10	0.51
1:D:132:LEU:HD13	1:D:188:LEU:CD1	2.41	0.51
1:A:342:MET:HE1	1:A:351:LEU:CD2	2.41	0.51
1:A:319:VAL:HG22	1:A:322:ARG:HE	1.76	0.51
1:B:225:PRO:O	1:B:229:GLN:HG2	2.10	0.51
1:A:196:THR:HG22	1:A:198:ASN:H	1.75	0.51
1:A:334:VAL:O	1:A:338:THR:HG22	2.11	0.51
1:C:192:TYR:CE2	1:C:200:LEU:HB2	2.46	0.51
1:C:267:ARG:HA	1:C:299:VAL:HG21	1.92	0.51
1:D:260:GLU:OE1	1:D:331:PHE:HB3	2.11	0.51
1:A:131:VAL:HG21	1:A:185:LEU:CD2	2.33	0.50
1:C:105:PHE:CZ	1:C:115:THR:HG21	2.45	0.50
1:C:288:PRO:CG	1:C:291:GLN:HE21	2.24	0.50
1:D:311:LEU:O	1:D:314:VAL:HG12	2.10	0.50
1:D:334:VAL:O	1:D:338:THR:HG22	2.11	0.50
1:C:266:ARG:HB2	1:C:299:VAL:CG1	2.42	0.50
1:A:123:PRO:HB2	1:A:316:TRP:CE2	2.47	0.50
1:A:210:SER:HA	2:A:363:HOH:O	2.12	0.50
1:B:219:GLN:HA	1:B:223:HIS:HB3	1.92	0.50
1:A:152:ARG:HB2	1:A:152:ARG:HH21	1.77	0.50
1:C:170:ASP:OD2	1:C:187:HIS:HE1	1.94	0.50
1:B:191:LYS:O	1:B:195:GLU:HG3	2.11	0.50
1:B:134:GLU:CD	1:B:346:ALA:HB3	2.37	0.50
1:C:268:GLU:HA	1:C:289:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:TYR:HB3	1:D:150:GLU:HA	1.93	0.50
1:C:118:SER:HA	1:C:165:VAL:HB	1.93	0.50
1:D:123:PRO:HB2	1:D:316:TRP:CE2	2.47	0.50
1:B:310:ASP:HA	1:B:337:TRP:HZ2	1.77	0.49
1:B:297:TYR:CD1	1:B:298:PRO:HD2	2.48	0.49
1:C:267:ARG:NH1	1:C:297:TYR:O	2.39	0.49
1:A:320:VAL:O	1:A:323:ILE:HG12	2.13	0.49
1:B:102:ILE:HG13	1:B:150:GLU:HB3	1.93	0.49
1:C:144:LEU:HA	1:C:150:GLU:OE1	2.13	0.49
1:A:187:HIS:HD2	1:B:210:SER:OG	1.96	0.49
1:C:134:GLU:HB3	1:C:201:LEU:HD11	1.95	0.49
1:C:348:ILE:O	1:C:352:ARG:HB2	2.13	0.49
1:A:185:LEU:HD13	1:A:308:ILE:HB	1.95	0.49
1:A:161:PRO:HB2	1:B:258:VAL:HG13	1.95	0.48
1:B:271:VAL:C	1:B:273:GLU:H	2.21	0.48
1:B:293:ARG:NH1	1:B:294:PHE:HE1	2.09	0.48
1:B:125:GLY:HA2	1:B:166:PRO:HB3	1.95	0.48
1:C:184:ILE:O	1:C:188:LEU:HG	2.13	0.48
1:B:251:GLU:O	1:B:255:VAL:HG13	2.13	0.48
1:C:145:ASP:OD1	1:C:148:LEU:HD13	2.14	0.48
1:C:259:VAL:HG23	1:C:334:VAL:HG22	1.95	0.48
1:B:273:GLU:O	1:B:273:GLU:HG2	2.13	0.48
1:C:275:ASP:OD1	1:C:278:ASN:HB2	2.13	0.48
1:C:288:PRO:HG2	1:C:291:GLN:HE21	1.77	0.48
1:A:171:HIS:HA	1:A:175:ASN:HD22	1.77	0.48
1:A:102:ILE:HG22	1:A:106:PHE:CE1	2.48	0.48
1:A:164:ARG:NH1	1:B:254:ARG:HH21	2.12	0.48
1:B:326:ASN:C	1:B:326:ASN:ND2	2.69	0.47
1:B:322:ARG:HG3	1:B:322:ARG:NH1	2.28	0.47
1:C:110:PRO:HG2	1:C:171:HIS:CD2	2.49	0.47
1:B:132:LEU:HD13	1:B:188:LEU:HD11	1.97	0.47
1:D:186:LEU:HD21	1:D:213:ASN:HD21	1.78	0.47
1:B:145:ASP:OD1	1:B:147:ASN:HB3	2.14	0.47
1:C:278:ASN:HB3	1:C:282:TYR:CZ	2.50	0.47
1:A:266:ARG:CB	1:A:299:VAL:HG13	2.42	0.47
1:D:314:VAL:HG13	1:D:315:PRO:CD	2.35	0.47
1:D:96:HIS:N	1:D:96:HIS:CD2	2.83	0.46
1:B:109:GLN:NE2	1:B:169:ILE:HG21	2.31	0.46
1:C:272:MET:HE2	1:C:282:TYR:HD1	1.80	0.46
1:D:260:GLU:OE1	1:D:334:VAL:HG23	2.15	0.46
1:A:243:SER:OG	1:B:239:GLN:NE2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:HG12	1:B:300:TRP:N	2.31	0.46
1:C:123:PRO:HB2	1:C:316:TRP:CE2	2.51	0.46
1:C:152:ARG:HG3	2:C:419:HOH:O	2.15	0.46
1:A:106:PHE:CZ	1:A:159:VAL:HG21	2.50	0.46
1:A:114:TYR:O	1:A:139:TYR:HA	2.15	0.46
1:C:160:ASN:ND2	1:C:164:ARG:O	2.47	0.46
1:C:278:ASN:HB3	1:C:282:TYR:CE1	2.51	0.46
1:A:171:HIS:HA	1:A:175:ASN:ND2	2.31	0.46
1:D:159:VAL:HG13	1:D:177:SER:OG	2.16	0.46
1:D:159:VAL:HG13	1:D:177:SER:CB	2.45	0.46
1:C:256:TYR:O	1:C:259:VAL:HG22	2.16	0.46
1:A:247:ARG:HH21	1:B:229:GLN:HE22	1.63	0.46
1:B:111:LEU:CD1	1:B:112:GLU:N	2.78	0.46
1:B:267:ARG:NH1	1:B:297:TYR:O	2.41	0.46
1:B:326:ASN:OD1	1:B:329:ILE:HD12	2.16	0.45
1:C:288:PRO:HG2	1:C:291:GLN:CG	2.38	0.45
1:A:314:VAL:HG22	1:A:341:MET:CE	2.46	0.45
1:D:224:ALA:HB3	1:D:225:PRO:HD3	1.98	0.45
1:A:256:TYR:O	1:A:259:VAL:HG22	2.15	0.45
1:A:266:ARG:CB	1:A:299:VAL:CG1	2.94	0.45
1:B:108:GLU:O	1:B:108:GLU:HG3	2.15	0.45
1:A:119:HIS:HE1	2:A:369:HOH:O	1.99	0.45
1:B:173:MET:O	1:B:174:ASP:HB3	2.17	0.45
1:C:237:HIS:HE1	1:D:243:SER:OG	1.99	0.45
1:D:326:ASN:ND2	1:D:329:ILE:H	2.12	0.44
1:A:159:VAL:HG13	1:A:169:ILE:HD11	1.99	0.44
1:A:266:ARG:HB3	1:A:299:VAL:CG1	2.46	0.44
1:D:344:ARG:HA	1:D:345:PRO:HD3	1.91	0.44
1:B:128:VAL:O	1:B:132:LEU:HB2	2.18	0.44
1:C:266:ARG:HB2	1:C:299:VAL:HG13	2.00	0.44
1:B:97:VAL:HA	1:B:148:LEU:O	2.17	0.44
1:D:223:HIS:CD2	1:D:227:ILE:HD11	2.53	0.44
1:D:170:ASP:CG	1:D:191:LYS:HZ2	2.24	0.44
1:D:186:LEU:HD21	1:D:213:ASN:ND2	2.33	0.44
1:B:253:ARG:NH1	1:B:325:ILE:HG12	2.33	0.44
1:B:274:LEU:HB2	2:B:372:HOH:O	2.18	0.44
1:A:118:SER:OG	1:A:125:GLY:HA3	2.18	0.43
1:A:128:VAL:HG12	1:A:132:LEU:HD22	1.99	0.43
1:D:189:VAL:HB	1:D:202:TRP:HB2	2.00	0.43
1:A:171:HIS:ND1	1:A:175:ASN:ND2	2.66	0.43
1:C:105:PHE:HD2	1:C:106:PHE:CD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLU:OE2	1:D:333:GLU:HB2	2.18	0.43
1:C:262:ALA:O	1:C:266:ARG:HG2	2.18	0.43
1:C:128:VAL:O	1:C:132:LEU:HB2	2.18	0.43
1:A:118:SER:HA	1:A:165:VAL:HB	1.99	0.43
1:A:241:ILE:HG21	1:B:241:ILE:CD1	2.49	0.43
1:A:243:SER:OG	1:B:237:HIS:HE1	2.02	0.43
1:C:146:PHE:HZ	1:C:165:VAL:HG13	1.82	0.43
1:C:201:LEU:HA	1:C:306:LEU:O	2.19	0.43
1:B:135:LEU:HD21	1:B:201:LEU:HD12	2.00	0.43
1:B:266:ARG:HB2	1:B:299:VAL:CG1	2.48	0.43
1:D:235:TYR:HB2	1:D:236:PHE:CE1	2.54	0.43
1:D:325:ILE:N	1:D:325:ILE:CD1	2.82	0.43
1:C:118:SER:OG	1:C:119:HIS:N	2.48	0.42
1:B:105:PHE:CZ	1:B:115:THR:HG21	2.54	0.42
1:A:259:VAL:HG23	1:A:334:VAL:CG2	2.49	0.42
1:A:118:SER:O	1:A:143:PHE:HA	2.19	0.42
1:A:152:ARG:HB2	1:A:152:ARG:NH2	2.34	0.42
1:C:198:ASN:HD22	1:C:199:PRO:N	2.17	0.42
1:C:217:PHE:CE2	1:D:182:GLY:HA3	2.54	0.42
1:B:201:LEU:HA	1:B:307:THR:HA	2.01	0.42
1:C:201:LEU:HA	1:C:307:THR:HA	2.01	0.42
1:D:109:GLN:HA	1:D:110:PRO:HD3	1.90	0.42
1:D:262:ALA:O	1:D:266:ARG:HG2	2.20	0.42
1:A:119:HIS:CE1	2:A:369:HOH:O	2.71	0.42
1:B:219:GLN:O	1:B:223:HIS:HB3	2.19	0.42
1:C:178:ILE:HD12	1:C:178:ILE:N	2.35	0.42
1:D:282:TYR:CD2	1:D:289:MET:HE3	2.55	0.42
1:A:119:HIS:HB2	1:A:146:PHE:CE1	2.55	0.41
1:C:102:ILE:N	1:C:102:ILE:HD12	2.36	0.41
1:C:102:ILE:O	1:C:106:PHE:HD1	2.03	0.41
1:C:116:LEU:C	1:C:116:LEU:CD2	2.92	0.41
1:C:219:GLN:HB2	1:C:313:PHE:CZ	2.56	0.41
1:D:272:MET:HE3	1:D:279:ALA:HB1	2.01	0.41
1:B:178:ILE:HD12	1:B:178:ILE:H	1.83	0.41
1:C:198:ASN:C	1:C:198:ASN:ND2	2.78	0.41
1:C:272:MET:HE1	1:C:282:TYR:CB	2.50	0.41
1:A:207:ALA:O	1:A:211:GLN:HG2	2.19	0.41
1:D:112:GLU:HG3	2:D:382:HOH:O	2.19	0.41
1:D:170:ASP:OD2	1:D:191:LYS:NZ	2.48	0.41
1:A:155:GLU:CD	1:A:155:GLU:H	2.28	0.41
1:A:298:PRO:HB3	1:A:340:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:C	1:A:198:ASN:ND2	2.78	0.41
1:A:109:GLN:HG3	1:A:110:PRO:HD2	2.03	0.41
1:A:119:HIS:O	1:A:121:SER:N	2.54	0.41
1:A:196:THR:HG22	1:A:198:ASN:N	2.36	0.41
1:C:225:PRO:O	1:C:229:GLN:HG2	2.21	0.41
1:C:254:ARG:NH1	1:D:162:ASN:ND2	2.63	0.41
1:A:202:TRP:CG	1:A:203:SER:N	2.86	0.41
1:B:219:GLN:HB2	1:B:313:PHE:CZ	2.55	0.41
1:C:101:ARG:NH2	1:C:142:ILE:HG23	2.35	0.41
1:C:155:GLU:O	1:C:158:SER:HB3	2.21	0.41
1:A:105:PHE:CE2	1:A:109:GLN:NE2	2.89	0.40
1:A:159:VAL:CG1	1:A:169:ILE:HD11	2.51	0.40
1:A:271:VAL:C	1:A:273:GLU:N	2.79	0.40
1:B:148:LEU:HD13	1:C:297:TYR:OH	2.21	0.40
1:B:274:LEU:HD23	1:B:294:PHE:CZ	2.56	0.40
1:C:154:PRO:HA	1:C:157:VAL:HG12	2.02	0.40
1:A:103:THR:C	1:A:105:PHE:H	2.29	0.40
1:A:187:HIS:CD2	1:B:210:SER:OG	2.74	0.40
1:A:102:ILE:O	1:A:105:PHE:HB3	2.21	0.40
1:A:314:VAL:HG22	1:A:341:MET:HE3	2.04	0.40
1:B:198:ASN:ND2	1:B:200:LEU:HG	2.36	0.40
1:B:229:GLN:HB2	1:B:248:TYR:CD2	2.56	0.40
1:C:294:PHE:HA	1:C:297:TYR:CD1	2.56	0.40
1:C:349:LYS:HZ3	1:C:354:GLU:C	2.29	0.40
1:D:281:ALA:HB1	1:D:287:THR:OG1	2.22	0.40
1:C:241:ILE:HG22	1:C:244:ALA:H	1.87	0.40
1:D:232:HIS:NE2	1:D:237:HIS:CD2	2.83	0.40

There are no symmetry-related clashes.

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	230/261 (88%)	214 (93%)	15 (6%)	1 (0%)	30	49
1	B	238/261 (91%)	222 (93%)	14 (6%)	2 (1%)	16	31
1	C	253/261 (97%)	239 (94%)	13 (5%)	1 (0%)	30	49
1	D	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
All	All	978/1044 (94%)	924 (94%)	50 (5%)	4 (0%)	30	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	278	ASN
1	A	120	ARG
1	B	274	LEU
1	B	275	ASP

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	202/224 (90%)	195 (96%)	7 (4%)	32	58
1	B	210/224 (94%)	201 (96%)	9 (4%)	26	51
1	C	218/224 (97%)	209 (96%)	9 (4%)	27	53
1	D	222/224 (99%)	211 (95%)	11 (5%)	22	44
All	All	852/896 (95%)	816 (96%)	36 (4%)	26	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	112	GLU
1	A	132	LEU
1	A	200	LEU
1	A	314	VAL
1	A	319	VAL
1	A	351	LEU

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Mol	Chain	Res	Type
1	B	108	GLU
1	B	111	LEU
1	B	112	GLU
1	B	148	LEU
1	B	159	VAL
1	B	293	ARG
1	B	302	VAL
1	B	306	LEU
1	B	326	ASN
1	C	111	LEU
1	C	116	LEU
1	C	132	LEU
1	C	190	ASN
1	C	200	LEU
1	C	267	ARG
1	C	272	MET
1	C	299	VAL
1	C	326	ASN
1	D	96	HIS
1	D	116	LEU
1	D	132	LEU
1	D	159	VAL
1	D	178	ILE
1	D	200	LEU
1	D	289	MET
1	D	314	VAL
1	D	339	LYS
1	D	351	LEU
1	D	354	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	A	140	ASN
1	A	147	ASN
1	A	160	ASN
1	A	162	ASN
1	A	175	ASN
1	A	187	HIS
1	A	198	ASN
1	A	209	GLN

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	213	ASN
1	A	219	GLN
1	A	229	GLN
1	A	237	HIS
1	A	317	ASN
1	A	340	HIS
1	B	109	GLN
1	B	151	HIS
1	B	162	ASN
1	B	175	ASN
1	B	187	HIS
1	B	198	ASN
1	B	209	GLN
1	B	213	ASN
1	B	219	GLN
1	B	229	GLN
1	B	237	HIS
1	B	239	GLN
1	B	318	ASN
1	B	326	ASN
1	C	107	GLN
1	C	119	HIS
1	C	138	HIS
1	C	162	ASN
1	C	187	HIS
1	C	198	ASN
1	C	209	GLN
1	C	211	GLN
1	C	213	ASN
1	C	219	GLN
1	C	229	GLN
1	C	237	HIS
1	C	239	GLN
1	C	291	GLN
1	C	317	ASN
1	D	96	HIS
1	D	109	GLN
1	D	138	HIS
1	D	147	ASN
1	D	162	ASN
1	D	175	ASN

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Mol	Chain	Res	Type
1	D	187	HIS
1	D	190	ASN
1	D	209	GLN
1	D	213	ASN
1	D	219	GLN
1	D	229	GLN
1	D	237	HIS
1	D	317	ASN
1	D	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 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	234/261 (89%)	0.01	11 (4%) 36 32	15, 27, 69, 80	0
1	B	242/261 (92%)	0.08	11 (4%) 38 33	17, 31, 63, 80	0
1	C	255/261 (97%)	-0.13	3 (1%) 76 73	13, 24, 58, 66	0
1	D	259/261 (99%)	-0.25	2 (0%) 82 80	12, 25, 44, 75	0
All	All	990/1044 (94%)	-0.08	27 (2%) 56 51	12, 27, 62, 80	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	LEU	4.2
1	A	102	ILE	3.5
1	B	111	LEU	3.3
1	B	271	VAL	3.3
1	A	103	THR	3.2
1	A	274	LEU	3.2
1	B	97	VAL	2.8
1	B	295	PHE	2.8
1	A	353	GLY	2.7
1	C	149	GLY	2.6
1	A	105	PHE	2.6
1	A	104	LYS	2.5
1	A	107	GLN	2.5
1	A	106	PHE	2.4
1	B	292	SER	2.4
1	C	148	LEU	2.3
1	A	100	SER	2.3
1	B	269	ALA	2.3
1	B	276	THR	2.2
1	D	96	HIS	2.2
1	A	157	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	296	ASP	2.1
1	B	272	MET	2.1
1	C	276	THR	2.1
1	B	297	TYR	2.0
1	D	97	VAL	2.0
1	A	275	ASP	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.