Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 01:28 pm GMT

PDB ID	:	1G6W
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

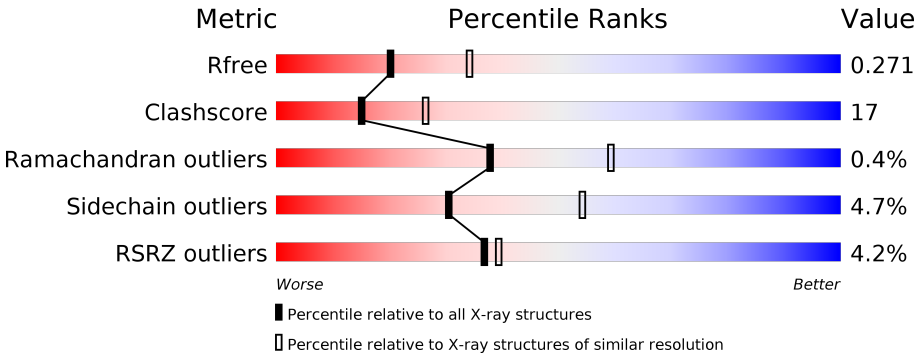
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	5% 58% 30% • 10%
1	B	261	7% 58% 30% • 7%
1	C	261	3% 60% 34% • •
1	D	261	2% 70% 27% • •

2 Entry composition (i)

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.

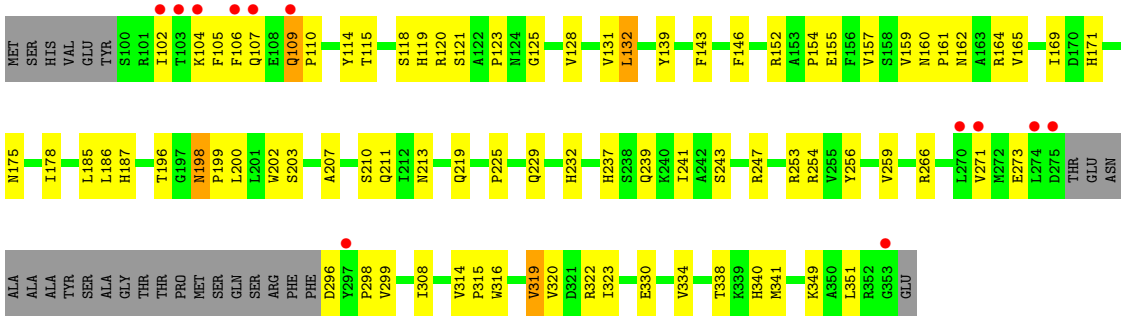
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	68	Total	O	0	0
			68	68		
2	C	69	Total	O	0	0
			69	69		
2	D	85	Total	O	0	0
			85	85		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

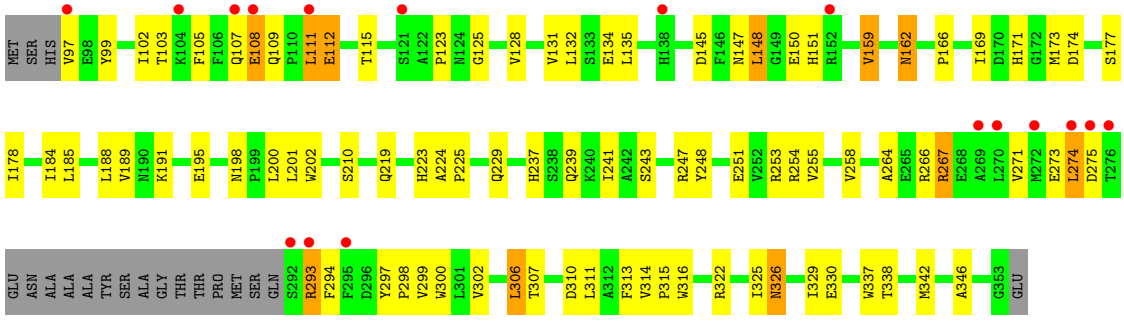
- Molecule 1: URE2 PROTEIN

Chain A:



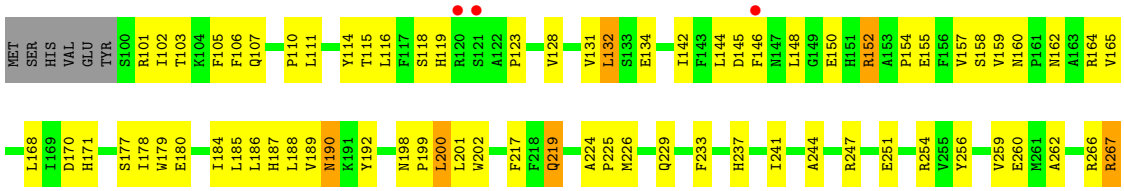
- Molecule 1: URE2 PROTEIN

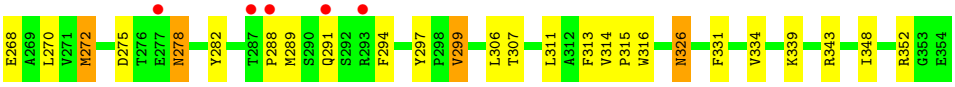
Chain B:



- Molecule 1: URE2 PROTEIN

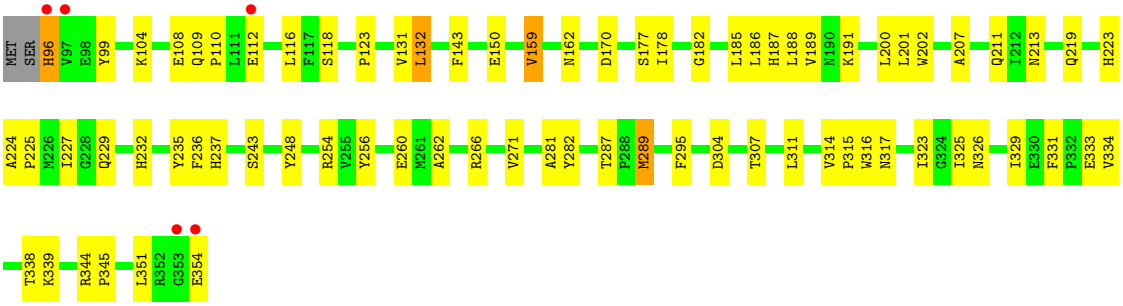
Chain C:





• Molecule 1: URE2 PROTEIN

Chain D:



4 Data and refinement statistics (i)

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 19.93 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 95.7 (19.93-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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%)	DCC
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 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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

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	0.37	0/1960	0.60	0/2661
1	B	0.36	0/2037	0.58	0/2765
1	C	0.37	0/2123	0.59	0/2884
1	D	0.38	0/2164	0.59	0/2939
All	All	0.37	0/8284	0.59	0/11249

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	1907	0	1876	77	0
1	B	1981	0	1943	76	0
1	C	2065	0	2018	81	0
1	D	2104	0	2049	56	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	268	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 17.

All (268) 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: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:D:282:TYR:HB3	1:D:289:MET:HE1	1.62	0.82
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
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: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:111:LEU:CD1	1:B:112:GLU:H	2.08	0.66
1:C:226:MET:HE2	1:C:251:GLU:HG2	1.77	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:B:326:ASN:C	1:B:326:ASN:HD22	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:103:THR:O	1:C:107:GLN:HG2	2.00	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
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: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:C:226:MET:HE3	1:C:251:GLU:HG2	1.85	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:326:ASN:HD22	1:C:326:ASN:C	2.07	0.58
1:C:198:ASN:HD22	1:C:199:PRO:CD	2.16	0.57
1:B:178:ILE:HD12	1:B:178:ILE:N	2.19	0.57
1:A:102:ILE:HG22	1:A:106:PHE:HE1	1.69	0.57
1:A:178:ILE:HD12	1:A:178:ILE:N	2.18	0.57
1:B:293:ARG:HH11	1:B:294:PHE:HE1	1.51	0.57
1:C:145:ASP:CG	1:C:148:LEU:HD13	2.25	0.56
1:A:198:ASN:HD22	1:A:199:PRO:CD	2.17	0.56
1:B:189:VAL:HB	1:B:202:TRP:HB2	1.88	0.56
1:A:229:GLN:HE22	1:B:247:ARG:HH21	1.53	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:C:233:PHE:HE1	1:D:248:TYR:HH	1.53	0.56
1:A:225:PRO:O	1:A:229:GLN:HG2	2.05	0.56
1:B:266:ARG:HB2	1:B:299:VAL:HG11	1.87	0.56
1:A:232:HIS:NE2	1:A:237:HIS:HD2	2.04	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG3	1:C:101:ARG:HH11	1.73	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:N	1:D:325:ILE:HD12	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:271:VAL:C	1:A:273:GLU:H	2.13	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:109:GLN:HG2	1:A:175:ASN:CG	2.30	0.51
1:A:105:PHE:CZ	1:A:115:THR:HG21	2.46	0.51
1:A:273:GLU:HA	1:A:273:GLU:OE2	2.10	0.51
1:A:349:LYS:C	1:A:349:LYS:HD3	2.31	0.51
1:D:170:ASP:OD2	1:D:187:HIS:HE1	1.93	0.51
1:D:132:LEU:HD13	1:D:188:LEU:CD1	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:210:SER:HA	2:A:363:HOH:O	2.12	0.50
1:A:123:PRO:HB2	1:A:316:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLN:HA	1:B:223:HIS:HB3	1.92	0.50
1:A:152:ARG:HH21	1:A:152:ARG:HB2	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:C:268:GLU:HA	1:C:289:MET:CE	2.42	0.50
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: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:C:272:MET:HE2	1:C:282:TYR:HD1	1.79	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:CD2	1:D:96:HIS:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLN:NE2	1:B:169:ILE:HG21	2.31	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
1:B:299:VAL:HG12	1:B:300:TRP:N	2.31	0.46
1:C:152:ARG:HG3	2:C:419:HOH:O	2.15	0.46
1:C:123:PRO:HB2	1:C:316:TRP:CE2	2.51	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:B:111:LEU:CD1	1:B:112:GLU:N	2.78	0.46
1:A:247:ARG:HH21	1:B:229:GLN:HE22	1.63	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:HG3	1:B:108:GLU:O	2.15	0.45
1:B:134:GLU:CD	1:B:346:ALA:HB3	2.37	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:B:326:ASN:C	1:B:326:ASN:ND2	2.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:243:SER:OG	1:B:237:HIS:HE1	2.02	0.43
1:A:241:ILE:HG21	1:B:241:ILE:CD1	2.49	0.43
1:B:271:VAL:C	1:B:273:GLU:H	2.21	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:NH2	1:A:152:ARG:HB2	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:170:ASP:CG	1:D:191:LYS:HZ2	2.21	0.42
1:D:271:VAL:HG11	1:D:289:MET:HE3	2.02	0.42
1:A:119:HIS:HB2	1:A:146:PHE:CE1	2.55	0.41
1:C:102:ILE:HD12	1:C:102:ILE:N	2.36	0.41
1:C:102:ILE:O	1:C:106:PHE:HD1	2.03	0.41
1:C:219:GLN:HB2	1:C:313:PHE:CZ	2.56	0.41
1:B:178:ILE:HD12	1:B:178:ILE:H	1.83	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: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:109:GLN:HG3	1:A:110:PRO:HD2	2.03	0.41
1:A:196:THR:HG22	1:A:198:ASN:N	2.36	0.41
1:C:254:ARG:NH1	1:D:162:ASN:ND2	2.63	0.41
1:A:119:HIS:O	1:A:121:SER:N	2.54	0.41
1:C:225:PRO:O	1:C:229:GLN:HG2	2.21	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: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: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: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:272:MET:HE1	1:C:282:TYR:CB	2.51	0.40
1:C:294:PHE:HA	1:C:297:TYR:CD1	2.56	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 (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	230/261 (88%)	214 (93%)	15 (6%)	1 (0%)	38 59
1	B	238/261 (91%)	222 (93%)	14 (6%)	2 (1%)	22 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	253/261 (97%)	239 (94%)	13 (5%)	1 (0%)	38 59
1	D	257/261 (98%)	249 (97%)	8 (3%)	0	100 100
All	All	978/1044 (94%)	924 (94%)	50 (5%)	4 (0%)	38 59

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 (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	202/224 (90%)	194 (96%)	8 (4%)	36 62
1	B	210/224 (94%)	199 (95%)	11 (5%)	27 49
1	C	218/224 (97%)	207 (95%)	11 (5%)	28 51
1	D	222/224 (99%)	212 (96%)	10 (4%)	32 56
All	All	852/896 (95%)	812 (95%)	40 (5%)	30 54

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	132	LEU
1	A	160	ASN
1	A	198	ASN
1	A	200	LEU
1	A	219	GLN
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	162	ASN
1	B	267	ARG
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	152	ARG
1	C	190	ASN
1	C	200	LEU
1	C	219	GLN
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	200	LEU
1	D	219	GLN
1	D	289	MET
1	D	339	LYS
1	D	351	LEU
1	D	354	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	119	HIS
1	A	147	ASN
1	A	160	ASN
1	A	162	ASN
1	A	175	ASN

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Mol	Chain	Res	Type
1	A	187	HIS
1	A	190	ASN
1	A	198	ASN
1	A	209	GLN
1	A	213	ASN
1	A	219	GLN
1	A	229	GLN
1	A	237	HIS
1	A	317	ASN
1	A	318	ASN
1	B	109	GLN
1	B	151	HIS
1	B	162	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	109	GLN
1	C	119	HIS
1	C	162	ASN
1	C	187	HIS
1	C	198	ASN
1	C	209	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	C	326	ASN
1	D	96	HIS
1	D	109	GLN
1	D	147	ASN
1	D	162	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	239	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	234/261 (89%)	0.13	12 (5%)	29	30	15, 27, 69, 80	0
1	B	242/261 (92%)	0.11	17 (7%)	17	17	17, 31, 63, 80	0
1	C	255/261 (97%)	-0.16	8 (3%)	49	52	13, 24, 58, 66	0
1	D	259/261 (99%)	-0.17	5 (1%)	67	69	12, 25, 44, 75	0
All	All	990/1044 (94%)	-0.03	42 (4%)	37	39	12, 27, 62, 80	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107	GLN	6.1
1	A	103	THR	5.5
1	A	353	GLY	4.9
1	D	96	HIS	4.5
1	A	106	PHE	4.1
1	D	354	GLU	4.0
1	D	353	GLY	3.9
1	B	276	THR	3.8
1	B	97	VAL	3.7
1	A	102	ILE	3.6
1	B	270	LEU	3.4
1	B	107	GLN	3.3
1	C	293	ARG	3.2
1	A	104	LYS	3.1
1	B	275	ASP	3.0
1	C	146	PHE	3.0
1	B	111	LEU	3.0
1	A	271	VAL	2.9
1	A	274	LEU	2.9
1	A	275	ASP	2.8
1	C	291	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	272	MET	2.7
1	A	109	GLN	2.7
1	B	269	ALA	2.7
1	C	121	SER	2.6
1	B	152	ARG	2.6
1	C	288	PRO	2.6
1	C	277	GLU	2.6
1	C	120	ARG	2.5
1	A	297	TYR	2.5
1	B	121	SER	2.5
1	B	295	PHE	2.5
1	D	97	VAL	2.4
1	B	292	SER	2.4
1	B	293	ARG	2.3
1	B	138	HIS	2.3
1	B	274	LEU	2.3
1	B	104	LYS	2.2
1	A	270	LEU	2.1
1	B	108	GLU	2.1
1	D	112	GLU	2.1
1	C	287	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.