Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:39 pm BST

PDB ID	:	1UOC
Title	:	X-ray structure of the RNase domain of the yeast Pop2 protein
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Deposited on	:	2003-09-16
Resolution	:	2.30 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 ①) were used in the production of this report:

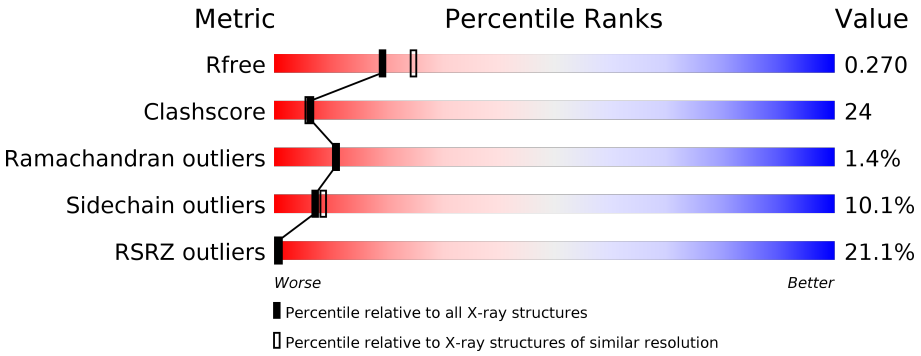
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	289	18% 53% 32% 6% 9%
1	B	289	19% 53% 29% 6% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4263 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 POP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2148	1392	340	405	11			
1	B	254	Total	C	N	O	S	0	0	0
			2066	1340	326	389	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Xe	0	0
			1	1		
3	A	1	Total	Xe	0	0
			1	1		

- Molecule 4 is water.

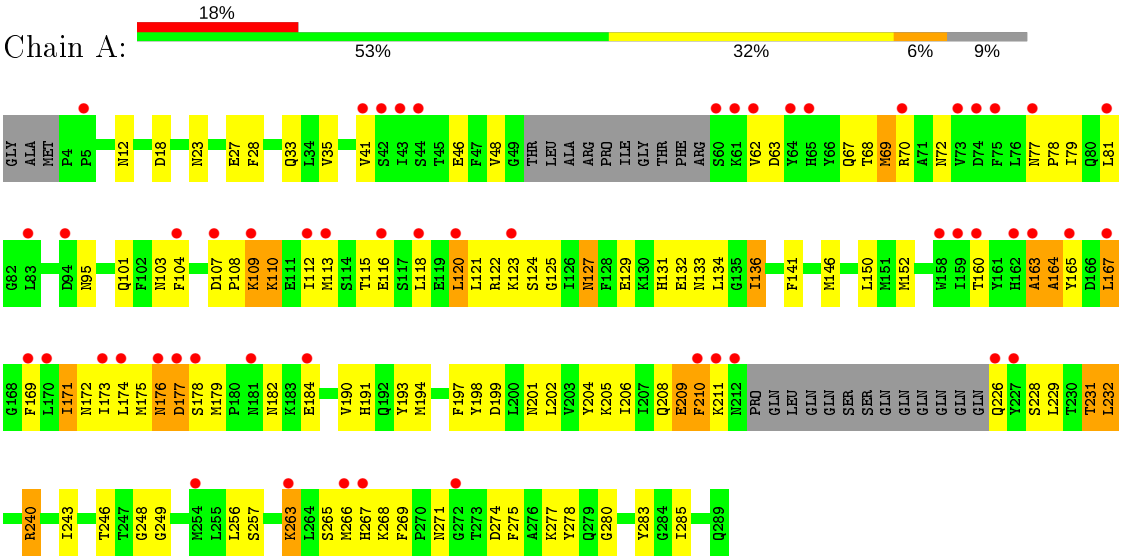
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	16	Total	O	0	0
			16	16		

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.

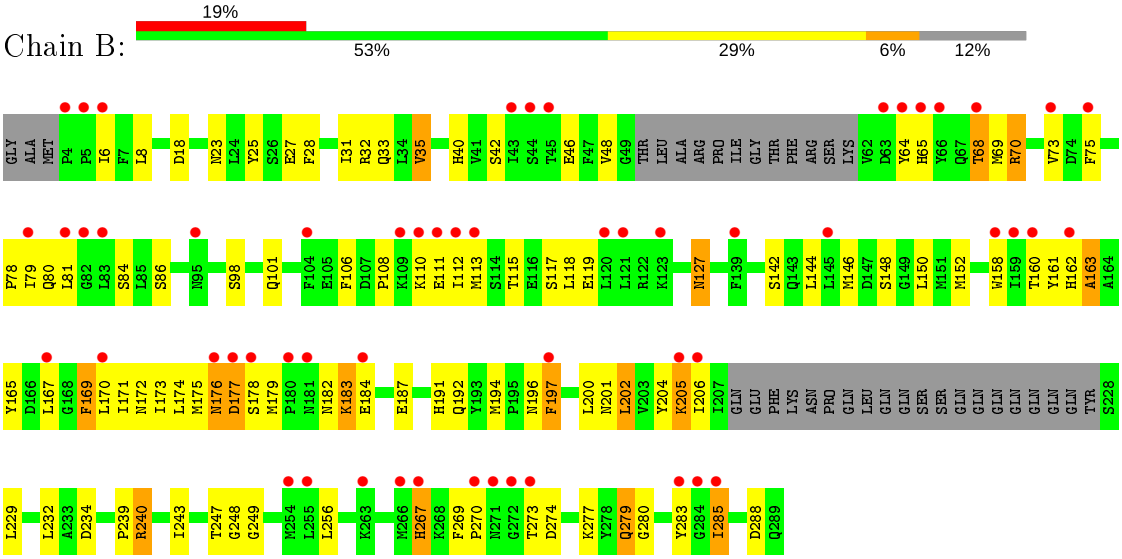
- Molecule 1: POP2

Chain A:



- Molecule 1: POP2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.58Å 79.44Å 101.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.97 – 2.30 28.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (9.97-2.30) 95.5 (28.90-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.64 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.265 0.247 , 0.270	Depositor DCC
R_{free} test set	2615 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4263	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: CA, XE

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	0.39	0/2207	0.62	0/2990
1	B	0.37	0/2123	0.61	0/2879
All	All	0.38	0/4330	0.62	0/5869

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	2148	0	2060	104	0
1	B	2066	0	1983	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
4	A	29	0	0	0	0
4	B	16	0	0	2	0
All	All	4263	0	4043	197	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 24.

All (197) 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:171:ILE:HG13	3:A:1291:XE:XE	2.50	0.89
1:A:205:LYS:O	1:A:209:GLU:HB2	1.73	0.88
1:A:101:GLN:HE21	1:A:248:GLY:H	1.20	0.88
1:A:202:LEU:HD11	1:A:278:TYR:CD2	2.08	0.88
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.38	0.86
1:B:35:VAL:HG11	1:B:150:LEU:HD22	1.59	0.84
1:B:171:ILE:HG12	3:B:1291:XE:XE	2.57	0.83
1:B:172:ASN:HD22	1:B:179:MET:HG2	1.43	0.82
1:A:211:LYS:HA	1:A:211:LYS:HE2	1.61	0.81
1:A:163:ALA:HB1	1:A:167:LEU:HD22	1.62	0.81
1:A:136:ILE:CD1	1:A:141:PHE:HB2	2.10	0.81
1:A:136:ILE:HD11	1:A:141:PHE:HB2	1.66	0.76
1:A:226:GLN:HB3	1:A:231:THR:HG21	1.68	0.75
1:B:183:LYS:HA	1:B:183:LYS:HZ1	1.52	0.75
1:B:182:ASN:ND2	1:B:184:GLU:HB3	2.02	0.75
1:B:101:GLN:HE21	1:B:248:GLY:H	1.33	0.74
1:A:110:LYS:HZ2	1:A:112:ILE:HD13	1.53	0.74
1:A:41:VAL:HG21	1:A:150:LEU:HD22	1.70	0.73
1:B:273:THR:HG21	1:B:277:LYS:HD3	1.71	0.73
1:A:35:VAL:HG21	1:A:150:LEU:HD23	1.69	0.73
1:A:228:SER:OG	1:A:231:THR:HG22	1.89	0.73
1:B:64:TYR:O	1:B:68:THR:HG22	1.88	0.72
1:A:263:LYS:HE3	1:A:263:LYS:HA	1.71	0.72
1:B:205:LYS:HA	1:B:205:LYS:NZ	2.04	0.72
1:B:170:LEU:O	1:B:174:LEU:HB2	1.92	0.70
1:A:48:VAL:HG12	1:A:121:LEU:HD11	1.74	0.70
1:B:98:SER:HB2	4:B:2007:HOH:O	1.92	0.69
1:A:167:LEU:HG	1:A:194:MET:HE1	1.75	0.69
1:A:101:GLN:NE2	1:A:248:GLY:H	1.90	0.69
1:B:183:LYS:HE3	1:B:187:GLU:HG3	1.74	0.68
1:A:127:ASN:C	1:A:127:ASN:HD22	1.97	0.68
1:A:240:ARG:HG2	1:A:240:ARG:NH1	2.10	0.67
1:A:167:LEU:HG	1:A:194:MET:CE	2.24	0.67
1:B:6:ILE:HD11	1:B:8:LEU:HD13	1.76	0.67
1:B:173:ILE:HG13	1:B:174:LEU:N	2.09	0.67
1:A:182:ASN:HD22	1:A:184:GLU:HG2	1.58	0.67
1:B:127:ASN:HD22	1:B:127:ASN:C	1.98	0.67
1:A:206:ILE:HD11	1:A:269:PHE:CE2	2.29	0.66
1:B:160:THR:OG1	1:B:163:ALA:HB2	1.96	0.66
1:B:183:LYS:HA	1:B:183:LYS:NZ	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HG21	1:A:163:ALA:HB2	1.79	0.64
1:B:101:GLN:NE2	1:B:248:GLY:H	1.95	0.64
1:B:158:TRP:HB2	1:B:197:PHE:HB2	1.79	0.63
1:A:163:ALA:O	1:A:165:TYR:N	2.33	0.62
1:A:48:VAL:HB	1:A:113:MET:CE	2.29	0.62
1:A:101:GLN:HE21	1:A:248:GLY:N	1.95	0.62
1:A:202:LEU:HD11	1:A:278:TYR:HD2	1.65	0.62
1:B:110:LYS:HB3	1:B:110:LYS:HZ2	1.66	0.61
1:A:210:PHE:HE2	1:A:271:ASN:HB3	1.64	0.61
1:B:69:MET:O	1:B:73:VAL:HG13	2.00	0.61
1:B:152:MET:HG2	1:B:192:GLN:O	2.02	0.60
1:B:35:VAL:CG1	1:B:150:LEU:HD22	2.31	0.59
1:A:226:GLN:HA	1:A:226:GLN:HE21	1.67	0.59
1:A:112:ILE:O	1:A:112:ILE:CG2	2.51	0.58
1:B:183:LYS:HE2	1:B:283:TYR:CD1	2.38	0.58
1:B:160:THR:CB	1:B:163:ALA:HB2	2.34	0.58
1:B:176:ASN:HB2	1:B:178:SER:OG	2.04	0.58
1:B:196:ASN:HA	1:B:279:GLN:OE1	2.04	0.57
1:B:267:HIS:CG	1:B:267:HIS:O	2.58	0.57
1:A:112:ILE:O	1:A:112:ILE:HG22	2.04	0.56
1:A:167:LEU:CG	1:A:194:MET:HE1	2.34	0.56
1:A:204:TYR:CE1	1:A:232:LEU:HD23	2.39	0.56
1:B:173:ILE:HG13	1:B:174:LEU:H	1.69	0.56
1:A:48:VAL:HB	1:A:113:MET:SD	2.45	0.56
1:B:169:PHE:CE1	1:B:173:ILE:HD13	2.41	0.56
1:B:81:LEU:C	1:B:81:LEU:HD23	2.26	0.56
1:B:234:ASP:OD1	1:B:240:ARG:NH1	2.38	0.55
1:B:40:HIS:HB2	1:B:86:SER:O	2.06	0.55
1:A:108:PRO:HG2	1:A:132:GLU:CD	2.27	0.55
1:B:113:MET:HB2	1:B:117:SER:HB2	1.87	0.55
1:B:46:GLU:O	1:B:79:ILE:HG22	2.07	0.54
1:B:191:HIS:HE1	1:B:280:GLY:O	1.89	0.54
1:A:123:LYS:C	1:A:125:GLY:H	2.11	0.54
1:A:133:ASN:O	1:A:134:LEU:HD23	2.08	0.54
1:B:175:MET:C	1:B:177:ASP:H	2.11	0.54
1:A:266:MET:O	1:A:267:HIS:ND1	2.41	0.54
1:A:70:ARG:HH21	1:A:70:ARG:HG3	1.73	0.53
1:B:23:ASN:O	1:B:27:GLU:HG2	2.09	0.53
1:B:243:ILE:O	1:B:249:GLY:HA3	2.09	0.53
1:B:31:ILE:O	1:B:35:VAL:HG22	2.09	0.53
1:A:127:ASN:ND2	1:A:129:GLU:H	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD12	1:A:169:PHE:HE2	1.72	0.53
1:B:269:PHE:HB3	1:B:270:PRO:CD	2.39	0.53
1:B:172:ASN:HD22	1:B:179:MET:CG	2.18	0.53
1:A:172:ASN:ND2	1:A:179:MET:HG2	2.24	0.53
1:B:110:LYS:HB3	1:B:110:LYS:NZ	2.24	0.52
1:B:167:LEU:HG	1:B:194:MET:HE1	1.91	0.52
1:A:202:LEU:O	1:A:206:ILE:HG23	2.09	0.52
1:A:116:GLU:O	1:A:120:LEU:HB2	2.09	0.52
1:A:208:GLN:HA	1:A:208:GLN:OE1	2.09	0.52
1:B:25:TYR:CE2	1:B:144:LEU:HD21	2.45	0.52
1:A:177:ASP:OD2	1:A:177:ASP:C	2.48	0.51
1:B:78:PRO:HG2	1:B:169:PHE:CE1	2.45	0.51
1:B:69:MET:HA	1:B:165:TYR:CZ	2.45	0.51
1:A:123:LYS:O	1:A:125:GLY:N	2.43	0.51
1:A:266:MET:O	1:A:268:LYS:HG2	2.11	0.51
1:B:240:ARG:HG2	1:B:240:ARG:HH11	1.74	0.51
1:B:277:LYS:HE3	1:B:285:ILE:HD12	1.92	0.51
1:A:48:VAL:HB	1:A:113:MET:HE2	1.92	0.51
1:B:205:LYS:HA	1:B:205:LYS:HZ2	1.75	0.51
1:A:67:GLN:HE22	1:A:70:ARG:NH1	2.09	0.51
1:A:160:THR:HG23	1:A:199:ASP:HA	1.93	0.51
1:A:160:THR:HG22	1:A:198:TYR:O	2.10	0.51
1:B:167:LEU:HG	1:B:194:MET:CE	2.42	0.50
1:B:35:VAL:HG11	1:B:150:LEU:CD2	2.36	0.50
1:B:98:SER:HB3	4:B:2010:HOH:O	2.11	0.50
1:A:69:MET:C	1:A:69:MET:HE2	2.32	0.50
1:A:101:GLN:HE22	1:A:246:THR:HB	1.75	0.50
1:A:226:GLN:HA	1:A:226:GLN:NE2	2.26	0.50
1:B:285:ILE:HG23	1:B:288:ASP:OD2	2.12	0.50
1:A:191:HIS:HE1	1:A:280:GLY:O	1.95	0.50
1:B:115:THR:O	1:B:119:GLU:HG2	2.11	0.50
1:A:104:PHE:CE2	1:A:136:ILE:HD11	2.47	0.49
1:B:161:TYR:HD1	1:B:200:LEU:HB3	1.77	0.49
1:A:152:MET:HE2	1:A:193:TYR:CE2	2.47	0.49
1:A:176:ASN:C	1:A:178:SER:H	2.15	0.49
1:B:148:SER:OG	1:B:150:LEU:HG	2.13	0.49
1:A:69:MET:HE2	1:A:69:MET:O	2.13	0.49
1:B:48:VAL:O	1:B:48:VAL:HG23	2.12	0.49
1:A:210:PHE:CE2	1:A:271:ASN:HB3	2.46	0.48
1:B:182:ASN:HD21	1:B:184:GLU:HB3	1.75	0.48
1:A:269:PHE:CE1	1:A:275:PHE:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:HB3	1:B:270:PRO:HD2	1.95	0.48
1:B:279:GLN:NE2	1:B:279:GLN:C	2.67	0.48
1:A:110:LYS:HB2	1:A:112:ILE:HD13	1.94	0.48
1:A:110:LYS:HB2	1:A:110:LYS:HZ3	1.79	0.47
1:B:106:PHE:O	1:B:108:PRO:HD3	2.14	0.47
1:B:206:ILE:HG21	1:B:269:PHE:CD2	2.49	0.47
1:A:108:PRO:HG2	1:A:132:GLU:OE2	2.14	0.47
1:B:205:LYS:HA	1:B:205:LYS:HZ1	1.79	0.47
1:B:80:GLN:NE2	1:B:247:THR:OG1	2.48	0.47
1:A:103:ASN:O	1:A:136:ILE:HG23	2.15	0.47
1:A:173:ILE:HG13	1:A:174:LEU:N	2.30	0.47
1:A:146:MET:HG2	1:A:174:LEU:HD22	1.97	0.47
1:A:127:ASN:HD22	1:A:129:GLU:H	1.61	0.47
1:B:183:LYS:O	1:B:187:GLU:HG3	2.15	0.47
1:A:172:ASN:HD22	1:A:179:MET:HG2	1.80	0.46
1:B:205:LYS:O	1:B:206:ILE:C	2.54	0.46
1:B:176:ASN:C	1:B:178:SER:N	2.69	0.46
1:A:176:ASN:O	1:A:177:ASP:OD2	2.34	0.46
1:A:267:HIS:CD2	1:A:274:ASP:OD1	2.69	0.46
1:A:67:GLN:NE2	1:A:67:GLN:HA	2.30	0.46
1:B:32:ARG:HG2	1:B:148:SER:O	2.15	0.46
1:B:110:LYS:HZ2	1:B:112:ILE:CG1	2.29	0.46
1:A:103:ASN:HB3	1:A:131:HIS:CE1	2.50	0.46
1:B:8:LEU:CD1	1:B:239:PRO:HG2	2.45	0.46
1:B:142:SER:HB2	1:B:174:LEU:HD12	1.96	0.46
1:B:234:ASP:CG	1:B:240:ARG:HH12	2.19	0.46
1:B:160:THR:HB	1:B:163:ALA:HB2	1.98	0.46
1:A:110:LYS:HB2	1:A:110:LYS:NZ	2.31	0.45
1:A:113:MET:CE	1:A:118:LEU:HD21	2.45	0.45
1:A:240:ARG:CG	1:A:240:ARG:NH1	2.78	0.45
1:B:162:HIS:NE2	1:B:201:ASN:ND2	2.64	0.45
1:A:226:GLN:HG3	1:A:228:SER:H	1.81	0.45
1:A:110:LYS:NZ	1:A:112:ILE:HD13	2.28	0.45
1:A:167:LEU:HG	1:A:194:MET:HE2	1.97	0.45
1:A:23:ASN:O	1:A:27:GLU:HG2	2.18	0.44
1:A:109:LYS:HA	1:A:109:LYS:HE2	1.98	0.44
1:A:113:MET:HE3	1:A:118:LEU:HD21	1.99	0.44
1:B:112:ILE:HG22	1:B:112:ILE:O	2.18	0.44
1:B:204:TYR:CD1	1:B:232:LEU:HD13	2.52	0.44
1:B:70:ARG:O	1:B:73:VAL:HG22	2.18	0.44
1:B:167:LEU:HD21	1:B:197:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LEU:O	1:B:206:ILE:HD13	2.18	0.43
1:A:199:ASP:OD1	1:A:201:ASN:HB3	2.18	0.43
1:A:232:LEU:CD1	1:A:257:SER:HB3	2.48	0.43
1:A:70:ARG:HG3	1:A:70:ARG:NH2	2.33	0.43
1:A:277:LYS:HG2	1:A:285:ILE:HD11	2.01	0.43
1:B:32:ARG:O	1:B:35:VAL:HG23	2.18	0.43
1:A:175:MET:C	1:A:177:ASP:H	2.22	0.43
1:A:127:ASN:C	1:A:127:ASN:ND2	2.69	0.42
1:A:171:ILE:HD12	1:A:190:VAL:HG23	2.01	0.42
1:B:161:TYR:CD1	1:B:200:LEU:HB3	2.53	0.42
1:B:240:ARG:CG	1:B:240:ARG:HH11	2.32	0.42
1:A:68:THR:O	1:A:72:ASN:ND2	2.53	0.42
1:B:267:HIS:CE1	1:B:274:ASP:OD1	2.73	0.42
1:B:65:HIS:O	1:B:68:THR:HG23	2.18	0.42
1:A:176:ASN:C	1:A:178:SER:N	2.72	0.42
1:B:70:ARG:HD2	1:B:70:ARG:O	2.20	0.42
1:A:123:LYS:C	1:A:125:GLY:N	2.73	0.42
1:B:175:MET:O	1:B:177:ASP:N	2.46	0.42
1:B:197:PHE:C	1:B:197:PHE:CD2	2.91	0.42
1:A:265:SER:O	1:A:266:MET:C	2.57	0.42
1:A:243:ILE:O	1:A:249:GLY:HA3	2.20	0.41
1:B:42:SER:OG	1:B:84:SER:HB3	2.20	0.41
1:A:206:ILE:HD11	1:A:269:PHE:CZ	2.55	0.41
1:A:46:GLU:O	1:A:79:ILE:HG22	2.20	0.41
1:A:211:LYS:CE	1:A:211:LYS:HA	2.42	0.41
1:B:110:LYS:C	1:B:112:ILE:H	2.24	0.41
1:A:163:ALA:O	1:A:164:ALA:C	2.59	0.41
1:A:62:VAL:HG13	1:A:283:TYR:HB3	2.01	0.41
1:A:77:ASN:HA	1:A:78:PRO:HD3	1.80	0.41
1:A:197:PHE:CE2	1:A:280:GLY:HA2	2.55	0.41
1:B:171:ILE:HA	1:B:171:ILE:HD13	1.88	0.41
1:B:183:LYS:HE3	1:B:183:LYS:O	2.20	0.40
1:A:35:VAL:HG21	1:A:150:LEU:CD2	2.46	0.40
1:B:110:LYS:HZ2	1:B:112:ILE:HD11	1.87	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	257/289 (89%)	243 (95%)	10 (4%)	4 (2%)	9 9
1	B	248/289 (86%)	234 (94%)	11 (4%)	3 (1%)	13 14
All	All	505/578 (87%)	477 (94%)	21 (4%)	7 (1%)	11 11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	SER
1	A	163	ALA
1	A	164	ALA
1	B	163	ALA
1	B	176	ASN
1	B	111	GLU
1	A	209	GLU

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	241/263 (92%)	215 (89%)	26 (11%)	6 7
1	B	232/263 (88%)	210 (90%)	22 (10%)	8 10
All	All	473/526 (90%)	425 (90%)	48 (10%)	7 9

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	18	ASP
1	A	28	PHE
1	A	33	GLN
1	A	63	ASP
1	A	69	MET
1	A	95	ASN
1	A	107	ASP
1	A	109	LYS
1	A	110	LYS
1	A	115	THR
1	A	120	LEU
1	A	122	ARG
1	A	127	ASN
1	A	136	ILE
1	A	167	LEU
1	A	171	ILE
1	A	176	ASN
1	A	177	ASP
1	A	210	PHE
1	A	229	LEU
1	A	231	THR
1	A	232	LEU
1	A	240	ARG
1	A	256	LEU
1	A	263	LYS
1	B	18	ASP
1	B	28	PHE
1	B	33	GLN
1	B	35	VAL
1	B	68	THR
1	B	70	ARG
1	B	75	PHE
1	B	118	LEU
1	B	127	ASN
1	B	146	MET
1	B	169	PHE
1	B	177	ASP
1	B	183	LYS
1	B	197	PHE
1	B	202	LEU
1	B	205	LYS
1	B	229	LEU

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Mol	Chain	Res	Type
1	B	240	ARG
1	B	256	LEU
1	B	267	HIS
1	B	279	GLN
1	B	285	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	67	GLN
1	A	72	ASN
1	A	80	GLN
1	A	91	ASN
1	A	95	ASN
1	A	101	GLN
1	A	103	ASN
1	A	127	ASN
1	A	172	ASN
1	A	181	ASN
1	A	182	ASN
1	A	201	ASN
1	A	226	GLN
1	A	289	GLN
1	B	80	GLN
1	B	89	ASN
1	B	91	ASN
1	B	95	ASN
1	B	101	GLN
1	B	103	ASN
1	B	127	ASN
1	B	172	ASN
1	B	182	ASN
1	B	191	HIS
1	B	201	ASN
1	B	250	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	263/289 (91%)	1.05	53 (20%) 1 1	24, 45, 81, 93	0
1	B	254/289 (87%)	1.18	56 (22%) 0 1	28, 50, 81, 95	0
All	All	517/578 (89%)	1.11	109 (21%) 1 1	24, 47, 81, 95	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	PRO	7.8
1	A	112	ILE	7.0
1	B	176	ASN	6.7
1	A	113	MET	6.3
1	A	75	PHE	5.7
1	B	177	ASP	5.4
1	A	64	TYR	5.2
1	A	170	LEU	4.9
1	B	270	PRO	4.9
1	A	73	VAL	4.7
1	B	273	THR	4.5
1	A	267	HIS	4.2
1	B	271	ASN	4.2
1	A	226	GLN	4.2
1	A	43	ILE	4.1
1	B	43	ILE	4.0
1	A	167	LEU	3.9
1	A	70	ARG	3.9
1	B	111	GLU	3.9
1	A	181	ASN	3.8
1	B	170	LEU	3.8
1	B	112	ILE	3.8
1	B	65	HIS	3.7
1	B	162	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASP	3.7
1	B	5	PRO	3.7
1	A	211	LYS	3.6
1	A	263	LYS	3.6
1	A	210	PHE	3.5
1	B	272	GLY	3.5
1	B	184	GLU	3.5
1	B	75	PHE	3.5
1	A	123	LYS	3.4
1	A	162	HIS	3.4
1	B	81	LEU	3.4
1	A	176	ASN	3.4
1	B	79	ILE	3.4
1	B	160	THR	3.4
1	B	159	ILE	3.4
1	B	266	MET	3.3
1	A	165	TYR	3.3
1	B	113	MET	3.2
1	A	212	ASN	3.2
1	A	118	LEU	3.2
1	A	266	MET	3.2
1	B	178	SER	3.1
1	A	81	LEU	3.1
1	A	177	ASP	3.1
1	B	285	ILE	3.0
1	B	123	LYS	3.0
1	A	178	SER	3.0
1	A	5	PRO	3.0
1	B	283	TYR	2.9
1	B	95	ASN	2.9
1	A	254	MET	2.9
1	B	263	LYS	2.9
1	A	60	SER	2.9
1	B	44	SER	2.9
1	B	64	TYR	2.9
1	A	184	GLU	2.8
1	B	45	THR	2.8
1	A	159	ILE	2.7
1	A	227	TYR	2.7
1	B	66	TYR	2.7
1	B	73	VAL	2.7
1	A	65	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	139	PHE	2.6
1	B	197	PHE	2.6
1	A	109	LYS	2.6
1	B	284	GLY	2.6
1	B	104	PHE	2.6
1	A	61	LYS	2.6
1	B	6	ILE	2.5
1	B	110	LYS	2.5
1	A	107	ASP	2.5
1	A	169	PHE	2.5
1	B	82	GLY	2.5
1	B	205	LYS	2.5
1	A	163	ALA	2.4
1	A	44	SER	2.4
1	A	83	LEU	2.4
1	A	174	LEU	2.4
1	A	41	VAL	2.4
1	A	158	TRP	2.4
1	A	62	VAL	2.4
1	A	94	ASP	2.4
1	A	160	THR	2.3
1	B	109	LYS	2.3
1	B	121	LEU	2.3
1	B	158	TRP	2.3
1	A	116	GLU	2.3
1	A	173	ILE	2.3
1	A	120	LEU	2.3
1	B	63	ASP	2.3
1	B	68	THR	2.2
1	A	272	GLY	2.2
1	B	206	ILE	2.2
1	B	167	LEU	2.2
1	B	254	MET	2.2
1	A	104	PHE	2.2
1	B	255	LEU	2.2
1	B	145	LEU	2.1
1	A	42	SER	2.1
1	B	181	ASN	2.1
1	B	180	PRO	2.1
1	B	267	HIS	2.1
1	B	83	LEU	2.1
1	A	77	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	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)

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
2	CA	A	1290	1/1	0.94	0.11	47,47,47,47	0
2	CA	B	1290	1/1	0.96	0.06	53,53,53,53	0
3	XE	B	1291	1/1	0.97	0.09	63,63,63,63	0
3	XE	A	1291	1/1	0.98	0.05	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.