



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:21 PM UTC

PDB ID : 1Y14 / pdb_00001y14
Title : Crystal structure of yeast subcomplex of Rpb4 and Rpb7
Authors : Armache, K.-J.; Mitterweger, S.; Meinhart, A.; Cramer, P.
Deposited on : 2004-11-17
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 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

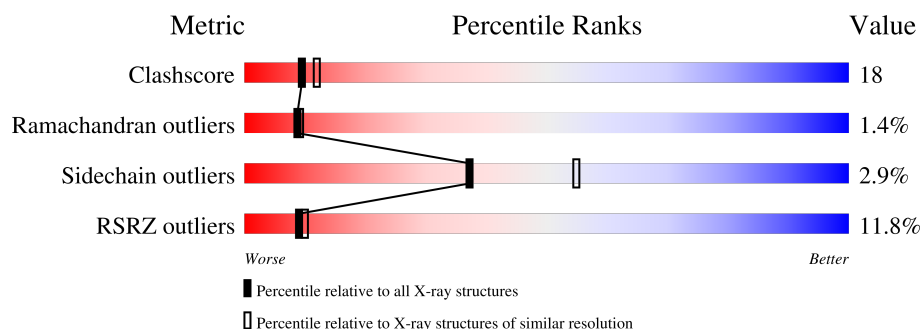
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	187	8% 50% 19% • 29%
1	C	187	7% 47% 23% • 27%
2	B	171	16% 55% 30% • • 10%
2	D	171	8% 58% 35% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4776 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 DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1059	659	185	213	2			
1	C	136	Total	C	N	O	S	0	0	0
			1087	677	192	216	2			

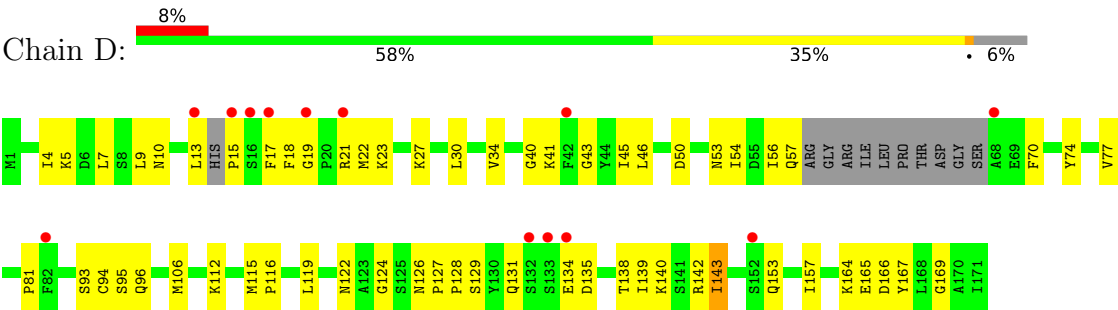
- Molecule 2 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	154	Total	C	N	O	S	0	0	0
			1220	790	198	224	8			
2	D	160	Total	C	N	O	S	0	0	0
			1256	811	203	234	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	30	Total	O	0	0
			30	30		
3	C	37	Total	O	0	0
			37	37		
3	D	44	Total	O	0	0
			44	44		

● Molecule 2: DNA-directed RNA polymerase II 19 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	103.65Å 114.81Å 80.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 95.2 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.29Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.228 , 0.274 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4776	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

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	0.42	0/1066	0.88	4/1432 (0.3%)
1	C	0.42	0/1095	0.91	4/1469 (0.3%)
2	B	0.44	0/1243	1.05	11/1670 (0.7%)
2	D	0.46	0/1280	1.02	5/1721 (0.3%)
All	All	0.44	0/4684	0.98	24/6292 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ARG	N-CA-C	8.86	123.88	112.89
1	A	155	ARG	N-CA-C	8.57	123.74	113.28
2	B	133	SER	N-CA-C	-7.54	102.94	113.20
2	D	46	LEU	N-CA-C	7.41	119.43	111.36
2	B	14	HIS	CA-C-N	7.32	128.99	119.84
2	B	14	HIS	C-N-CA	7.32	128.99	119.84
2	B	4	ILE	N-CA-C	-6.80	97.94	107.80
2	B	41	LYS	N-CA-C	6.63	118.16	111.07
2	B	46	LEU	N-CA-C	6.52	119.71	111.69
1	A	51	ASN	N-CA-C	-6.50	102.14	110.53
1	A	195	ILE	CA-C-N	6.22	126.68	119.47
1	A	195	ILE	C-N-CA	6.22	126.68	119.47
2	D	4	ILE	N-CA-C	-5.92	99.22	107.80
2	D	43	GLY	N-CA-C	5.88	123.19	112.37
2	D	77	VAL	N-CA-C	-5.84	101.18	108.89
1	C	51	ASN	N-CA-C	-5.67	102.38	110.59
2	B	34	VAL	N-CA-C	5.50	118.46	112.96
1	C	201	LYS	N-CA-C	-5.40	107.94	114.75
1	C	134	THR	N-CA-C	5.38	118.47	110.14
2	B	56	ILE	N-CA-C	5.32	120.40	109.34
2	D	143	ILE	N-CA-C	5.29	115.33	108.35
2	B	135	ASP	N-CA-C	5.16	117.34	110.53
2	B	33	GLU	N-CA-C	5.12	118.68	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	MET	N-CA-C	5.10	117.42	109.52

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	1059	0	1083	30	0
1	C	1087	0	1116	41	0
2	B	1220	0	1239	61	0
2	D	1256	0	1272	45	0
3	A	43	0	0	0	0
3	B	30	0	0	0	0
3	C	37	0	0	1	0
3	D	44	0	0	0	0
All	All	4776	0	4710	167	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 (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:GLY:H	2:D:22:MET:HE2	1.29	0.97
1:C:130:LEU:HD21	1:C:145:MET:HE2	1.50	0.93
2:D:112:LYS:HA	2:D:115:MET:HE3	1.54	0.89
2:B:138:THR:HG22	2:B:139:ILE:H	1.42	0.85
2:D:126:ASN:HD22	2:D:127:PRO:HA	1.44	0.82
2:B:56:ILE:O	2:B:57:GLN:HG2	1.82	0.79
2:B:99:PHE:HE2	2:B:115:MET:HE3	1.49	0.77
2:D:13:LEU:HD21	2:D:17:PHE:HB2	1.68	0.76
2:B:138:THR:HG22	2:B:139:ILE:N	2.00	0.76
2:B:134:GLU:HG3	2:B:135:ASP:H	1.51	0.75
1:C:76:LYS:O	1:C:77:HIS:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ASN:HD22	2:B:131:GLN:NE2	1.86	0.73
2:D:122:ASN:HD22	2:D:131:GLN:NE2	1.88	0.72
2:B:132:SER:C	2:B:134:GLU:H	1.99	0.71
2:D:81:PRO:HB3	2:D:106:MET:HE1	1.73	0.70
1:A:47:LEU:HD23	2:B:5:LYS:HD3	1.73	0.69
2:B:81:PRO:HB3	2:B:106:MET:HE1	1.72	0.69
1:C:67:ARG:HD2	3:C:235:HOH:O	1.92	0.69
1:C:130:LEU:HD13	1:C:142:LYS:HG2	1.73	0.69
2:D:34:VAL:HG12	2:D:45:ILE:HG21	1.75	0.69
1:A:118:THR:HB	1:A:121:LYS:HB2	1.76	0.68
1:A:175:PHE:O	1:A:179:GLN:HG3	1.94	0.67
1:C:141:LEU:O	1:C:145:MET:HG2	1.94	0.66
2:D:126:ASN:HD22	2:D:127:PRO:CA	2.08	0.66
1:A:120:GLU:HA	1:A:123:LEU:HD12	1.78	0.66
2:D:34:VAL:HG11	2:D:74:TYR:OH	1.95	0.65
2:B:99:PHE:CE2	2:B:115:MET:HE3	2.33	0.63
2:D:15:PRO:HA	2:D:18:PHE:CE1	2.33	0.63
2:D:34:VAL:HG13	2:D:45:ILE:HD12	1.81	0.63
1:C:134:THR:HG22	1:C:135:GLY:N	2.13	0.62
2:B:164:LYS:NZ	2:D:153:GLN:HE21	1.97	0.62
2:D:5:LYS:HD3	2:D:7:LEU:HD21	1.81	0.61
2:B:164:LYS:HZ2	2:D:153:GLN:HE21	1.48	0.61
1:A:138:ASN:ND2	1:A:141:LEU:H	1.99	0.61
2:B:116:PRO:HD3	2:B:163:ILE:HG13	1.83	0.61
1:C:175:PHE:O	1:C:179:GLN:HG3	2.00	0.61
2:D:96:GLN:O	2:D:112:LYS:HD3	2.01	0.61
2:B:143:ILE:HG13	2:B:169:GLY:C	2.26	0.61
1:C:127:ASP:O	1:C:131:GLU:HG3	2.02	0.60
1:C:119:ARG:HH21	1:C:155:ARG:HD2	1.66	0.59
2:B:14:HIS:CB	2:B:15:PRO:HD2	2.32	0.59
2:B:122:ASN:ND2	2:B:131:GLN:NE2	2.50	0.59
2:B:44:TYR:HE1	2:B:157:ILE:HD11	1.66	0.58
2:B:44:TYR:CE1	2:B:157:ILE:HD11	2.38	0.58
1:C:153:ARG:HE	1:C:218:GLU:CD	2.12	0.57
1:C:61:GLU:O	1:C:65:GLU:HG3	2.04	0.57
2:B:138:THR:CG2	2:B:139:ILE:H	2.15	0.57
2:B:15:PRO:HD3	2:B:18:PHE:CZ	2.41	0.56
2:B:132:SER:C	2:B:134:GLU:N	2.64	0.56
1:A:155:ARG:HG2	1:A:155:ARG:HH11	1.70	0.55
1:A:206:GLU:O	1:A:209:ARG:HG3	2.07	0.55
2:B:153:GLN:HE21	2:D:164:LYS:NZ	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:HG2	1:A:47:LEU:N	2.22	0.55
1:C:153:ARG:NE	1:C:218:GLU:OE2	2.38	0.55
1:A:130:LEU:HD21	1:A:145:MET:SD	2.47	0.55
1:A:47:LEU:CD2	2:B:5:LYS:HD3	2.36	0.55
2:B:50:ASP:OD2	2:B:53:ASN:HB2	2.06	0.54
2:B:14:HIS:O	2:B:16:SER:N	2.41	0.54
1:C:134:THR:CG2	1:C:135:GLY:N	2.70	0.54
2:B:138:THR:CG2	2:B:139:ILE:N	2.70	0.54
1:C:219:THR:CG2	1:C:221:TYR:HB3	2.38	0.53
2:B:6:ASP:OD1	2:B:75:ARG:HG2	2.08	0.53
2:D:13:LEU:HD21	2:D:17:PHE:CB	2.37	0.53
1:C:119:ARG:HH21	1:C:155:ARG:CD	2.20	0.53
1:C:119:ARG:HH21	1:C:155:ARG:NE	2.06	0.53
1:A:67:ARG:HE	1:A:132:GLN:NE2	2.06	0.53
1:A:155:ARG:HD3	1:A:219:THR:HG21	1.90	0.52
2:D:139:ILE:O	2:D:140:LYS:HB2	2.08	0.52
1:C:75:LYS:HD3	1:C:75:LYS:H	1.74	0.52
2:B:115:MET:HE1	2:B:130:TYR:CG	2.45	0.52
1:A:142:LYS:HG2	1:A:146:GLN:NE2	2.24	0.52
2:D:13:LEU:HD21	2:D:17:PHE:H	1.74	0.52
2:B:17:PHE:O	2:B:18:PHE:C	2.54	0.51
1:C:167:LEU:HB3	1:C:177:VAL:HG13	1.92	0.51
1:C:122:GLU:O	1:C:126:ILE:HG13	2.10	0.51
2:B:40:GLY:O	2:B:80:LYS:NZ	2.44	0.51
2:B:81:PRO:CB	2:B:106:MET:HE1	2.38	0.51
2:D:166:ASP:O	2:D:167:TYR:HB2	2.11	0.51
2:B:14:HIS:HB3	2:B:15:PRO:HD2	1.93	0.50
2:D:143:ILE:HG13	2:D:169:GLY:C	2.35	0.50
1:C:130:LEU:CD1	1:C:142:LYS:HG2	2.41	0.50
1:A:137:ASN:O	1:A:138:ASN:C	2.55	0.50
1:A:209:ARG:HD2	1:A:210:ILE:N	2.27	0.50
2:D:112:LYS:CA	2:D:115:MET:HE3	2.34	0.50
2:B:122:ASN:ND2	2:B:131:GLN:HE22	2.10	0.49
1:A:48:ILE:HD12	2:B:75:ARG:NH2	2.27	0.49
2:B:122:ASN:HD22	2:B:131:GLN:HE22	1.58	0.49
2:B:85:GLU:HG2	2:B:87:VAL:HG13	1.93	0.49
1:A:72:ARG:O	1:A:74:GLN:HG3	2.11	0.49
2:D:23:LYS:HG3	2:D:56:ILE:HD12	1.94	0.49
1:A:137:ASN:CG	1:A:138:ASN:H	2.21	0.48
2:B:22:MET:O	2:B:26:LEU:HG	2.13	0.48
1:C:209:ARG:O	1:C:213:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:LEU:C	2:D:13:LEU:HD23	2.39	0.48
2:B:138:THR:O	2:B:141:SER:HB2	2.13	0.47
2:B:153:GLN:HE21	2:D:164:LYS:HZ2	1.61	0.47
1:C:75:LYS:H	1:C:75:LYS:CD	2.26	0.47
1:C:153:ARG:HD3	1:C:154:PHE:CZ	2.49	0.47
2:D:27:LYS:HE2	2:D:54:ILE:HB	1.96	0.47
1:C:130:LEU:HD21	1:C:145:MET:CE	2.35	0.47
1:C:155:ARG:HG3	1:C:219:THR:HG21	1.96	0.47
2:B:25:TYR:OH	2:B:29:LYS:HE3	2.14	0.47
2:B:97:HIS:HD2	2:D:95:SER:OG	1.98	0.47
2:B:114:LEU:HB3	2:B:162:SER:CB	2.45	0.47
1:C:176:GLU:O	1:C:180:LEU:HB2	2.16	0.46
1:A:119:ARG:NH1	1:A:155:ARG:HD2	2.30	0.46
2:D:34:VAL:CG1	2:D:45:ILE:HG21	2.42	0.46
2:D:116:PRO:HD2	2:D:119:LEU:HD12	1.97	0.46
2:B:5:LYS:HG3	2:B:7:LEU:HD21	1.97	0.46
1:C:219:THR:HG22	1:C:221:TYR:HB3	1.98	0.46
1:A:138:ASN:C	1:A:138:ASN:HD22	2.23	0.46
1:C:220:LEU:O	1:C:221:TYR:C	2.58	0.45
2:D:40:GLY:HA2	2:D:157:ILE:HG12	1.98	0.45
1:C:221:TYR:CD1	1:C:221:TYR:O	2.69	0.45
1:C:198:LEU:O	1:C:199:ASN:C	2.60	0.45
1:A:48:ILE:HD12	2:B:75:ARG:HH22	1.81	0.45
2:D:5:LYS:CD	2:D:7:LEU:HD21	2.46	0.45
2:B:81:PRO:CD	2:B:157:ILE:HD12	2.47	0.45
2:D:94:CYS:HB2	2:D:128:PRO:HB2	1.99	0.45
2:D:134:GLU:HG3	2:D:135:ASP:N	2.32	0.45
1:C:75:LYS:HD3	1:C:75:LYS:N	2.32	0.44
2:B:170:ALA:O	2:B:171:ILE:HB	2.18	0.44
1:A:155:ARG:HG2	1:A:155:ARG:NH1	2.33	0.44
2:B:5:LYS:HG3	2:B:7:LEU:CD2	2.48	0.44
1:A:46:GLU:HG2	1:A:47:LEU:H	1.82	0.44
1:A:118:THR:HG21	1:A:121:LYS:HG3	1.98	0.44
1:C:168:LYS:C	1:C:170:THR:H	2.25	0.44
2:D:126:ASN:HA	2:D:127:PRO:C	2.42	0.44
2:B:9:LEU:HD22	2:B:34:VAL:HG13	2.00	0.44
2:B:56:ILE:O	2:B:57:GLN:CG	2.61	0.43
1:A:162:ALA:HA	1:A:165:GLN:HG2	2.00	0.43
1:C:63:LEU:HD12	1:C:145:MET:HE1	1.99	0.43
1:C:126:ILE:HG23	1:C:145:MET:HE3	2.00	0.43
2:D:13:LEU:HD21	2:D:17:PHE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:ASN:C	2:D:124:GLY:H	2.26	0.43
2:B:56:ILE:HG22	2:B:57:GLN:N	2.33	0.43
2:B:14:HIS:CG	2:B:15:PRO:HD2	2.54	0.43
1:A:120:GLU:O	1:A:123:LEU:HB2	2.19	0.43
2:B:81:PRO:HD2	2:B:157:ILE:HD12	2.00	0.42
2:D:21:ARG:HD3	2:D:21:ARG:HA	1.76	0.42
1:A:142:LYS:HG2	1:A:146:GLN:HE21	1.84	0.42
2:B:97:HIS:HE1	2:D:93:SER:OG	2.01	0.42
2:B:49:LEU:HD21	2:B:77:VAL:HG23	2.00	0.42
1:C:153:ARG:CG	1:C:218:GLU:HG3	2.50	0.42
2:D:9:LEU:HD23	2:D:30:LEU:HD12	2.01	0.42
2:B:50:ASP:CG	2:B:53:ASN:HB2	2.44	0.42
1:C:156:ASP:OD2	1:C:158:GLU:HB2	2.19	0.42
2:B:55:ASP:OD2	2:B:73:LYS:HD2	2.20	0.42
2:D:126:ASN:ND2	2:D:127:PRO:HA	2.24	0.42
2:B:115:MET:HE1	2:B:130:TYR:CD2	2.55	0.42
1:C:153:ARG:NH2	1:C:215:SER:HA	2.35	0.42
2:D:50:ASP:OD2	2:D:53:ASN:HB2	2.19	0.42
1:C:134:THR:HG21	1:C:138:ASN:HB3	2.02	0.41
1:C:137:ASN:C	1:C:137:ASN:ND2	2.77	0.41
1:A:204:ASP:O	1:A:208:GLU:HG2	2.20	0.41
2:D:13:LEU:HD21	2:D:17:PHE:CA	2.51	0.41
2:D:126:ASN:HD22	2:D:127:PRO:N	2.18	0.41
2:B:13:LEU:HD23	2:B:22:MET:HE3	2.03	0.41
1:C:120:GLU:N	1:C:120:GLU:CD	2.78	0.41
2:B:139:ILE:O	2:B:140:LYS:HB2	2.21	0.41
1:A:54:GLU:O	1:A:58:VAL:HG23	2.22	0.41
2:B:114:LEU:HB3	2:B:162:SER:HB3	2.03	0.41
1:C:158:GLU:H	1:C:158:GLU:CD	2.29	0.40
2:D:129:SER:HB3	2:D:138:THR:HB	2.03	0.40
2:D:70:PHE:CD1	2:D:70:PHE:N	2.89	0.40
1:A:128:VAL:O	1:A:131:GLU:HB3	2.22	0.40
2:B:116:PRO:HG3	2:B:164:LYS:HA	2.03	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	129/187 (69%)	121 (94%)	5 (4%)	3 (2%)	5	4
1	C	132/187 (71%)	126 (96%)	5 (4%)	1 (1%)	16	20
2	B	148/171 (86%)	135 (91%)	10 (7%)	3 (2%)	6	5
2	D	154/171 (90%)	146 (95%)	7 (4%)	1 (1%)	21	27
All	All	563/716 (79%)	528 (94%)	27 (5%)	8 (1%)	9	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	PRO
1	A	73	SER
2	B	134	GLU
1	C	136	GLY
1	A	138	ASN
2	B	18	PHE
1	A	72	ARG
2	D	41	LYS

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	119/169 (70%)	116 (98%)	3 (2%)	42	60
1	C	122/169 (72%)	117 (96%)	5 (4%)	27	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	139/152 (91%)	136 (98%)	3 (2%)	45	65
2	D	143/152 (94%)	139 (97%)	4 (3%)	38	56
All	All	523/642 (82%)	508 (97%)	15 (3%)	37	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	199	ASN
1	A	209	ARG
2	B	14	HIS
2	B	15	PRO
2	B	141	SER
1	C	75	LYS
1	C	137	ASN
1	C	139	LYS
1	C	146	GLN
1	C	180	LEU
2	D	10	ASN
2	D	57	GLN
2	D	142	ARG
2	D	165	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	138	ASN
1	A	146	GLN
1	A	199	ASN
2	B	10	ASN
2	B	24	GLN
2	B	97	HIS
2	B	131	GLN
2	B	153	GLN
1	C	137	ASN
1	C	143	ASN
2	D	10	ASN
2	D	71	ASN
2	D	97	HIS

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Mol	Chain	Res	Type
2	D	102	GLN
2	D	126	ASN
2	D	131	GLN
2	D	153	GLN

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	133/187 (71%)	0.50	15 (11%) 10 11	28, 47, 86, 99	0
1	C	136/187 (72%)	0.42	13 (9%) 13 15	30, 51, 93, 100	0
2	B	154/171 (90%)	0.72	28 (18%) 3 4	29, 51, 92, 99	0
2	D	160/171 (93%)	0.44	13 (8%) 18 19	27, 47, 89, 99	0
All	All	583/716 (81%)	0.52	69 (11%) 9 10	27, 49, 92, 100	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	13	LEU	5.4
2	D	15	PRO	5.3
2	B	123	ALA	4.8
1	C	47	LEU	4.6
2	B	14	HIS	4.4
2	B	57	GLN	4.2
2	B	129	SER	4.1
2	B	136	VAL	3.9
2	B	13	LEU	3.7
2	D	21	ARG	3.7
2	B	20	PRO	3.7
2	B	17	PHE	3.6
2	D	17	PHE	3.6
2	B	16	SER	3.5
1	A	135	GLY	3.5
2	D	42	PHE	3.5
2	B	19	GLY	3.4
2	D	68	ALA	3.4
2	B	120	THR	3.4
1	A	72	ARG	3.4
2	B	131	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	137	ASN	3.3
1	A	47	LEU	3.2
1	C	123	LEU	3.2
2	B	12	THR	3.2
1	A	73	SER	3.2
1	C	199	ASN	3.1
2	D	16	SER	3.1
2	D	132	SER	3.1
2	B	116	PRO	3.1
2	B	18	PHE	2.9
1	C	137	ASN	2.8
2	B	25	TYR	2.8
2	B	121	PHE	2.8
1	C	77	HIS	2.7
1	A	120	GLU	2.7
1	C	221	TYR	2.7
1	A	205	ASP	2.7
2	B	122	ASN	2.7
1	A	71	LYS	2.7
2	D	133	SER	2.7
2	B	118	ASP	2.7
2	D	82	PHE	2.6
2	D	152	SER	2.6
1	C	46	GLU	2.6
2	B	15	PRO	2.6
2	B	70	PHE	2.6
2	B	171	ILE	2.6
1	C	119	ARG	2.5
2	D	134	GLU	2.5
2	B	113	HIS	2.4
1	A	74	GLN	2.4
1	A	69	ALA	2.3
1	C	126	ILE	2.3
2	B	21	ARG	2.3
2	B	117	GLN	2.3
1	A	209	ARG	2.2
1	A	128	VAL	2.2
1	C	118	THR	2.2
1	A	126	ILE	2.1
1	C	165	GLN	2.1
1	A	118	THR	2.1
1	A	165	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	119	LEU	2.1
1	C	200	ASN	2.1
2	D	19	GLY	2.1
2	B	132	SER	2.0
2	B	133	SER	2.0
1	C	138	ASN	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.