



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:05 AM UTC

PDB ID : 1OK7 / pdb_00001ok7
Title : A Conserved protein binding-site on Bacterial Sliding Clamps
Authors : Burnouf, D.Y.; Olieric, V.; Wagner, J.; Fujii, S.; Reinbolt, J.; Fuchs, R.P.P.;
Dumas, P.
Deposited on : 2003-07-18
Resolution : 1.65 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

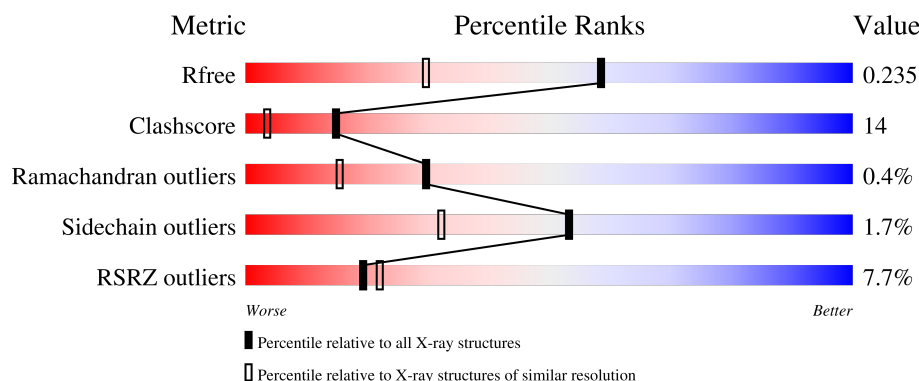
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	366	7% 75% 22% .
1	B	366	9% 77% 22% .
2	C	16	6% 31% 12% 56%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6235 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 POLYMERASE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	5	0
			2866	1799	501	545	21			
1	B	366	Total	C	N	O	S	0	3	0
			2853	1792	500	541	20			

- Molecule 2 is a protein called DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			56	36	11	9			

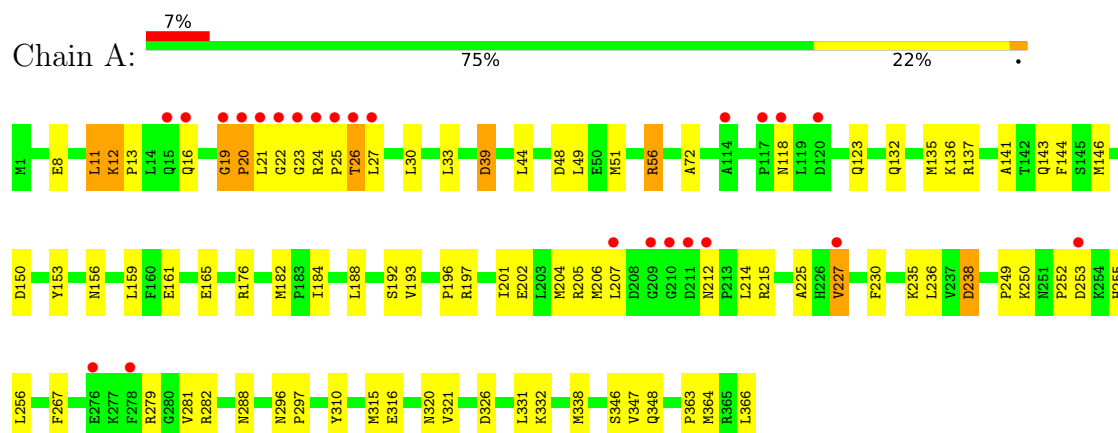
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total	O	0	0
			227	227		
3	B	231	Total	O	0	0
			231	231		
3	C	2	Total	O	0	0
			2	2		

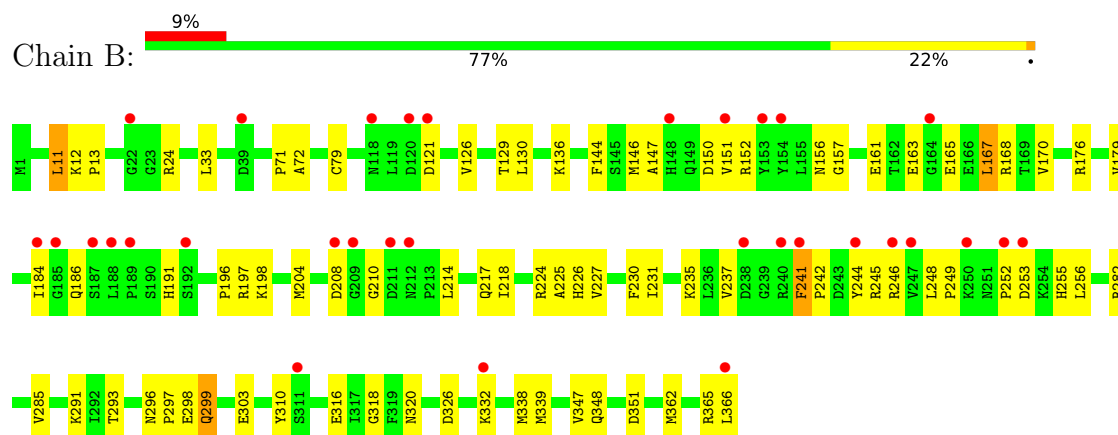
3 Residue-property plots [i](#)

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.

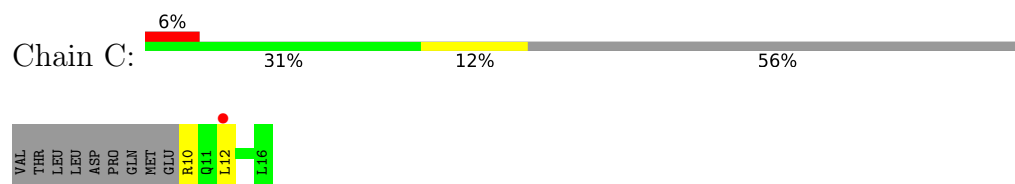
• Molecule 1: DNA POLYMERASE III



• Molecule 1: DNA POLYMERASE III



• Molecule 2: DNA POLYMERASE IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	41.23Å 65.22Å 73.38Å 73.11° 85.58° 85.80°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-1.65) 96.7 (20.00-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 1.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.229 0.207 , 0.235	Depositor DCC
R_{free} test set	4293 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.5	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	0.95	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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	0.55	1/2934 (0.0%)	0.93	5/3969 (0.1%)
1	B	0.53	0/2917	0.95	7/3948 (0.2%)
2	C	0.38	0/55	0.92	0/71
All	All	0.54	1/5906 (0.0%)	0.94	12/7988 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	315	MET	SD-CE	-5.30	1.66	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	LEU	N-CA-C	8.45	120.18	110.97
1	A	253	ASP	N-CA-C	7.05	119.82	111.71
1	A	279	ARG	N-CA-C	5.74	118.03	109.25
1	B	241	PHE	CA-C-N	5.54	125.55	119.89
1	B	241	PHE	C-N-CA	5.54	125.55	119.89
1	B	351	ASP	N-CA-C	-5.47	101.75	109.96
1	B	253	ASP	N-CA-C	5.46	117.94	111.33
1	A	321	VAL	N-CA-C	5.46	115.66	110.42
1	A	11	LEU	N-CA-C	5.24	117.41	111.02
1	B	167	LEU	N-CA-C	-5.16	101.29	109.59
1	A	235	LYS	N-CA-C	-5.03	103.77	110.55
1	B	320	ASN	N-CA-C	-5.02	100.89	108.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39[B]	ASP	Mainchain

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	2866	0	2874	88	0
1	B	2853	0	2870	72	0
2	C	56	0	65	4	0
3	A	227	0	0	8	0
3	B	231	0	0	2	0
3	C	2	0	0	0	0
All	All	6235	0	5809	160	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 14.

All (160) 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:338[B]:MET:HG3	1:A:347:VAL:HG21	1.49	0.95
1:B:249:PRO:HB2	1:B:252:PRO:HG3	1.50	0.91
1:B:150:ASP:H	1:B:156:ASN:HD21	1.18	0.86
1:A:214:LEU:CD1	1:A:227:VAL:HG22	2.06	0.85
1:A:214:LEU:HD12	1:A:227:VAL:HG22	1.59	0.83
1:B:163:GLU:HG3	1:B:168:ARG:NH2	1.94	0.83
1:B:161:GLU:CD	1:B:168:ARG:HH21	1.87	0.83
1:B:163:GLU:HG3	1:B:168:ARG:HH22	1.44	0.83
1:A:338[B]:MET:HG3	1:A:347:VAL:CG2	2.11	0.80
1:A:320:ASN:HD22	1:A:364[A]:MET:HE1	1.47	0.79
1:A:206:MET:HE2	1:A:227:VAL:HG23	1.66	0.77
1:A:27:LEU:H	1:A:27:LEU:HD12	1.49	0.77
1:A:137:ARG:HD2	1:A:182[B]:MET:SD	2.25	0.76
1:A:215:ARG:HH11	1:A:215:ARG:HB3	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASP:H	1:A:156:ASN:HD21	1.37	0.73
1:A:184:ILE:HD11	1:A:188:LEU:HD11	1.70	0.72
1:B:249:PRO:HD2	1:B:348:GLN:HE21	1.53	0.72
1:A:33:LEU:HG	1:A:72:ALA:HB2	1.73	0.70
1:B:24:ARG:HG2	1:B:24:ARG:HH11	1.57	0.69
1:A:338[B]:MET:CG	1:A:347:VAL:HG21	2.22	0.68
1:B:246:ARG:HG3	1:B:246:ARG:HH11	1.59	0.68
1:A:33:LEU:HG	1:A:72:ALA:CB	2.25	0.67
1:B:217:GLN:HE21	1:B:226[A]:HIS:HE1	1.41	0.67
1:B:165:GLU:O	1:B:165:GLU:HG2	1.93	0.67
1:A:249:PRO:HD2	1:A:348:GLN:HE21	1.58	0.66
1:A:26:THR:HG22	1:A:27:LEU:HD12	1.77	0.66
1:A:123[A]:GLN:NE2	3:A:2085:HOH:O	2.20	0.66
1:A:165:GLU:HG2	1:A:165:GLU:O	1.97	0.65
1:B:170:VAL:HG22	1:B:179:VAL:HG23	1.77	0.64
1:A:282:ARG:HH21	1:A:366:LEU:HB2	1.61	0.64
1:B:291:LYS:HE3	1:B:303:GLU:OE1	1.98	0.63
1:B:318:GLY:HA3	1:B:366:LEU:HD23	1.81	0.63
1:A:288:ASN:HD22	1:A:310:TYR:H	1.44	0.63
1:B:129:THR:H	1:B:186:GLN:HE22	1.46	0.61
1:B:126:VAL:CG1	1:B:218:ILE:HB	2.30	0.61
1:B:150:ASP:H	1:B:156:ASN:ND2	1.95	0.61
1:A:51:MET:HE3	1:A:202:GLU:HG2	1.81	0.61
1:A:48:ASP:O	1:A:49:LEU:HB2	2.01	0.61
1:A:16:GLN:HG2	1:A:230:PHE:CD1	2.35	0.61
1:A:27:LEU:H	1:A:27:LEU:CD1	2.14	0.61
1:A:320:ASN:HB2	1:A:364[A]:MET:HE3	1.83	0.60
1:B:33:LEU:HG	1:B:72:ALA:HB2	1.83	0.60
1:B:365:ARG:O	2:C:10:ARG:HG2	2.02	0.59
1:B:129:THR:H	1:B:186:GLN:NE2	2.01	0.59
1:B:249:PRO:HB2	1:B:252:PRO:CG	2.28	0.59
1:B:249:PRO:CB	1:B:252:PRO:HG3	2.28	0.58
1:A:143:GLN:HG3	1:A:146:MET:HE2	1.84	0.58
1:A:26:THR:CG2	1:A:27:LEU:HD12	2.33	0.57
1:A:215:ARG:HB3	1:A:215:ARG:NH1	2.18	0.57
1:B:24:ARG:HG2	1:B:24:ARG:NH1	2.19	0.57
1:A:161:GLU:CD	3:A:2104:HOH:O	2.47	0.57
1:A:206:MET:HE2	1:A:227:VAL:CG2	2.36	0.56
1:B:71:PRO:HG3	3:B:2023:HOH:O	2.06	0.56
1:A:21:LEU:HD21	3:A:2012:HOH:O	2.05	0.55
1:A:51:MET:HE1	1:A:202:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD11	1:A:192:SER:OG	2.08	0.53
1:A:27:LEU:HD12	1:A:27:LEU:N	2.20	0.53
1:A:144:PHE:CD2	1:A:326:ASP:HB3	2.44	0.53
1:A:12:LYS:HB3	1:A:12:LYS:NZ	2.23	0.53
1:A:19:GLY:HA3	1:A:205:ARG:NH1	2.23	0.52
1:B:298:GLU:O	1:B:299:GLN:HB2	2.10	0.52
1:A:118:ASN:HA	3:A:2077:HOH:O	2.08	0.52
1:A:282:ARG:HD2	3:A:2169:HOH:O	2.10	0.52
1:B:332:LYS:HG3	1:B:332:LYS:O	2.10	0.52
1:B:291:LYS:HE2	1:B:293:THR:CG2	2.40	0.52
1:B:161:GLU:CD	1:B:168:ARG:NH2	2.64	0.51
1:A:12:LYS:HB3	1:A:13:PRO:HD3	1.91	0.51
1:A:320:ASN:HD22	1:A:364[A]:MET:CE	2.21	0.51
1:B:296:ASN:HB2	1:B:297:PRO:CD	2.40	0.51
1:B:217:GLN:NE2	1:B:226[A]:HIS:HE1	2.06	0.51
1:B:184:ILE:HG22	1:B:184:ILE:O	2.11	0.51
1:B:168:ARG:NH2	1:B:245:ARG:NH2	2.60	0.50
1:A:12:LYS:HB3	1:A:12:LYS:HZ2	1.77	0.49
1:A:21:LEU:HG	1:A:22:GLY:N	2.27	0.49
1:A:21:LEU:HG	1:A:22:GLY:H	1.78	0.49
1:B:365:ARG:O	2:C:10:ARG:HB3	2.12	0.49
1:A:27:LEU:HB2	1:A:30:LEU:HG	1.94	0.48
1:A:153:TYR:H	1:A:153:TYR:HD1	1.60	0.48
1:B:33:LEU:HG	1:B:72:ALA:CB	2.43	0.48
1:B:338:MET:HE3	1:B:347:VAL:HG21	1.95	0.48
1:B:126:VAL:HG12	1:B:218:ILE:HB	1.93	0.48
1:A:153:TYR:CD1	1:A:153:TYR:N	2.81	0.48
1:A:320:ASN:ND2	1:A:364[A]:MET:HE1	2.24	0.48
1:B:291:LYS:HE3	1:B:303:GLU:CD	2.39	0.47
1:A:20:PRO:O	1:A:21:LEU:HB2	2.13	0.47
1:A:136:LYS:CB	1:A:204:MET:HE1	2.45	0.47
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.97	0.47
1:B:252:PRO:HB2	1:B:339:MET:HB3	1.97	0.47
1:A:19:GLY:C	1:A:205:ARG:HH12	2.22	0.46
1:A:256:LEU:C	1:A:256:LEU:HD23	2.40	0.46
1:B:282:ARG:NH1	1:B:316:GLU:OE1	2.48	0.46
1:B:318:GLY:HA3	1:B:366:LEU:CD2	2.45	0.46
1:A:25:PRO:O	1:A:26:THR:O	2.34	0.46
1:A:193:VAL:HB	1:A:236:LEU:HD13	1.96	0.46
1:A:267:PHE:CE1	1:A:281:VAL:HG21	2.51	0.45
1:B:252:PRO:O	1:B:255:HIS:CE1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLN:HG3	1:A:212:ASN:O	2.16	0.45
1:B:196:PRO:HG3	1:B:237:VAL:HG23	1.99	0.45
1:B:165:GLU:HA	1:B:186:GLN:O	2.16	0.45
1:B:241:PHE:HA	1:B:242:PRO:HD3	1.87	0.45
1:B:235:LYS:HE2	3:B:2161:HOH:O	2.16	0.45
1:B:12:LYS:HB3	1:B:13:PRO:HD3	1.99	0.45
1:B:285:VAL:HG12	1:B:310:TYR:CD2	2.52	0.45
1:A:51:MET:CE	1:A:202:GLU:HG2	2.47	0.45
1:A:346:SER:HA	1:A:363:PRO:HD3	1.99	0.45
1:A:288:ASN:ND2	1:A:310:TYR:H	2.11	0.44
1:B:226[B]:HIS:CD2	1:B:231:ILE:HG12	2.52	0.44
1:A:136:LYS:HB2	1:A:204:MET:HE1	1.99	0.44
1:B:184:ILE:O	1:B:184:ILE:CG2	2.65	0.44
1:A:26:THR:HG22	1:A:27:LEU:N	2.33	0.44
1:B:244:TYR:O	1:B:248:LEU:HG	2.18	0.44
1:B:226[B]:HIS:HD2	1:B:230:PHE:O	2.01	0.43
1:A:250:LYS:HG3	3:A:2146:HOH:O	2.17	0.43
1:B:256:LEU:C	1:B:256:LEU:HD23	2.43	0.43
1:A:282:ARG:HD3	1:A:316:GLU:HG2	2.01	0.43
1:B:147:ALA:HB1	1:B:150:ASP:HB2	2.00	0.43
1:B:152:ARG:HD3	1:B:152:ARG:H	1.83	0.43
1:B:365:ARG:O	2:C:10:ARG:CB	2.66	0.43
1:A:206:MET:HG3	1:A:227:VAL:HG21	2.00	0.43
1:A:282:ARG:HH21	1:A:366:LEU:CB	2.30	0.43
1:B:150:ASP:OD1	1:B:151:VAL:N	2.52	0.43
1:A:331:LEU:O	1:A:332:LYS:C	2.62	0.43
1:B:226[B]:HIS:CD2	1:B:230:PHE:O	2.72	0.43
1:A:56:ARG:HG3	3:A:2027:HOH:O	2.20	0.42
1:A:143:GLN:OE1	1:A:201:ILE:HD13	2.19	0.42
1:A:153:TYR:CE2	1:A:238:ASP:O	2.73	0.42
1:A:137:ARG:HH11	1:A:141:ALA:HB2	1.85	0.42
1:B:130:LEU:HD21	1:B:214:LEU:HD23	2.01	0.42
1:B:214:LEU:HD13	1:B:227:VAL:CG2	2.50	0.42
1:A:8:GLU:N	1:A:8:GLU:CD	2.78	0.42
1:B:197:ARG:HH21	1:B:198:LYS:NZ	2.18	0.42
1:B:249:PRO:HD2	1:B:348:GLN:NE2	2.28	0.42
1:A:135:MET:HG3	1:A:207:LEU:HD21	2.02	0.41
1:A:23:GLY:O	1:A:24:ARG:C	2.63	0.41
1:A:252:PRO:O	1:A:255:HIS:CE1	2.74	0.41
1:A:137:ARG:NH1	1:A:141:ALA:HB2	2.36	0.41
1:B:11:LEU:HD13	1:B:79[B]:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PHE:CD2	1:B:326:ASP:HB3	2.56	0.41
1:B:146:MET:HE3	1:B:157:GLY:C	2.46	0.41
1:A:143:GLN:CG	1:A:146:MET:HE2	2.51	0.41
1:A:44:LEU:HD22	1:A:44:LEU:N	2.36	0.41
1:A:196:PRO:HG2	3:A:2139:HOH:O	2.21	0.41
1:B:224:ARG:HG2	1:B:226[A]:HIS:CE1	2.56	0.41
1:A:19:GLY:CA	1:A:205:ARG:HH12	2.34	0.41
1:A:19:GLY:O	1:A:21:LEU:N	2.54	0.41
1:B:362:MET:HG3	2:C:12:LEU:HB2	2.03	0.41
1:B:366:LEU:HD22	1:B:366:LEU:N	2.36	0.41
1:A:143:GLN:OE1	1:A:201:ILE:CD1	2.69	0.40
1:B:136:LYS:HA	1:B:204:MET:HE1	2.03	0.40
1:A:150:ASP:H	1:A:156:ASN:ND2	2.13	0.40
1:A:214:LEU:HD11	1:A:225:ALA:HB1	2.03	0.40
1:B:291:LYS:HE2	1:B:293:THR:HG21	2.03	0.40
1:A:197:ARG:O	1:A:201:ILE:HG12	2.22	0.40
1:A:296:ASN:HB2	1:A:297:PRO:CD	2.52	0.40
1:A:8:GLU:CD	1:A:8:GLU:H	2.29	0.40
1:A:282:ARG:HD3	1:A:316:GLU:CG	2.52	0.40
1:B:208:ASP:OD2	1:B:210:GLY:HA3	2.22	0.40
1:B:217:GLN:NE2	1:B:226[A]:HIS:CE1	2.88	0.40
1:B:241:PHE:CD1	1:B:242:PRO:HD2	2.57	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	369/366 (101%)	356 (96%)	10 (3%)	3 (1%)	16	4
1	B	367/366 (100%)	359 (98%)	8 (2%)	0	100	100
2	C	5/16 (31%)	4 (80%)	1 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	741/748 (99%)	719 (97%)	19 (3%)	3 (0%)	30 15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	20	PRO
1	A	19	GLY

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	318/313 (102%)	312 (98%)	6 (2%)	50 28
1	B	316/313 (101%)	311 (98%)	5 (2%)	55 34
2	C	6/15 (40%)	6 (100%)	0	100 100
All	All	640/641 (100%)	629 (98%)	11 (2%)	53 32

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	LYS
1	A	56	ARG
1	A	176	ARG
1	A	227	VAL
1	A	238	ASP
1	B	121	ASP
1	B	167	LEU
1	B	176	ARG
1	B	191	HIS
1	B	299	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	148	HIS
1	A	156	ASN
1	A	212	ASN
1	A	255	HIS
1	A	288	ASN
1	A	320	ASN
1	A	329	ASN
1	A	348	GLN
1	B	16	GLN
1	B	61	GLN
1	B	91	GLN
1	B	123	GLN
1	B	156	ASN
1	B	175	HIS
1	B	186	GLN
1	B	217	GLN
1	B	255	HIS
1	B	329	ASN
1	B	348	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	366/366 (100%)	0.33	24 (6%)	24 27	10, 20, 43, 79	5 (1%)
1	B	366/366 (100%)	0.39	32 (8%)	16 17	10, 21, 42, 51	4 (1%)
2	C	7/16 (43%)	1.56	1 (14%)	6 6	19, 20, 26, 29	7 (100%)
All	All	739/748 (98%)	0.37	57 (7%)	19 22	10, 20, 43, 79	16 (2%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	LEU	7.1
1	B	39	ASP	6.6
1	A	19	GLY	4.8
1	A	207	LEU	4.7
1	B	22	GLY	4.7
1	B	240	ARG	4.3
1	B	188	LEU	4.0
1	B	366	LEU	3.9
1	A	27	LEU	3.7
1	A	23	GLY	3.6
1	B	211	ASP	3.6
1	A	20	PRO	3.5
1	B	247	VAL	3.4
1	B	246	ARG	3.3
1	B	151	VAL	3.3
1	A	278	PHE	3.3
1	A	22	GLY	3.2
1	A	25	PRO	3.2
1	A	210	GLY	3.1
1	A	26	THR	3.1
1	B	185	GLY	3.0
1	B	189	PRO	3.0
1	A	212	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	24	ARG	2.9
1	B	153	TYR	2.9
1	A	209	GLY	2.9
1	B	121	ASP	2.9
1	B	212	ASN	2.9
1	B	332	LYS	2.8
1	B	148	HIS	2.7
1	B	253	ASP	2.7
1	B	208	ASP	2.7
1	B	241	PHE	2.6
1	B	184	ILE	2.6
1	B	252	PRO	2.6
1	B	238	ASP	2.5
1	A	120	ASP	2.4
1	B	250	LYS	2.4
1	B	154	TYR	2.3
1	A	227	VAL	2.3
1	A	253	ASP	2.3
1	A	114	ALA	2.2
1	B	118	ASN	2.2
1	B	187	SER	2.2
1	A	16	GLN	2.1
1	B	209	GLY	2.1
2	C	12	LEU	2.1
1	A	118	ASN	2.1
1	B	120	ASP	2.1
1	A	276	GLU	2.1
1	A	117	PRO	2.0
1	A	15	GLN	2.0
1	B	164	GLY	2.0
1	B	244	TYR	2.0
1	A	211	ASP	2.0
1	B	192	SER	2.0
1	B	311	SER	2.0

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

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.