



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:13 AM UTC

PDB ID : 3C7V / pdb_00003c7v
Title : Structural Insight into the Kinetics and Delta-Cp of interactions between
TEM-1 Beta-Lactamase and BLIP
Authors : Wang, J.; Chow, D.-C.
Deposited on : 2008-02-08
Resolution : 2.07 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

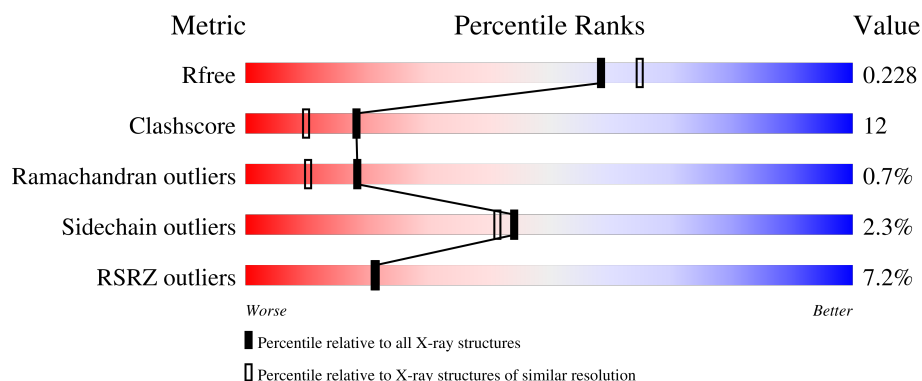
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	263	6% 77% 21% .
1	C	263	11% 70% 28% .
2	B	165	4% 86% 13% .
2	D	165	5% 82% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6689 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2030	1268	360	391	11			
1	C	263	Total	C	N	O	S	0	0	0
			2030	1268	360	391	11			

- Molecule 2 is a protein called Beta-lactamase inhibitory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1228	772	207	242	7			
2	D	165	Total	C	N	O	S	0	0	0
			1228	772	207	242	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	51	ALA	TYR	engineered mutation	UNP P35804
D	51	ALA	TYR	engineered mutation	UNP P35804

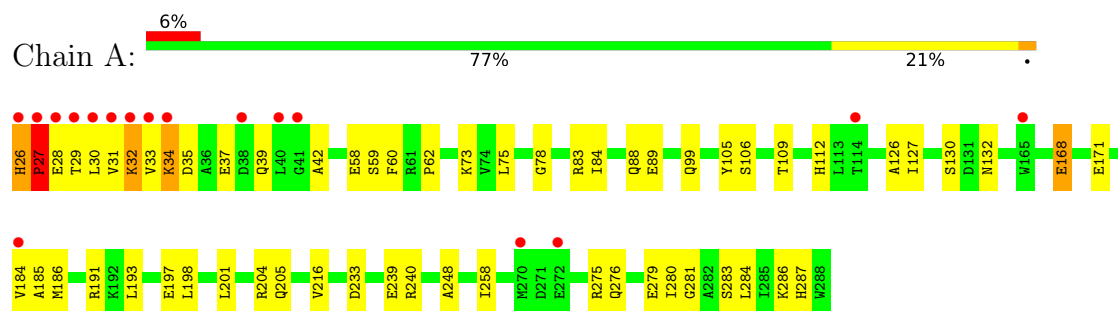
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	47	Total	O	0	0
			47	47		
3	C	43	Total	O	0	0
			43	43		
3	D	30	Total	O	0	0
			30	30		

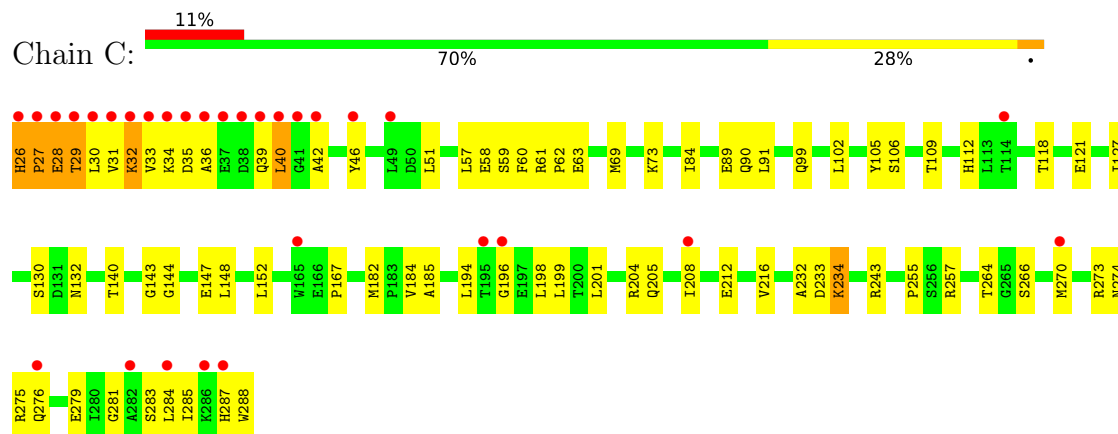
3 Residue-property plots

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.

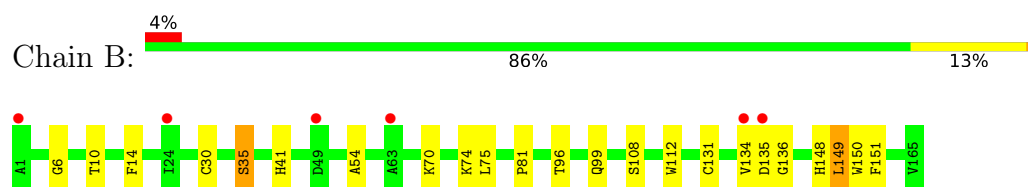
• Molecule 1: Beta-lactamase



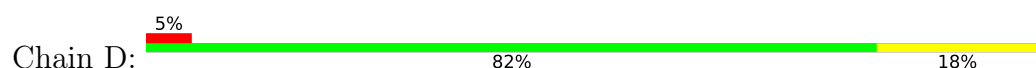
• Molecule 1: Beta-lactamase



• Molecule 2: Beta-lactamase inhibitory protein



• Molecule 2: Beta-lactamase inhibitory protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.67Å 129.04Å 78.90Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	35.09 – 2.07 35.09 – 2.07	Depositor EDS
% Data completeness (in resolution range)	92.9 (35.09-2.07) 92.8 (35.09-2.07)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.238 (Not available) , 0.228	Depositor DCC
R_{free} test set	2789 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6689	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 5.81% 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	0.76	0/2064	0.95	7/2794 (0.3%)
1	C	0.71	0/2064	0.93	4/2794 (0.1%)
2	B	0.74	0/1256	0.93	2/1704 (0.1%)
2	D	0.66	0/1256	0.88	2/1704 (0.1%)
All	All	0.72	0/6640	0.93	15/8996 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLU	N-CA-C	-6.71	104.72	113.17
1	C	144	GLY	CA-C-N	6.35	126.84	119.47
1	C	144	GLY	C-N-CA	6.35	126.84	119.47
2	B	112	TRP	N-CA-C	-6.20	103.83	111.40
2	B	136	GLY	N-CA-C	6.06	120.53	112.77
1	A	233	ASP	N-CA-C	5.75	116.97	108.86
1	A	216	VAL	N-CA-C	5.59	117.48	112.17
1	A	168	GLU	N-CA-C	5.51	118.05	111.71
1	C	216	VAL	N-CA-C	5.40	117.30	112.17
1	C	233	ASP	N-CA-C	5.40	116.47	108.86
1	A	78	GLY	N-CA-C	-5.28	106.02	112.77
2	D	52	ALA	N-CA-C	-5.27	103.08	110.50
1	A	127	ILE	N-CA-C	5.24	115.90	110.82
1	A	248	ALA	N-CA-C	-5.20	99.82	108.34
2	D	75	LEU	N-CA-C	-5.12	107.17	113.41

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	2030	0	2040	52	0
1	C	2030	0	2040	80	0
2	B	1228	0	1167	18	0
2	D	1228	0	1167	18	0
3	A	53	0	0	0	0
3	B	47	0	0	0	0
3	C	43	0	0	4	0
3	D	30	0	0	1	0
All	All	6689	0	6414	157	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 12.

All (157) 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:C:140:THR:HG21	3:C:319:HOH:O	1.50	1.09
1:C:90:GLN:HB2	3:C:290:HOH:O	1.53	1.07
1:C:26:HIS:HB2	1:C:58:GLU:OE1	1.58	1.03
1:C:30:LEU:HD21	1:C:59:SER:O	1.71	0.89
1:C:84:ILE:HD13	1:C:91:LEU:HG	1.58	0.84
1:A:26:HIS:HD1	1:A:26:HIS:N	1.76	0.83
1:C:26:HIS:N	1:C:27:PRO:CD	2.42	0.82
1:C:27:PRO:HD2	1:C:287:HIS:O	1.78	0.82
1:A:26:HIS:N	1:A:27:PRO:CD	2.45	0.79
1:A:32:LYS:HG3	1:A:280:ILE:HD13	1.65	0.78
1:C:30:LEU:HD11	1:C:58:GLU:HG2	1.68	0.75
1:A:26:HIS:N	1:A:26:HIS:ND1	2.30	0.73
1:C:26:HIS:CD2	1:C:57:LEU:O	2.42	0.72
1:C:194:LEU:HD22	1:C:208:ILE:CG1	2.20	0.72
1:C:28:GLU:HG2	1:C:29:THR:H	1.54	0.71
1:A:83:ARG:HA	1:A:88:GLN:HE21	1.54	0.71
1:C:127:ILE:O	1:C:234:LYS:HE3	1.93	0.68
1:A:32:LYS:HE2	1:A:279:GLU:HB3	1.76	0.67
1:A:99:GLN:HG2	2:B:150:TRP:CG	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:CB	3:C:290:HOH:O	2.22	0.66
1:C:99:GLN:HG2	2:D:150:TRP:CG	2.30	0.66
1:C:27:PRO:HB2	1:C:287:HIS:CD2	2.32	0.65
1:A:26:HIS:HB2	1:A:58:GLU:OE2	1.96	0.65
1:C:105:TYR:CZ	2:D:74:LYS:HE3	2.31	0.65
2:D:134:VAL:HG13	3:D:181:HOH:O	1.96	0.65
1:C:31:VAL:O	1:C:34:LYS:HB3	1.97	0.65
1:A:26:HIS:N	1:A:27:PRO:HD3	2.11	0.64
1:A:29:THR:HG21	1:A:58:GLU:OE1	1.97	0.64
1:C:275:ARG:O	1:C:279:GLU:HG3	1.98	0.64
1:A:37:GLU:HG3	1:A:42:ALA:O	1.99	0.63
1:A:275:ARG:O	1:A:279:GLU:HG3	1.97	0.63
1:C:234:LYS:HE2	3:C:300:HOH:O	1.98	0.63
2:D:96:THR:H	2:D:99:GLN:NE2	1.97	0.62
1:A:26:HIS:HB2	1:A:58:GLU:CD	2.25	0.62
1:C:194:LEU:HB3	1:C:208:ILE:HD11	1.81	0.62
1:A:201:LEU:HD22	1:A:204:ARG:NH2	2.15	0.61
1:A:27:PRO:HD2	1:A:287:HIS:O	2.00	0.61
2:D:96:THR:H	2:D:99:GLN:HE21	1.49	0.61
1:A:83:ARG:HA	1:A:88:GLN:NE2	2.16	0.60
1:A:191:ARG:HB2	1:A:258:ILE:HD12	1.83	0.60
1:C:29:THR:HB	1:C:58:GLU:OE2	2.01	0.60
1:C:35:ASP:O	1:C:39:GLN:HG2	2.01	0.60
1:C:26:HIS:N	1:C:26:HIS:ND1	2.47	0.60
1:C:99:GLN:HG3	2:D:148:HIS:CE1	2.37	0.60
1:C:281:GLY:O	1:C:285:ILE:HG12	2.01	0.60
1:C:27:PRO:HB2	1:C:287:HIS:HD2	1.68	0.59
1:C:89:GLU:HG3	1:C:90:GLN:N	2.18	0.58
1:A:105:TYR:CZ	2:B:74:LYS:HE2	2.39	0.58
1:C:99:GLN:NE2	1:C:102:LEU:HD12	2.18	0.58
1:A:35:ASP:O	1:A:39:GLN:HG2	2.03	0.57
1:C:26:HIS:HD2	1:C:57:LEU:O	1.84	0.57
2:D:8:LYS:HD3	2:D:25:ALA:HA	1.87	0.57
1:C:118:THR:OG1	1:C:121:GLU:HG3	2.06	0.56
1:C:30:LEU:CD2	1:C:60:PHE:HB2	2.35	0.56
1:A:32:LYS:NZ	1:A:32:LYS:HB2	2.21	0.55
1:A:99:GLN:HE21	2:B:148:HIS:CE1	2.25	0.55
1:C:40:LEU:HD13	1:C:276:GLN:HG3	1.88	0.54
2:B:131:CYS:SG	2:B:149:LEU:HD22	2.47	0.54
1:A:168:GLU:O	1:A:171:GLU:HG3	2.07	0.54
2:B:96:THR:H	2:B:99:GLN:NE2	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:HIS:N	1:C:26:HIS:HD1	2.06	0.53
1:C:26:HIS:N	1:C:27:PRO:HD3	2.21	0.53
2:D:81:PRO:HA	2:D:108:SER:HA	1.90	0.53
2:B:134:VAL:HG13	2:B:135:ASP:H	1.73	0.53
1:C:270:MET:HE3	1:C:274:ASN:HD21	1.72	0.53
2:D:12:ILE:HD13	2:D:21:VAL:HG13	1.89	0.53
1:A:29:THR:CG2	1:A:58:GLU:OE1	2.57	0.53
1:A:34:LYS:HD3	1:A:35:ASP:N	2.24	0.53
1:A:59:SER:HB2	1:A:62:PRO:HB3	1.91	0.53
1:A:99:GLN:HG3	2:B:148:HIS:CE1	2.43	0.53
1:C:106:SER:HB3	1:C:109:THR:OG1	2.09	0.52
1:C:84:ILE:CD1	1:C:91:LEU:HG	2.36	0.52
1:C:194:LEU:HD22	1:C:208:ILE:HG13	1.89	0.52
1:C:212:GLU:HA	1:C:232:ALA:HA	1.91	0.52
1:A:193:LEU:HD23	1:A:198:LEU:HD23	1.91	0.52
1:C:26:HIS:N	1:C:287:HIS:O	2.42	0.52
2:D:3:VAL:O	2:D:5:THR:HG23	2.10	0.52
1:C:36:ALA:O	1:C:40:LEU:HB2	2.11	0.51
1:C:26:HIS:N	1:C:27:PRO:HD2	2.22	0.51
1:A:26:HIS:CB	1:A:58:GLU:CD	2.83	0.50
1:C:42:ALA:HB1	1:C:264:THR:O	2.11	0.50
1:C:270:MET:HG3	1:C:273:ARG:NH1	2.27	0.50
1:A:84:ILE:HD13	1:A:89:GLU:C	2.36	0.50
1:A:112:HIS:HE1	2:B:35:SER:O	1.94	0.50
1:C:99:GLN:HG2	2:D:150:TRP:CB	2.41	0.50
1:A:276:GLN:O	1:A:280:ILE:HG12	2.11	0.50
2:B:6:GLY:O	2:B:10:THR:HG23	2.12	0.50
1:C:201:LEU:O	1:C:205:GLN:HG3	2.11	0.50
2:B:54:ALA:HB2	2:B:75:LEU:HD11	1.95	0.49
1:C:270:MET:HG3	1:C:273:ARG:HH12	1.78	0.49
1:A:32:LYS:HB2	1:A:32:LYS:HZ3	1.79	0.48
1:C:32:LYS:O	1:C:32:LYS:HE3	2.13	0.48
2:B:134:VAL:HG13	2:B:135:ASP:N	2.29	0.48
1:C:28:GLU:O	1:C:29:THR:CB	2.62	0.48
1:C:99:GLN:HE21	1:C:102:LEU:HD12	1.79	0.48
1:C:148:LEU:O	1:C:152:LEU:HG	2.14	0.48
1:A:28:GLU:HB3	1:A:287:HIS:CE1	2.49	0.47
1:A:29:THR:HA	1:A:283:SER:OG	2.14	0.47
1:A:105:TYR:OH	2:B:74:LYS:HE2	2.14	0.47
1:C:29:THR:HG21	1:C:284:LEU:HB3	1.95	0.47
1:C:61:ARG:N	1:C:62:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:VAL:HG13	1:A:185:ALA:N	2.30	0.47
1:C:57:LEU:HD12	1:C:257:ARG:HD3	1.97	0.47
1:A:106:SER:HB3	1:A:109:THR:OG1	2.13	0.47
1:C:143:GLY:HA3	1:C:147:GLU:HG3	1.95	0.47
1:C:28:GLU:HG2	1:C:29:THR:N	2.28	0.46
1:C:28:GLU:O	1:C:29:THR:HB	2.16	0.46
2:B:54:ALA:HB2	2:B:75:LEU:CD1	2.45	0.46
1:C:198:LEU:C	1:C:198:LEU:HD13	2.41	0.46
2:B:151:PHE:CD1	2:B:151:PHE:N	2.84	0.46
2:B:30:CYS:HA	2:B:41:HIS:O	2.15	0.46
1:C:30:LEU:HD11	1:C:58:GLU:CG	2.43	0.45
1:C:112:HIS:HE1	2:D:35:SER:O	2.00	0.44
1:A:33:VAL:HG22	1:A:280:ILE:HD12	1.98	0.44
1:A:75:LEU:HD11	1:A:186:MET:HE1	1.98	0.44
1:C:26:HIS:O	1:C:58:GLU:OE1	2.34	0.44
1:C:284:LEU:C	1:C:284:LEU:HD12	2.42	0.44
1:C:194:LEU:HD22	1:C:208:ILE:HG12	1.98	0.44
1:A:32:LYS:NZ	1:A:32:LYS:CB	2.80	0.44
1:C:30:LEU:HD23	1:C:60:PHE:HB2	2.00	0.44
1:A:29:THR:O	1:A:33:VAL:HG23	2.18	0.44
1:C:31:VAL:HG13	1:C:32:LYS:N	2.32	0.43
2:D:18:ARG:NH1	2:D:38:ASP:O	2.49	0.43
2:D:118:ALA:O	2:D:119:TYR:C	2.61	0.43
1:C:63:GLU:O	1:C:182:MET:HE2	2.19	0.43
2:D:16:MET:O	2:D:66:LYS:HA	2.19	0.43
1:A:126:ALA:O	1:A:130:SER:HA	2.18	0.43
1:A:29:THR:HG23	1:A:30:LEU:HD22	2.01	0.42
1:A:286:LYS:HD3	1:A:287:HIS:CE1	2.54	0.42
2:D:68:ASP:C	2:D:68:ASP:OD1	2.63	0.42
1:A:26:HIS:N	1:A:27:PRO:HD2	2.32	0.42
1:A:239:GLU:O	1:A:240:ARG:HB2	2.19	0.42
1:A:30:LEU:CD1	1:A:60:PHE:HB2	2.49	0.42
1:C:73:LYS:NZ	1:C:132:ASN:ND2	2.67	0.42
2:B:96:THR:H	2:B:99:GLN:HE21	1.67	0.42
1:C:32:LYS:HE3	1:C:35:ASP:HB2	2.01	0.42
1:C:69:MET:HE1	1:C:243:ARG:C	2.44	0.42
2:D:95:MET:HA	2:D:99:GLN:NE2	2.35	0.41
1:C:184:VAL:HG13	1:C:185:ALA:N	2.35	0.41
1:C:42:ALA:HB2	1:C:266:SER:CA	2.50	0.41
1:A:73:LYS:NZ	1:A:132:ASN:ND2	2.69	0.41
1:A:33:VAL:HA	1:A:280:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:HB2	1:C:266:SER:HA	2.02	0.41
1:C:285:ILE:O	1:C:288:TRP:HB2	2.21	0.41
2:B:81:PRO:HA	2:B:108:SER:HA	2.02	0.41
1:C:29:THR:HA	1:C:283:SER:OG	2.21	0.41
1:C:26:HIS:O	1:C:27:PRO:C	2.64	0.41
1:C:30:LEU:CD1	1:C:58:GLU:CG	2.99	0.41
1:C:51:LEU:HD23	1:C:255:PRO:O	2.21	0.41
1:A:281:GLY:O	1:A:284:LEU:HG	2.21	0.40
1:A:73:LYS:NZ	1:A:132:ASN:HD22	2.20	0.40
1:C:30:LEU:HA	1:C:33:VAL:CG2	2.51	0.40
1:A:28:GLU:O	1:A:31:VAL:HG12	2.22	0.40
1:C:30:LEU:CD1	1:C:46:TYR:HE2	2.34	0.40
1:C:199:LEU:O	1:C:204:ARG:NH2	2.53	0.40
2:D:69:SER:HB2	2:D:115:TYR:CD2	2.56	0.40
2:B:14:PHE:CE2	2:B:70:LYS:HG3	2.56	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	261/263 (99%)	253 (97%)	7 (3%)	1 (0%)	30	23
1	C	261/263 (99%)	251 (96%)	6 (2%)	4 (2%)	8	2
2	B	163/165 (99%)	156 (96%)	7 (4%)	0	100	100
2	D	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	21	13
All	All	848/856 (99%)	818 (96%)	24 (3%)	6 (1%)	18	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	PRO
1	C	27	PRO
1	C	28	GLU
1	C	29	THR
1	C	196	GLY
2	D	134	VAL

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	218/218 (100%)	213 (98%)	5 (2%)	44	41
1	C	218/218 (100%)	212 (97%)	6 (3%)	38	34
2	B	125/125 (100%)	123 (98%)	2 (2%)	55	55
2	D	125/125 (100%)	122 (98%)	3 (2%)	43	40
All	All	686/686 (100%)	670 (98%)	16 (2%)	44	41

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	27	PRO
1	A	32	LYS
1	A	34	LYS
1	A	205	GLN
2	B	35	SER
2	B	149	LEU
1	C	26	HIS
1	C	32	LYS
1	C	40	LEU
1	C	130	SER
1	C	167	PRO
1	C	234	LYS
2	D	128	SER
2	D	149	LEU
2	D	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	88	GLN
1	A	90	GLN
1	A	96	HIS
1	A	99	GLN
1	A	100	ASN
1	A	112	HIS
1	A	132	ASN
1	A	154	ASN
2	B	13	GLN
2	B	19	GLN
2	B	45	HIS
2	B	99	GLN
1	C	26	HIS
1	C	96	HIS
1	C	99	GLN
1	C	112	HIS
1	C	132	ASN
1	C	154	ASN
1	C	267	GLN
2	D	19	GLN
2	D	45	HIS
2	D	99	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	263/263 (100%)	0.24	17 (6%) 25 24	14, 26, 62, 112	0
1	C	263/263 (100%)	0.59	30 (11%) 10 10	18, 31, 69, 104	0
2	B	165/165 (100%)	0.10	6 (3%) 46 47	14, 24, 40, 65	0
2	D	165/165 (100%)	0.38	9 (5%) 30 30	19, 30, 45, 72	0
All	All	856/856 (100%)	0.35	62 (7%) 21 21	14, 28, 56, 112	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	27	PRO	10.8
1	A	27	PRO	9.3
1	C	31	VAL	9.3
1	C	30	LEU	9.1
1	C	33	VAL	8.2
1	C	36	ALA	8.0
1	C	26	HIS	6.5
2	D	1	ALA	6.1
1	A	26	HIS	6.1
1	C	29	THR	6.0
2	B	1	ALA	5.9
1	C	40	LEU	5.9
1	A	31	VAL	5.7
1	A	29	THR	5.6
1	A	30	LEU	5.0
1	C	41	GLY	4.3
1	C	46	TYR	4.0
2	D	165	VAL	4.0
1	A	41	GLY	4.0
1	C	270	MET	3.9
2	B	135	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	32	LYS	3.7
1	C	39	GLN	3.6
1	A	34	LYS	3.5
1	C	208	ILE	3.3
1	C	284	LEU	3.3
2	D	122	THR	3.2
1	C	37	GLU	3.1
1	C	286	LYS	3.1
1	A	28	GLU	3.1
1	A	165	TRP	3.0
1	C	34	LYS	3.0
1	C	165	TRP	3.0
1	C	196	GLY	2.9
1	C	28	GLU	2.8
1	A	270	MET	2.8
1	C	32	LYS	2.8
2	D	15	GLY	2.7
1	C	42	ALA	2.7
1	C	282	ALA	2.6
1	A	38	ASP	2.6
1	A	40	LEU	2.6
2	B	49	ASP	2.6
1	A	184	VAL	2.5
2	D	63	ALA	2.5
1	A	272	GLU	2.5
2	B	63	ALA	2.4
2	D	2	GLY	2.4
1	C	195	THR	2.4
1	C	276	GLN	2.3
2	D	61	ALA	2.3
1	C	287	HIS	2.2
1	A	33	VAL	2.2
1	C	114	THR	2.2
1	C	35	ASP	2.2
2	D	3	VAL	2.2
2	B	134	VAL	2.1
2	D	64	ASP	2.1
1	A	114	THR	2.1
1	C	49	LEU	2.1
1	C	38	ASP	2.1
2	B	24	ILE	2.1

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.