



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:52 AM UTC

PDB ID : 1KHY / pdb_00001khy
Title : The Crystal Structure of ClpB N Terminal Domain, Implication to the Peptide Binding Function of ClpB
Authors : Jingzhi, L.; Bingdong, S.
Deposited on : 2001-12-01
Resolution : 1.95 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:

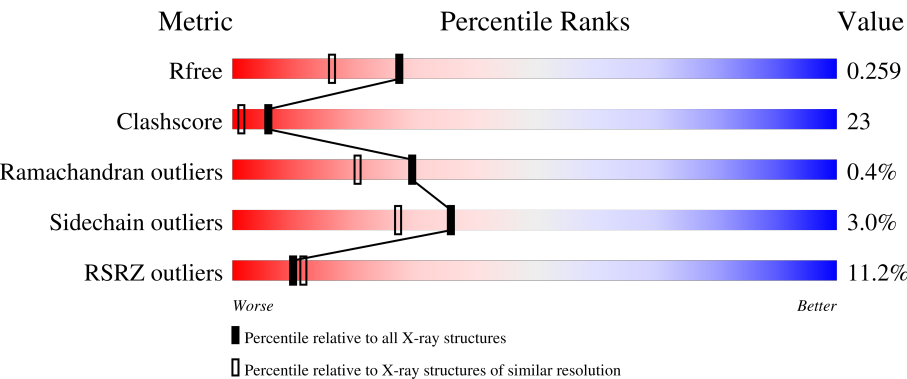
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	148	5% 57% 29% • 11%
1	B	148	3% 70% 19% • 10%
1	C	148	11% 57% 32% • 9%
1	D	148	21% 58% 33% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4304 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 CLPB PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	132	Total	C	N	O	S	Se	0	0	0
			992	616	179	195	1	1			
1	B	133	Total	C	N	O	S	Se	0	0	0
			1000	622	180	196	1	1			
1	C	135	Total	C	N	O	S	Se	0	0	0
			1015	630	182	200	1	2			
1	D	140	Total	C	N	O	S	Se	0	0	0
			1043	645	187	208	1	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P63284
A	35	MSE	MET	modified residue	UNP P63284
A	143	MSE	MET	modified residue	UNP P63284
B	1	MSE	MET	modified residue	UNP P63284
B	35	MSE	MET	modified residue	UNP P63284
B	143	MSE	MET	modified residue	UNP P63284
C	1	MSE	MET	modified residue	UNP P63284
C	35	MSE	MET	modified residue	UNP P63284
C	143	MSE	MET	modified residue	UNP P63284
D	1	MSE	MET	modified residue	UNP P63284
D	35	MSE	MET	modified residue	UNP P63284
D	143	MSE	MET	modified residue	UNP P63284

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	75	Total	O	0	0
			75	75		

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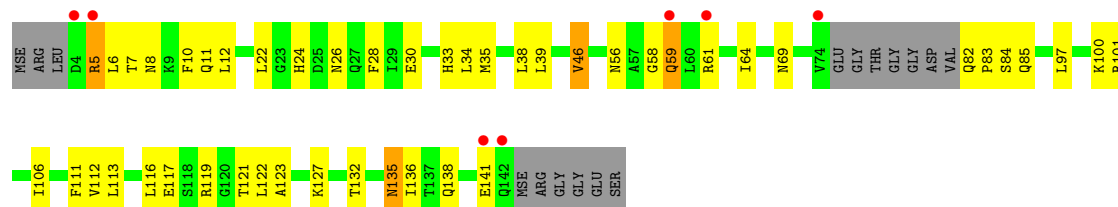
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	63	Total 63	O 63	0	0
2	D	52	Total 52	O 52	0	0

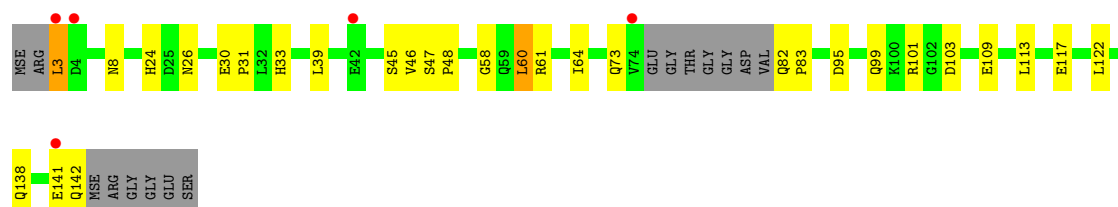
3 Residue-property plots [i](#)

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.

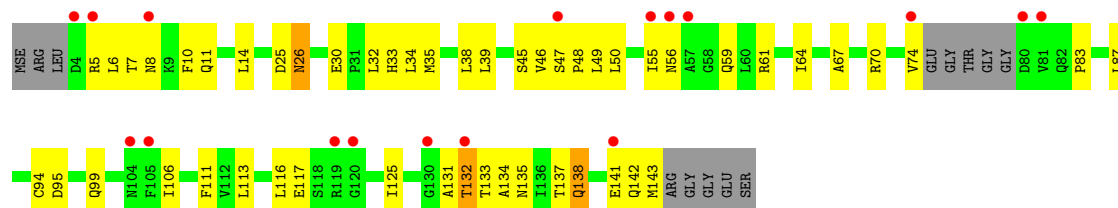
• Molecule 1: CLPB PROTEIN



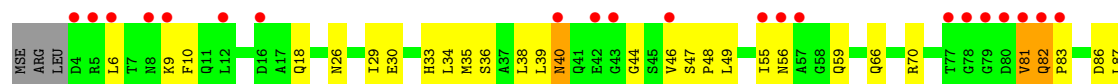
• Molecule 1: CLPB PROTEIN

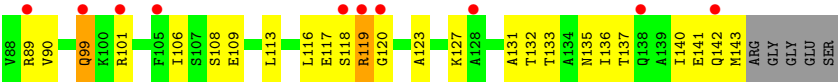


• Molecule 1: CLPB PROTEIN



• Molecule 1: CLPB PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.21Å 52.60Å 56.84Å 90.45° 111.73° 107.05°	Depositor
Resolution (Å)	30.00 – 1.95 30.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	90.6 (30.00-1.95) 96.5 (30.00-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.95 (at 1.95Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.259 0.222 , 0.259	Depositor DCC
R_{free} test set	3585 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4304	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1428e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0/999	0.82	3/1351 (0.2%)
1	B	0.37	0/1007	0.80	1/1362 (0.1%)
1	C	0.35	0/1021	0.84	2/1379 (0.1%)
1	D	0.36	0/1050	0.85	1/1419 (0.1%)
All	All	0.36	0/4077	0.83	7/5511 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	VAL	N-CA-C	6.93	117.08	110.42
1	D	81	VAL	N-CA-C	5.71	115.82	107.37
1	B	46	VAL	N-CA-C	5.38	115.58	110.53
1	A	121	THR	N-CA-C	5.22	116.66	111.07
1	C	26	ASN	N-CA-C	-5.11	102.12	110.20
1	A	5	ARG	N-CA-C	-5.09	106.92	113.02
1	C	5	ARG	N-CA-C	-5.08	106.33	112.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	992	0	1010	44	0
1	B	1000	0	1021	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1015	0	1032	58	0
1	D	1043	0	1055	63	0
2	A	64	0	0	2	0
2	B	75	0	0	4	0
2	C	63	0	0	3	0
2	D	52	0	0	2	0
All	All	4304	0	4118	187	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 23.

All (187) 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:D:35:MSE:HE2	1:D:39:LEU:HG	1.31	1.12
1:D:35:MSE:HE1	1:D:46:VAL:HG11	1.35	1.06
1:A:30:GLU:H	1:A:33:HIS:HD2	1.11	0.98
1:B:30:GLU:H	1:B:33:HIS:HD2	1.09	0.98
1:C:30:GLU:H	1:C:33:HIS:HD2	1.14	0.96
1:D:30:GLU:H	1:D:33:HIS:HD2	1.14	0.88
1:D:89:ARG:HH22	1:D:118:SER:HB3	1.40	0.86
1:C:132:THR:HG22	1:C:135:ASN:H	1.41	0.84
1:C:35:MSE:HE1	1:C:46:VAL:HG11	1.58	0.84
1:B:82:GLN:N	1:B:83:PRO:HD3	1.96	0.80
1:C:138:GLN:NE2	1:C:142:GLN:OE1	2.13	0.80
1:D:30:GLU:H	1:D:33:HIS:CD2	1.99	0.79
1:C:132:THR:HG23	1:C:134:ALA:H	1.48	0.78
1:C:56:ASN:HD22	1:C:59:GLN:HB2	1.48	0.78
1:C:116:LEU:HD21	1:C:132:THR:C	2.10	0.76
1:C:47:SER:HB2	1:C:48:PRO:HD3	1.68	0.74
1:A:132:THR:H	1:A:135:ASN:HD21	1.34	0.74
1:B:26:ASN:HD22	1:B:33:HIS:HE1	1.35	0.73
1:D:47:SER:HB2	1:D:48:PRO:HD3	1.70	0.73
1:C:138:GLN:C	1:C:138:GLN:HE21	1.97	0.72
1:D:120:GLY:H	1:D:123:ALA:HB3	1.53	0.72
1:A:138:GLN:O	1:A:141:GLU:HG2	1.88	0.72
1:B:30:GLU:H	1:B:33:HIS:CD2	2.01	0.72
1:C:8:ASN:HB3	2:C:177:HOH:O	1.90	0.71
1:A:35:MSE:HE1	1:A:112:VAL:HG22	1.72	0.70
1:A:26:ASN:HD22	1:A:33:HIS:HE1	1.37	0.70
1:A:30:GLU:H	1:A:33:HIS:CD2	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:GLN:HG3	1:D:81:VAL:HG13	1.74	0.70
1:C:56:ASN:ND2	1:C:59:GLN:HB2	2.08	0.69
1:A:35:MSE:HG3	1:A:122:LEU:HD11	1.75	0.68
1:D:35:MSE:CE	1:D:46:VAL:HG11	2.20	0.68
1:B:26:ASN:HD22	1:B:33:HIS:CE1	2.13	0.66
1:D:119:ARG:HH11	1:D:127:LYS:NZ	1.94	0.66
1:A:26:ASN:HD22	1:A:33:HIS:CE1	2.13	0.66
1:A:35:MSE:HG2	1:A:111:PHE:HE2	1.61	0.65
1:A:56:ASN:ND2	1:A:59:GLN:H	1.94	0.65
1:C:137:THR:O	1:C:141:GLU:HG3	1.96	0.65
1:A:135:ASN:HD22	1:A:136:ILE:N	1.95	0.64
1:D:137:THR:O	1:D:141:GLU:HG3	1.97	0.64
1:D:56:ASN:HD22	1:D:59:GLN:HB2	1.61	0.63
1:D:9:LYS:HE3	1:D:44:GLY:HA2	1.80	0.63
1:A:58:GLY:O	1:A:61:ARG:HG2	2.00	0.62
1:B:109:GLU:H	1:B:109:GLU:CD	2.08	0.62
1:C:132:THR:CG2	1:C:134:ALA:H	2.13	0.62
1:D:56:ASN:HD22	1:D:59:GLN:CB	2.12	0.62
1:D:6:LEU:HD23	1:D:106:ILE:HB	1.80	0.61
1:A:56:ASN:HD22	1:A:59:GLN:H	1.48	0.61
1:C:30:GLU:H	1:C:33:HIS:CD2	2.05	0.61
1:C:32:LEU:HD21	1:C:125:ILE:HD12	1.81	0.61
1:B:26:ASN:ND2	1:B:33:HIS:HE1	1.99	0.61
1:D:36:SER:O	1:D:40:ASN:ND2	2.34	0.60
1:C:49:LEU:HD13	1:C:143:MSE:HE1	1.83	0.60
1:D:119:ARG:NH1	1:D:127:LYS:HZ2	1.99	0.60
1:D:18:GLN:HG3	1:D:81:VAL:CG1	2.31	0.60
1:A:82:GLN:N	1:A:83:PRO:CD	2.65	0.60
1:A:132:THR:H	1:A:135:ASN:ND2	1.99	0.60
1:D:127:LYS:HE3	2:D:178:HOH:O	2.01	0.60
1:A:138:GLN:HA	1:A:141:GLU:CD	2.28	0.59
1:D:35:MSE:HE3	1:D:38:LEU:HB2	1.83	0.59
1:D:132:THR:N	1:D:135:ASN:HD21	2.01	0.59
1:D:101:ARG:O	1:D:101:ARG:HD2	2.04	0.58
1:A:26:ASN:ND2	1:A:33:HIS:HE1	2.02	0.57
1:B:141:GLU:HB3	2:B:199:HOH:O	2.04	0.57
1:C:113:LEU:O	1:C:117:GLU:HG3	2.03	0.57
1:D:89:ARG:NH2	1:D:118:SER:HB3	2.15	0.57
1:D:119:ARG:NH1	1:D:127:LYS:NZ	2.53	0.56
1:C:132:THR:HG22	1:C:135:ASN:N	2.16	0.56
1:B:82:GLN:N	1:B:83:PRO:CD	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ASN:HD22	1:D:33:HIS:HE1	1.53	0.56
1:C:116:LEU:HD21	1:C:133:THR:N	2.19	0.56
1:C:132:THR:CG2	1:C:134:ALA:N	2.68	0.56
1:D:49:LEU:HD22	1:D:109:GLU:HG2	1.89	0.55
1:C:95:ASP:O	1:C:99:GLN:HG3	2.06	0.55
1:B:3:LEU:HD23	2:B:221:HOH:O	2.06	0.55
1:C:39:LEU:HD21	1:C:50:LEU:HD11	1.89	0.54
1:A:113:LEU:O	1:A:117:GLU:HG3	2.07	0.54
1:B:60:LEU:HD13	1:B:64:ILE:HG12	1.88	0.54
1:B:82:GLN:HB3	2:B:195:HOH:O	2.05	0.54
1:D:26:ASN:ND2	1:D:33:HIS:HE1	2.05	0.54
1:A:38:LEU:HB3	1:A:46:VAL:HG21	1.88	0.54
1:B:138:GLN:O	1:B:142:GLN:HG3	2.08	0.54
1:C:67:ALA:HB2	1:C:125:ILE:HD11	1.90	0.54
1:D:40:ASN:ND2	1:D:40:ASN:H	2.06	0.53
1:C:10:PHE:HE2	1:C:34:LEU:HD21	1.74	0.53
1:D:29:ILE:HG13	1:D:81:VAL:HG22	1.91	0.53
1:A:24:HIS:HE1	1:A:69:ASN:OD1	1.91	0.53
1:D:132:THR:H	1:D:135:ASN:ND2	2.06	0.53
1:C:116:LEU:HD23	1:C:133:THR:HA	1.91	0.53
1:C:138:GLN:NE2	1:C:138:GLN:O	2.41	0.52
1:C:138:GLN:HE21	1:C:138:GLN:CA	2.19	0.52
1:C:45:SER:O	1:C:48:PRO:HD2	2.08	0.52
1:C:26:ASN:HD22	1:C:33:HIS:CE1	2.28	0.52
1:A:8:ASN:CB	1:D:101:ARG:HH11	2.22	0.52
1:D:132:THR:H	1:D:135:ASN:HD21	1.54	0.52
1:D:35:MSE:HE3	1:D:35:MSE:HA	1.91	0.52
1:B:24:HIS:O	1:B:73:GLN:HG2	2.09	0.52
1:D:113:LEU:O	1:D:117:GLU:HG3	2.09	0.52
1:D:89:ARG:HH12	1:D:118:SER:CB	2.23	0.52
1:A:85:GLN:HG2	2:A:165:HOH:O	2.10	0.51
1:D:119:ARG:HH11	1:D:127:LYS:HZ2	1.57	0.51
1:C:45:SER:C	1:C:48:PRO:HD2	2.35	0.51
1:A:22:LEU:C	1:A:22:LEU:HD23	2.35	0.51
1:C:138:GLN:NE2	1:C:138:GLN:CA	2.74	0.51
1:D:119:ARG:HA	2:D:178:HOH:O	2.10	0.51
1:C:26:ASN:HD22	1:C:33:HIS:HE1	1.59	0.51
1:C:26:ASN:ND2	1:C:33:HIS:HE1	2.08	0.51
1:B:47:SER:N	1:B:48:PRO:HD2	2.26	0.51
1:B:95:ASP:O	1:B:99:GLN:HG3	2.11	0.50
1:D:142:GLN:O	1:D:143:MSE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ILE:HD13	1:D:131:ALA:HB2	1.93	0.50
1:A:35:MSE:HG2	1:A:111:PHE:CE2	2.44	0.50
1:B:60:LEU:CD1	1:B:64:ILE:HG12	2.41	0.50
1:C:35:MSE:HE2	1:C:39:LEU:HG	1.94	0.50
1:C:83:PRO:HB3	1:C:87:LEU:HD23	1.92	0.50
1:B:39:LEU:HD11	1:B:60:LEU:HD12	1.94	0.49
1:A:12:LEU:HD12	1:D:101:ARG:HH12	1.77	0.49
1:A:35:MSE:HB3	1:A:64:ILE:HD13	1.94	0.49
1:A:8:ASN:HB3	1:D:101:ARG:HH11	1.78	0.49
1:C:132:THR:HG23	1:C:133:THR:N	2.27	0.49
1:D:141:GLU:C	1:D:143:MSE:H	2.21	0.49
1:A:10:PHE:HE2	1:A:34:LEU:HD21	1.77	0.49
1:A:123:ALA:O	1:A:127:LYS:HG3	2.13	0.48
1:D:83:PRO:HB3	1:D:87:LEU:HD23	1.96	0.48
1:C:67:ALA:CB	1:C:125:ILE:HD11	2.44	0.47
1:A:97:LEU:O	1:A:101:ARG:HG3	2.14	0.47
1:D:56:ASN:ND2	1:D:59:GLN:H	2.12	0.47
1:C:56:ASN:HD22	1:C:59:GLN:CB	2.24	0.47
1:C:94:CYS:SG	1:C:111:PHE:HA	2.55	0.47
1:D:38:LEU:HB3	1:D:46:VAL:HG21	1.96	0.47
1:D:55:ILE:CD1	1:D:131:ALA:HB2	2.44	0.46
1:C:6:LEU:HD23	1:C:106:ILE:HB	1.96	0.46
1:D:40:ASN:ND2	1:D:40:ASN:N	2.63	0.45
1:D:82:GLN:H	1:D:82:GLN:HG2	1.46	0.45
1:C:39:LEU:HD12	1:C:64:ILE:HD12	1.99	0.45
1:C:39:LEU:CD1	1:C:64:ILE:HD12	2.46	0.45
1:A:56:ASN:HD22	1:A:59:GLN:CB	2.29	0.45
1:A:135:ASN:HD22	1:A:135:ASN:C	2.24	0.45
2:A:162:HOH:O	1:D:99:GLN:HG3	2.15	0.45
1:B:45:SER:O	1:B:48:PRO:HG2	2.17	0.45
1:A:6:LEU:HD23	1:A:106:ILE:HB	1.97	0.45
1:A:28:PHE:HB3	1:A:84:SER:HB3	1.98	0.45
1:C:7:THR:O	1:C:11:GLN:HG3	2.16	0.45
1:C:35:MSE:CE	1:C:39:LEU:HG	2.47	0.45
1:D:89:ARG:HH11	1:D:89:ARG:HG2	1.82	0.45
1:C:55:ILE:HD13	1:C:131:ALA:HB2	2.00	0.44
1:C:132:THR:HG21	1:C:134:ALA:HB3	1.99	0.44
1:D:35:MSE:HE3	1:D:35:MSE:O	2.17	0.44
1:A:26:ASN:ND2	1:A:33:HIS:CE1	2.80	0.44
1:D:66:GLN:HG2	1:D:70:ARG:NH2	2.31	0.44
1:B:113:LEU:O	1:B:117:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ASN:ND2	1:C:33:HIS:CE1	2.86	0.44
1:D:30:GLU:N	1:D:33:HIS:HD2	1.97	0.44
1:D:136:ILE:O	1:D:140:ILE:HG13	2.17	0.44
1:C:61:ARG:NE	2:C:169:HOH:O	2.42	0.44
1:D:10:PHE:HE2	1:D:34:LEU:HD21	1.82	0.44
1:D:116:LEU:CD1	1:D:136:ILE:HG13	2.48	0.44
1:C:46:VAL:O	1:C:50:LEU:HG	2.18	0.44
1:C:70:ARG:NH2	2:C:150:HOH:O	2.50	0.44
1:C:132:THR:HB	1:C:135:ASN:ND2	2.33	0.44
1:D:86:ASP:O	1:D:90:VAL:HG23	2.18	0.43
1:C:116:LEU:CD2	1:C:132:THR:C	2.88	0.43
1:A:7:THR:O	1:A:11:GLN:HG3	2.18	0.43
1:D:123:ALA:HB1	1:D:127:LYS:HE2	2.01	0.43
1:D:113:LEU:HD11	1:D:133:THR:HG23	2.01	0.43
1:D:132:THR:N	1:D:135:ASN:ND2	2.65	0.43
1:A:138:GLN:C	1:A:141:GLU:HG2	2.44	0.42
1:A:38:LEU:HD13	1:A:46:VAL:HG21	2.01	0.42
1:A:39:LEU:CD1	1:A:64:ILE:HD12	2.50	0.42
1:B:60:LEU:HD13	1:B:60:LEU:O	2.20	0.42
1:C:132:THR:CG2	1:C:134:ALA:HB3	2.50	0.42
1:B:101:ARG:NH1	1:B:103:ASP:OD2	2.53	0.42
1:A:30:GLU:N	1:A:33:HIS:HD2	1.95	0.41
1:C:38:LEU:HB3	1:C:46:VAL:HG21	2.02	0.41
1:D:29:ILE:CG1	1:D:81:VAL:HG22	2.50	0.41
1:A:35:MSE:HG3	1:A:122:LEU:CD1	2.47	0.41
1:B:101:ARG:HG3	2:B:179:HOH:O	2.19	0.41
1:A:97:LEU:HD23	1:A:100:LYS:HE3	2.03	0.41
1:A:138:GLN:O	1:A:141:GLU:CG	2.63	0.41
1:B:58:GLY:HA2	1:B:61:ARG:HH11	1.85	0.41
1:A:56:ASN:HD22	1:A:59:GLN:HB3	1.85	0.41
1:B:31:PRO:HB2	1:B:122:LEU:HD23	2.03	0.41
1:C:35:MSE:CE	1:C:46:VAL:HG11	2.41	0.41
1:C:25:ASP:HB3	1:C:74:VAL:HG23	2.03	0.41
1:D:38:LEU:HD22	1:D:108:SER:HB3	2.03	0.41
1:C:49:LEU:CD1	1:C:143:MSE:HE1	2.49	0.40
1:C:132:THR:HG22	1:C:134:ALA:N	2.37	0.40
1:D:56:ASN:ND2	1:D:59:GLN:HB2	2.32	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	128/148 (86%)	127 (99%)	0	1 (1%)	16	8
1	B	129/148 (87%)	128 (99%)	1 (1%)	0	100	100
1	C	131/148 (88%)	130 (99%)	1 (1%)	0	100	100
1	D	138/148 (93%)	136 (99%)	1 (1%)	1 (1%)	18	10
All	All	526/592 (89%)	521 (99%)	3 (1%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	119	ARG
1	A	119	ARG

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	107/115 (93%)	103 (96%)	4 (4%)	30	20
1	B	108/115 (94%)	105 (97%)	3 (3%)	38	30
1	C	110/115 (96%)	107 (97%)	3 (3%)	39	32
1	D	112/115 (97%)	109 (97%)	3 (3%)	39	32
All	All	437/460 (95%)	424 (97%)	13 (3%)	36	27

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	59	GLN
1	A	116	LEU
1	A	135	ASN
1	B	3	LEU
1	B	8	ASN
1	B	60	LEU
1	C	14	LEU
1	C	132	THR
1	C	138	GLN
1	D	40	ASN
1	D	82	GLN
1	D	99	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	26	ASN
1	A	27	GLN
1	A	33	HIS
1	A	56	ASN
1	A	66	GLN
1	A	85	GLN
1	A	135	ASN
1	A	138	GLN
1	B	26	ASN
1	B	33	HIS
1	B	59	GLN
1	B	66	GLN
1	B	73	GLN
1	B	99	GLN
1	B	142	GLN
1	C	26	ASN
1	C	33	HIS
1	C	56	ASN
1	C	65	ASN
1	C	99	GLN
1	C	104	ASN
1	C	138	GLN
1	C	142	GLN
1	D	8	ASN
1	D	18	GLN

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Mol	Chain	Res	Type
1	D	26	ASN
1	D	33	HIS
1	D	40	ASN
1	D	56	ASN
1	D	135	ASN
1	D	142	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	131/148 (88%)	0.27	7 (5%) 32 37	4, 14, 32, 53	0
1	B	132/148 (89%)	0.18	5 (3%) 44 50	5, 12, 29, 41	0
1	C	133/148 (89%)	0.79	17 (12%) 7 9	7, 18, 40, 73	0
1	D	138/148 (93%)	1.06	31 (22%) 2 2	8, 21, 51, 79	0
All	All	534/592 (90%)	0.58	60 (11%) 10 12	4, 16, 40, 79	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	79	GLY	8.2
1	C	74	VAL	6.6
1	D	4	ASP	6.1
1	D	80	ASP	5.4
1	D	40	ASN	5.2
1	D	5	ARG	5.0
1	C	119	ARG	4.8
1	D	81	VAL	4.6
1	C	4	ASP	4.4
1	B	3	LEU	4.2
1	C	81	VAL	4.2
1	D	78	GLY	4.1
1	A	59	GLN	3.9
1	A	5	ARG	3.9
1	C	105	PHE	3.8
1	D	119	ARG	3.6
1	D	120	GLY	3.6
1	D	77	THR	3.6
1	A	4	ASP	3.5
1	C	8	ASN	3.5
1	B	4	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	5	ARG	3.4
1	D	142	GLN	3.3
1	C	56	ASN	3.3
1	C	80	ASP	3.3
1	C	104	ASN	3.1
1	C	47	SER	3.1
1	B	74	VAL	3.0
1	A	142	GLN	2.9
1	D	128	ALA	2.8
1	A	61	ARG	2.8
1	C	141	GLU	2.6
1	D	138	GLN	2.6
1	D	43	GLY	2.5
1	A	141	GLU	2.5
1	C	55	ILE	2.5
1	D	42	GLU	2.5
1	D	6	LEU	2.5
1	C	57	ALA	2.5
1	D	12	LEU	2.4
1	D	55	ILE	2.4
1	C	132	THR	2.4
1	D	57	ALA	2.4
1	D	82	GLN	2.4
1	D	99	GLN	2.4
1	D	118	SER	2.4
1	D	9	LYS	2.3
1	D	56	ASN	2.3
1	B	141	GLU	2.3
1	C	120	GLY	2.2
1	A	74	VAL	2.1
1	D	89	ARG	2.1
1	D	101	ARG	2.1
1	C	130	GLY	2.1
1	D	46	VAL	2.1
1	B	42	GLU	2.0
1	D	105	PHE	2.0
1	D	8	ASN	2.0
1	D	16	ASP	2.0
1	D	83	PRO	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.