



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 7CT2 / pdb_00007ct2
Title : New Delhi metallo-beta-lactamase 1 (NDM1) mutant - H116Q
Authors : Kong, W.P.; Chen, Y.W.; Wong, K.Y.
Deposited on : 2020-08-17
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

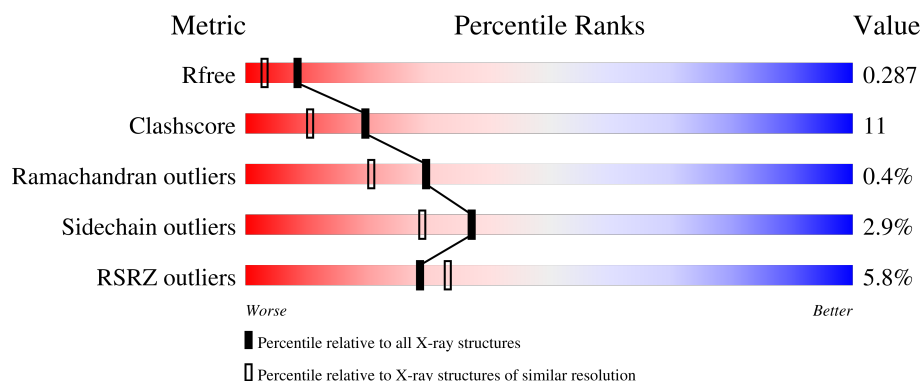
1 Overall quality at a glance

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	252	6% 73% 17% • 9%
1	B	252	4% 73% 16% • 9%
1	C	252	4% 73% 18% 9%
1	D	252	8% 69% 21% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7410 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 Metallo beta lactamase NDM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1702	1068	302	324	8			
1	B	229	Total	C	N	O	S	0	0	0
			1702	1068	302	324	8			
1	C	229	Total	C	N	O	S	0	0	0
			1702	1068	302	324	8			
1	D	229	Total	C	N	O	S	0	0	0
			1702	1068	302	324	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP E9NWK5
A	20	SER	-	expression tag	UNP E9NWK5
A	21	HIS	-	expression tag	UNP E9NWK5
A	22	MET	-	expression tag	UNP E9NWK5
A	23	ALA	-	expression tag	UNP E9NWK5
A	24	SER	-	expression tag	UNP E9NWK5
A	25	MET	-	expression tag	UNP E9NWK5
A	26	THR	-	expression tag	UNP E9NWK5
A	27	GLY	-	expression tag	UNP E9NWK5
A	28	GLY	-	expression tag	UNP E9NWK5
A	29	GLN	-	expression tag	UNP E9NWK5
A	30	GLN	-	expression tag	UNP E9NWK5
A	31	MET	-	expression tag	UNP E9NWK5
A	32	GLY	-	expression tag	UNP E9NWK5
A	33	ARG	-	expression tag	UNP E9NWK5
A	34	GLY	-	expression tag	UNP E9NWK5
A	35	SER	-	expression tag	UNP E9NWK5
A	120	GLN	HIS	engineered mutation	UNP E9NWK5
B	19	GLY	-	expression tag	UNP E9NWK5
B	20	SER	-	expression tag	UNP E9NWK5
B	21	HIS	-	expression tag	UNP E9NWK5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	22	MET	-	expression tag	UNP E9NWK5
B	23	ALA	-	expression tag	UNP E9NWK5
B	24	SER	-	expression tag	UNP E9NWK5
B	25	MET	-	expression tag	UNP E9NWK5
B	26	THR	-	expression tag	UNP E9NWK5
B	27	GLY	-	expression tag	UNP E9NWK5
B	28	GLY	-	expression tag	UNP E9NWK5
B	29	GLN	-	expression tag	UNP E9NWK5
B	30	GLN	-	expression tag	UNP E9NWK5
B	31	MET	-	expression tag	UNP E9NWK5
B	32	GLY	-	expression tag	UNP E9NWK5
B	33	ARG	-	expression tag	UNP E9NWK5
B	34	GLY	-	expression tag	UNP E9NWK5
B	35	SER	-	expression tag	UNP E9NWK5
B	120	GLN	HIS	engineered mutation	UNP E9NWK5
C	19	GLY	-	expression tag	UNP E9NWK5
C	20	SER	-	expression tag	UNP E9NWK5
C	21	HIS	-	expression tag	UNP E9NWK5
C	22	MET	-	expression tag	UNP E9NWK5
C	23	ALA	-	expression tag	UNP E9NWK5
C	24	SER	-	expression tag	UNP E9NWK5
C	25	MET	-	expression tag	UNP E9NWK5
C	26	THR	-	expression tag	UNP E9NWK5
C	27	GLY	-	expression tag	UNP E9NWK5
C	28	GLY	-	expression tag	UNP E9NWK5
C	29	GLN	-	expression tag	UNP E9NWK5
C	30	GLN	-	expression tag	UNP E9NWK5
C	31	MET	-	expression tag	UNP E9NWK5
C	32	GLY	-	expression tag	UNP E9NWK5
C	33	ARG	-	expression tag	UNP E9NWK5
C	34	GLY	-	expression tag	UNP E9NWK5
C	35	SER	-	expression tag	UNP E9NWK5
C	120	GLN	HIS	engineered mutation	UNP E9NWK5
D	19	GLY	-	expression tag	UNP E9NWK5
D	20	SER	-	expression tag	UNP E9NWK5
D	21	HIS	-	expression tag	UNP E9NWK5
D	22	MET	-	expression tag	UNP E9NWK5
D	23	ALA	-	expression tag	UNP E9NWK5
D	24	SER	-	expression tag	UNP E9NWK5
D	25	MET	-	expression tag	UNP E9NWK5
D	26	THR	-	expression tag	UNP E9NWK5
D	27	GLY	-	expression tag	UNP E9NWK5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	GLY	-	expression tag	UNP E9NWK5
D	29	GLN	-	expression tag	UNP E9NWK5
D	30	GLN	-	expression tag	UNP E9NWK5
D	31	MET	-	expression tag	UNP E9NWK5
D	32	GLY	-	expression tag	UNP E9NWK5
D	33	ARG	-	expression tag	UNP E9NWK5
D	34	GLY	-	expression tag	UNP E9NWK5
D	35	SER	-	expression tag	UNP E9NWK5
D	120	GLN	HIS	engineered mutation	UNP E9NWK5

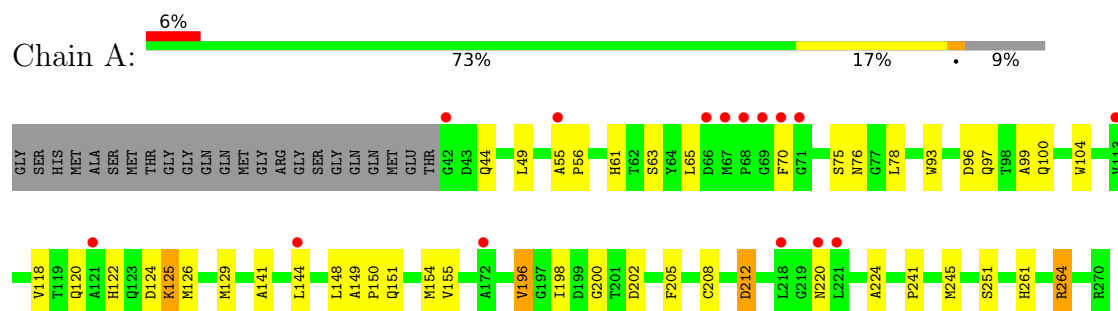
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	138	Total	O	0	0
			138	138		
2	B	139	Total	O	0	0
			139	139		
2	C	177	Total	O	0	0
			177	177		
2	D	148	Total	O	0	0
			148	148		

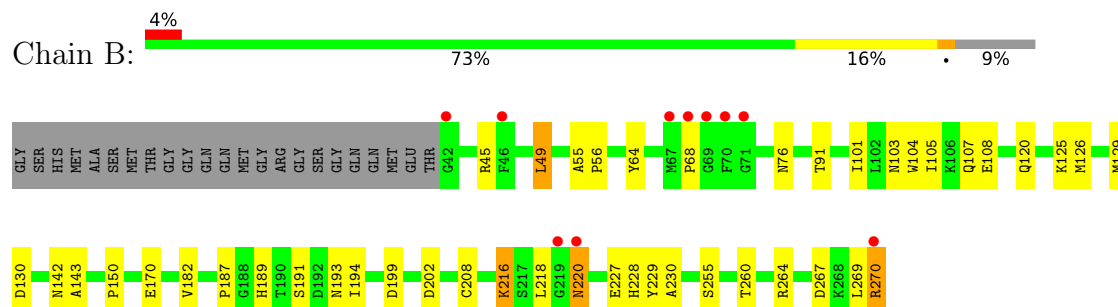
3 Residue-property plots

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.

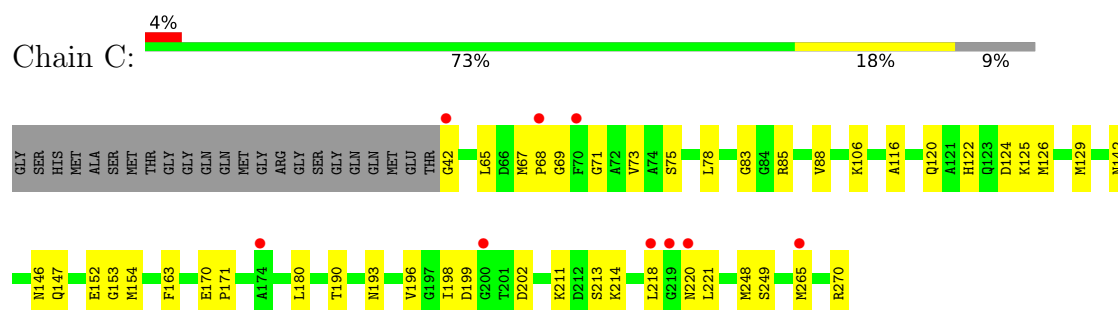
• Molecule 1: Metallo beta lactamase NDM-1



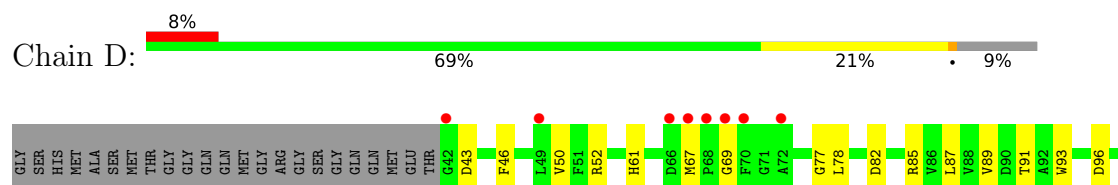
• Molecule 1: Metallo beta lactamase NDM-1

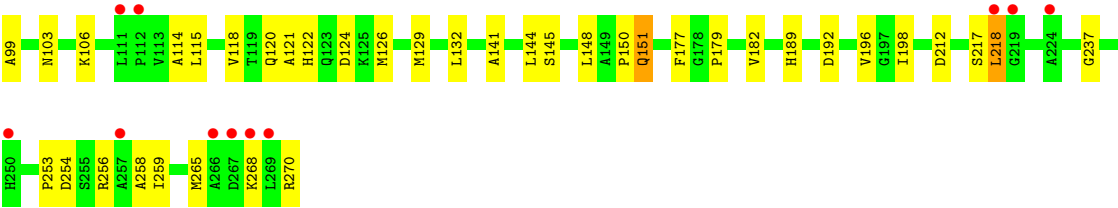


• Molecule 1: Metallo beta lactamase NDM-1



• Molecule 1: Metallo beta lactamase NDM-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.63Å 68.55Å 69.41Å 87.95° 88.82° 77.58°	Depositor
Resolution (Å)	30.54 – 1.95 30.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.54-1.95) 89.3 (30.54-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.222 , 0.286 0.225 , 0.287	Depositor DCC
R_{free} test set	2787 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7410	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.47% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CSO

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	0.68	0/1733	1.21	4/2357 (0.2%)
1	B	0.69	0/1733	1.20	3/2357 (0.1%)
1	C	0.67	0/1733	1.18	2/2357 (0.1%)
1	D	0.67	0/1733	1.15	3/2357 (0.1%)
All	All	0.68	0/6932	1.19	12/9428 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	HIS	CA-CB-CG	7.26	121.06	113.80
1	B	202	ASP	CB-CA-C	-6.59	99.42	110.56
1	B	150	PRO	CB-CA-C	-5.98	102.28	112.26
1	A	202	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	220	ASN	CB-CA-C	-5.76	100.68	109.89
1	A	76	ASN	CB-CA-C	-5.53	99.59	109.71
1	C	142	ASN	CB-CA-C	-5.50	102.07	109.71
1	D	177	PHE	CB-CA-C	-5.31	102.17	110.94
1	A	212	ASP	CB-CA-C	5.20	118.93	109.62
1	D	254	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	163	PHE	CA-CB-CG	-5.12	108.68	113.80
1	D	151	GLN	CB-CA-C	-5.07	100.33	110.42

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	1702	0	1650	35	0
1	B	1702	0	1650	38	0
1	C	1702	0	1650	34	0
1	D	1702	0	1650	47	0
2	A	138	0	0	9	0
2	B	139	0	0	9	0
2	C	177	0	0	12	0
2	D	148	0	0	15	0
All	All	7410	0	6600	154	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 11.

All (154) 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:42:GLY:HA2	2:C:425:HOH:O	1.53	1.07
1:D:148:LEU:HB2	2:D:304:HOH:O	1.60	1.01
1:B:130:ASP:OD2	2:B:301:HOH:O	1.85	0.93
1:D:43:ASP:OD1	1:D:52:ARG:HB2	1.70	0.92
1:C:67:MET:HG2	1:C:73:VAL:HG12	1.52	0.90
1:C:211:LYS:HE3	1:C:218:LEU:O	1.72	0.88
1:B:64:TYR:OH	2:B:302:HOH:O	1.91	0.80
1:A:44:GLN:OE1	2:A:301:HOH:O	1.99	0.79
1:C:67:MET:HG2	1:C:73:VAL:CG1	2.14	0.78
1:B:45:ARG:HB2	1:B:45:ARG:NH1	1.99	0.77
1:B:270:ARG:NH2	2:B:304:HOH:O	2.17	0.73
1:A:55:ALA:HB1	1:A:56:PRO:HD2	1.70	0.72
1:D:120:GLN:HE22	1:D:189:HIS:HD2	1.34	0.72
1:C:213:SER:HB2	2:C:347:HOH:O	1.88	0.71
1:B:126:MET:O	1:B:129:MET:HG2	1.91	0.70
1:B:45:ARG:HB2	1:B:45:ARG:HH11	1.57	0.70
1:A:70:PHE:HB3	2:A:414:HOH:O	1.93	0.68
1:B:267:ASP:HA	1:B:270:ARG:HD3	1.76	0.67
1:D:121:ALA:CB	2:D:304:HOH:O	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:O	2:B:303:HOH:O	2.12	0.67
1:B:218:LEU:HD12	1:B:269:LEU:HD11	1.77	0.67
1:C:67:MET:CG	1:C:73:VAL:CG1	2.73	0.66
1:C:180:LEU:HD22	1:C:196:VAL:HG11	1.78	0.66
1:B:220:ASN:HD21	1:B:269:LEU:HD22	1.61	0.65
1:B:228:HIS:C	1:B:270:ARG:HH22	2.05	0.65
1:D:69:GLY:N	2:D:305:HOH:O	2.30	0.65
1:D:91:THR:HG22	1:D:132:LEU:HD11	1.77	0.65
1:B:120:GLN:HE22	1:B:208:CSO:HB3	1.61	0.64
1:C:220:ASN:ND2	2:C:306:HOH:O	2.29	0.64
1:B:120:GLN:HB3	1:B:125:LYS:HD3	1.79	0.64
1:D:151:GLN:HG3	2:D:351:HOH:O	1.97	0.64
1:C:180:LEU:HD22	1:C:196:VAL:CG1	2.28	0.63
1:D:61:HIS:CE1	1:D:77:GLY:HA3	2.34	0.63
1:C:67:MET:CG	1:C:73:VAL:HG11	2.29	0.62
1:C:146:ASN:C	2:C:304:HOH:O	2.42	0.62
1:B:120:GLN:HE22	1:B:208:CSO:CB	2.12	0.62
1:B:230:ALA:H	1:B:270:ARG:NH2	1.98	0.61
1:C:69:GLY:HA3	2:D:342:HOH:O	2.01	0.61
1:A:126:MET:O	1:A:129:MET:HG2	2.01	0.61
1:D:121:ALA:HB3	2:D:304:HOH:O	2.01	0.60
1:D:126:MET:O	1:D:129:MET:HG2	1.99	0.60
1:C:67:MET:HG3	1:C:73:VAL:HG11	1.81	0.60
1:A:261:HIS:CD2	2:A:350:HOH:O	2.55	0.60
1:D:91:THR:O	2:D:301:HOH:O	2.16	0.60
1:D:122:HIS:HB3	2:D:348:HOH:O	2.01	0.60
1:C:88:VAL:O	1:C:116:ALA:HA	2.01	0.60
1:A:245:MET:HE1	2:A:412:HOH:O	2.01	0.59
1:A:261:HIS:HD2	2:A:350:HOH:O	1.84	0.59
1:D:67:MET:O	2:D:302:HOH:O	2.16	0.59
1:D:270:ARG:HD2	2:D:309:HOH:O	2.02	0.59
1:D:46:PHE:HD1	2:D:394:HOH:O	1.86	0.58
1:A:65:LEU:HD22	1:A:93:TRP:CE3	2.39	0.58
1:A:55:ALA:HB1	1:A:56:PRO:CD	2.35	0.57
1:B:229:TYR:N	1:B:270:ARG:HH22	2.02	0.57
1:C:220:ASN:O	1:C:221:LEU:HD23	2.05	0.57
1:C:124:ASP:OD1	1:C:124:ASP:N	2.37	0.57
1:A:264:ARG:HH11	1:A:264:ARG:HG3	1.70	0.56
1:D:67:MET:C	2:D:302:HOH:O	2.49	0.55
1:D:265:MET:O	1:D:268:LYS:N	2.40	0.55
1:C:78:LEU:HD13	1:C:198:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD21	1:C:265:MET:HB3	1.89	0.54
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.89	0.54
1:A:129:MET:HG3	1:A:155:VAL:O	2.08	0.54
1:D:78:LEU:HD13	1:D:198:ILE:HD11	1.90	0.54
1:D:87:LEU:HD22	1:D:115:LEU:HG	1.90	0.53
1:D:118:VAL:CG2	1:D:141:ALA:HB2	2.39	0.53
1:C:214:LYS:HA	2:C:349:HOH:O	2.08	0.52
1:D:218:LEU:HD21	1:D:265:MET:HB3	1.91	0.52
1:A:96:ASP:O	1:A:99:ALA:HB3	2.09	0.52
1:B:55:ALA:HB1	1:B:56:PRO:HD2	1.91	0.52
1:B:255:SER:HB2	2:B:325:HOH:O	2.09	0.52
1:A:125:LYS:N	1:A:125:LYS:HD2	2.25	0.52
1:B:220:ASN:ND2	1:B:269:LEU:HD22	2.23	0.51
1:C:106:LYS:HA	2:C:421:HOH:O	2.10	0.51
1:C:85:ARG:HB2	2:C:429:HOH:O	2.10	0.51
1:D:256:ARG:C	1:D:258:ALA:H	2.19	0.50
1:B:216:LYS:NZ	2:B:310:HOH:O	2.44	0.50
1:D:120:GLN:NE2	1:D:189:HIS:HD2	2.05	0.50
1:D:96:ASP:O	1:D:99:ALA:HB3	2.11	0.50
1:C:126:MET:O	1:C:129:MET:HG2	2.11	0.50
1:B:230:ALA:H	1:B:270:ARG:HH22	1.59	0.50
1:D:150:PRO:HG3	2:D:429:HOH:O	2.12	0.50
1:B:260:THR:HG22	2:B:403:HOH:O	2.11	0.49
1:D:256:ARG:C	1:D:258:ALA:N	2.66	0.49
1:B:227:GLU:O	1:B:270:ARG:NH2	2.44	0.49
1:B:270:ARG:OXT	2:B:305:HOH:O	2.20	0.49
1:D:85:ARG:HD3	1:D:114:ALA:CB	2.42	0.49
1:D:120:GLN:HE22	1:D:189:HIS:CD2	2.23	0.49
1:A:264:ARG:HG3	1:A:264:ARG:NH1	2.27	0.49
1:B:104:TRP:CE2	1:B:108:GLU:HG3	2.48	0.49
1:A:124:ASP:OD2	1:A:125:LYS:HE3	2.13	0.49
1:A:118:VAL:HG23	1:A:141:ALA:HB2	1.94	0.49
1:B:182:VAL:HG13	1:B:194:ILE:HD12	1.95	0.49
1:D:82:ASP:OD2	1:D:85:ARG:NH1	2.46	0.48
1:A:220:ASN:HB2	1:A:224:ALA:CB	2.43	0.48
1:A:49:LEU:HD11	1:A:100:GLN:HB2	1.94	0.48
1:D:182:VAL:HG22	1:D:196:VAL:HG22	1.95	0.48
1:C:120:GLN:HB3	1:C:125:LYS:HD3	1.94	0.48
1:C:152:GLU:HB3	2:C:319:HOH:O	2.12	0.48
1:D:93:TRP:CZ3	1:D:124:ASP:HB3	2.49	0.48
1:D:121:ALA:HB2	2:D:304:HOH:O	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:SER:HA	2:D:304:HOH:O	2.13	0.47
1:C:67:MET:N	1:C:71:GLY:O	2.38	0.47
1:B:230:ALA:H	1:B:270:ARG:CZ	2.28	0.47
1:D:78:LEU:HB2	1:D:89:VAL:HB	1.97	0.47
1:A:148:LEU:O	1:A:151:GLN:HG2	2.15	0.47
1:A:65:LEU:CD2	1:A:93:TRP:CE3	2.98	0.47
1:D:82:ASP:CG	1:D:179:PRO:HD3	2.40	0.47
1:B:187:PRO:HB3	1:B:191:SER:HA	1.96	0.46
1:B:76:ASN:O	2:B:306:HOH:O	2.21	0.46
1:A:44:GLN:NE2	1:A:104:TRP:HE1	2.13	0.46
1:A:78:LEU:HD13	1:A:198:ILE:HD11	1.98	0.46
1:A:49:LEU:HD22	1:A:63:SER:HB3	1.98	0.46
1:C:75:SER:HA	1:C:249:SER:O	2.16	0.45
1:C:153:GLY:O	1:C:154:MET:HE2	2.16	0.45
1:D:148:LEU:HD22	1:D:151:GLN:HE22	1.80	0.45
1:A:154:MET:HE3	2:A:374:HOH:O	2.15	0.45
1:D:148:LEU:O	1:D:151:GLN:HB2	2.17	0.45
1:A:120:GLN:OE1	1:A:122:HIS:ND1	2.49	0.45
1:A:241:PRO:HD2	2:A:321:HOH:O	2.15	0.45
1:A:44:GLN:HB2	2:A:366:HOH:O	2.17	0.45
1:A:196:VAL:O	1:A:205:PHE:N	2.40	0.45
1:B:55:ALA:O	1:B:56:PRO:C	2.59	0.44
1:B:267:ASP:O	1:B:270:ARG:HB2	2.17	0.44
1:C:270:ARG:HD3	2:C:369:HOH:O	2.17	0.44
1:C:218:LEU:CD2	1:C:265:MET:HB3	2.48	0.44
1:C:171:PRO:HD2	2:C:402:HOH:O	2.18	0.44
1:D:85:ARG:HD3	1:D:114:ALA:HB2	1.99	0.44
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.86	0.44
1:A:120:GLN:NE2	1:A:208:CSO:HB3	2.33	0.43
1:D:118:VAL:HG22	1:D:141:ALA:HB2	1.99	0.43
1:B:103:ASN:O	1:B:107:GLN:HG2	2.19	0.43
1:C:65:LEU:O	1:C:73:VAL:HG12	2.17	0.43
1:D:93:TRP:CH2	1:D:124:ASP:HB3	2.53	0.43
1:A:144:LEU:O	1:A:144:LEU:HD12	2.19	0.43
1:D:103:ASN:O	1:D:106:LYS:HB3	2.19	0.42
1:B:218:LEU:CD1	1:B:269:LEU:HD11	2.48	0.42
1:D:61:HIS:NE2	1:D:77:GLY:HA3	2.35	0.42
1:B:189:HIS:H	1:B:193:ASN:HD21	1.68	0.42
1:C:147:GLN:HA	2:C:304:HOH:O	2.20	0.41
1:D:144:LEU:HG	1:D:192:ASP:HB3	2.02	0.41
1:D:237:GLY:HA2	1:D:259:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:LEU:CD2	1:D:265:MET:HB3	2.50	0.41
1:B:49:LEU:HD22	1:B:101:ILE:CG1	2.50	0.41
1:C:190:THR:H	1:C:193:ASN:ND2	2.19	0.41
1:D:43:ASP:HB3	1:D:50:VAL:CG1	2.51	0.41
1:A:65:LEU:HB2	1:A:93:TRP:CD2	2.56	0.41
1:A:200:GLY:O	2:A:302:HOH:O	2.21	0.41
1:B:55:ALA:HB1	1:B:56:PRO:CD	2.51	0.41
1:A:49:LEU:HD11	1:A:97:GLN:O	2.21	0.40
1:B:142:ASN:O	1:B:143:ALA:C	2.63	0.40
1:C:270:ARG:HG3	2:C:353:HOH:O	2.21	0.40
1:B:104:TRP:O	1:B:105:ILE:C	2.63	0.40
1:D:121:ALA:HA	1:D:126:MET:SD	2.61	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	226/252 (90%)	218 (96%)	8 (4%)	0	100	100
1	B	226/252 (90%)	219 (97%)	6 (3%)	1 (0%)	30	21
1	C	226/252 (90%)	219 (97%)	5 (2%)	2 (1%)	14	6
1	D	226/252 (90%)	209 (92%)	16 (7%)	1 (0%)	30	21
All	All	904/1008 (90%)	865 (96%)	35 (4%)	4 (0%)	30	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	253	PRO
1	C	83	GLY
1	C	68	PRO

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Mol	Chain	Res	Type
1	B	68	PRO

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	170/186 (91%)	164 (96%)	6 (4%)	32	22
1	B	170/186 (91%)	164 (96%)	6 (4%)	32	22
1	C	170/186 (91%)	165 (97%)	5 (3%)	37	29
1	D	170/186 (91%)	167 (98%)	3 (2%)	51	47
All	All	680/744 (91%)	660 (97%)	20 (3%)	37	29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	A	125	LYS
1	A	196	VAL
1	A	212	ASP
1	A	251	SER
1	A	264	ARG
1	B	49	LEU
1	B	170	GLU
1	B	199	ASP
1	B	216	LYS
1	B	264	ARG
1	B	270	ARG
1	C	122	HIS
1	C	170	GLU
1	C	199	ASP
1	C	202	ASP
1	C	248	MET
1	D	212	ASP
1	D	217	SER
1	D	218	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	120	GLN
1	A	193	ASN
1	A	261	HIS
1	B	60	GLN
1	B	76	ASN
1	B	120	GLN
1	B	147	GLN
1	B	166	ASN
1	B	193	ASN
1	C	151	GLN
1	C	193	ASN
1	C	220	ASN
1	D	60	GLN
1	D	76	ASN
1	D	120	GLN
1	D	151	GLN
1	D	176	ASN
1	D	189	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	A	208	1	3,6,7	0.89	0	1,6,8	0.81	0
1	CSO	C	208	1	3,6,7	0.63	0	1,6,8	0.34	0
1	CSO	D	208	1	3,6,7	0.58	0	1,6,8	1.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	B	208	1	3,6,7	1.31	0	1,6,8	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	A	208	1	-	1/1/5/7	-
1	CSO	C	208	1	-	1/1/5/7	-
1	CSO	D	208	1	-	0/1/5/7	-
1	CSO	B	208	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	208	CSO	N-CA-CB-SG
1	B	208	CSO	N-CA-CB-SG
1	C	208	CSO	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	208	CSO	1	0
1	B	208	CSO	2	0

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	228/252 (90%)	0.68	15 (6%) 24 28	13, 22, 39, 101	0
1	B	228/252 (90%)	0.59	10 (4%) 39 45	14, 21, 38, 78	0
1	C	228/252 (90%)	0.65	9 (3%) 43 50	14, 22, 39, 92	0
1	D	228/252 (90%)	0.85	19 (8%) 17 20	14, 24, 54, 135	0
All	All	912/1008 (90%)	0.69	53 (5%) 29 33	13, 23, 45, 135	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	269	LEU	7.4
1	D	68	PRO	6.4
1	D	69	GLY	6.3
1	C	70	PHE	5.6
1	D	70	PHE	5.2
1	A	68	PRO	4.8
1	A	70	PHE	4.4
1	D	257	ALA	4.0
1	D	67	MET	4.0
1	A	67	MET	3.9
1	D	66	ASP	3.6
1	B	70	PHE	3.5
1	D	42	GLY	3.4
1	C	68	PRO	3.2
1	C	219	GLY	3.1
1	D	218	LEU	3.1
1	A	69	GLY	3.0
1	B	71	GLY	3.0
1	B	68	PRO	3.0
1	A	42	GLY	2.9
1	C	42	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	218	LEU	2.8
1	D	219	GLY	2.8
1	C	218	LEU	2.8
1	A	71	GLY	2.7
1	C	200	GLY	2.7
1	B	42	GLY	2.7
1	A	121	ALA	2.6
1	D	224	ALA	2.5
1	B	67	MET	2.5
1	D	266	ALA	2.4
1	B	46	PHE	2.4
1	C	220	ASN	2.4
1	D	250	HIS	2.4
1	B	219	GLY	2.4
1	D	72	ALA	2.3
1	A	221	LEU	2.3
1	C	265	MET	2.3
1	B	69	GLY	2.3
1	C	174	ALA	2.3
1	D	49	LEU	2.2
1	D	268	LYS	2.2
1	B	220	ASN	2.2
1	D	267	ASP	2.2
1	A	113	VAL	2.1
1	B	270	ARG	2.1
1	D	111	LEU	2.1
1	A	172	ALA	2.1
1	D	112	PRO	2.1
1	A	144	LEU	2.1
1	A	55	ALA	2.1
1	A	66	ASP	2.0
1	A	220	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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
1	CSO	C	208	7/8	0.81	0.16	26,30,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSO	D	208	7/8	0.82	0.19	34,37,40,43	0
1	CSO	A	208	7/8	0.89	0.13	22,26,38,43	0
1	CSO	B	208	7/8	0.89	0.10	22,23,40,40	0

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.