



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2022 – 12:13 PM JST

PDB ID : 7CT2  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

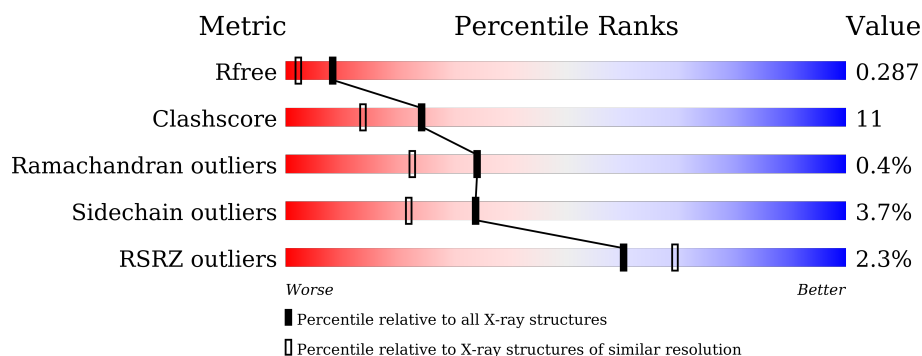
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	252	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	252	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div></div> <div>9%</div> </div> </div>
1	D	252	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>21%</div> <div></div> <div>9%</div> </div> </div>

## 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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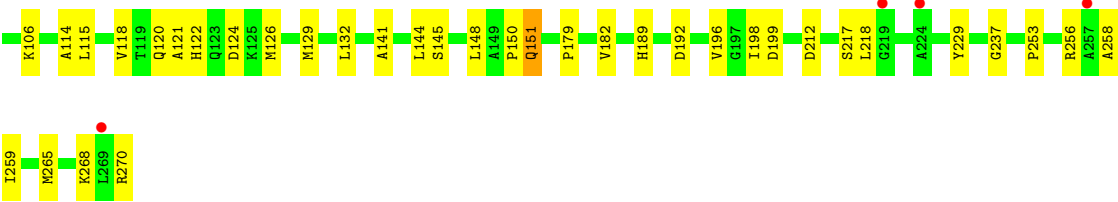
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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	GLY	-	expression tag	UNP E9NWK5
D	29	GLN	-	expression tag	UNP E9NWK5
D	30	GLN	-	expression tag	UNP E9NWK5
D	31	MET	-	expression tag	UNP E9NWK5
D	32	GLY	-	expression tag	UNP E9NWK5
D	33	ARG	-	expression 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 138 138	0	0
2	B	139	Total O 139 139	0	0
2	C	177	Total O 177 177	0	0
2	D	148	Total O 148 148	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.63Å 68.55Å 69.41Å 87.95° 88.82° 77.58°	Depositor
Resolution (Å)	30.54 – 1.95 38.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.54-1.95) 89.3 (38.30-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.44	0/1733	0.83	1/2357 (0.0%)
1	B	0.45	0/1733	0.83	1/2357 (0.0%)
1	C	0.44	0/1733	0.83	0/2357
1	D	0.44	0/1733	0.77	1/2357 (0.0%)
All	All	0.44	0/6932	0.82	3/9428 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ASP	CB-CA-C	-5.49	99.42	110.40
1	A	76	ASN	CB-CA-C	-5.40	99.59	110.40
1	D	151	GLN	CB-CA-C	-5.03	100.33	110.40

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	33	0
1	B	1702	0	1650	35	0
1	C	1702	0	1649	33	0
1	D	1702	0	1650	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	138	0	0	7	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	6599	148	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 (148) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:228:HIS:C	1:B:270:ARG:HH22	2.05	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: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:C:146:ASN:C	2:C:304:HOH:O	2.42	0.57
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:256:ARG:C	1:D:258:ALA:N	2.66	0.49
1:B:260:THR:HG22	2:B:403:HOH:O	2.11	0.49
1:D:67:MET:C	2:D:302:HOH:O	2.49	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
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: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:B:216:LYS:NZ	2:B:310:HOH:O	2.44	0.46
1:C:75:SER:HA	1:C:249:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:HD22	1:D:151:GLN:HE22	1.80	0.45
1:D:256:ARG:C	1:D:258:ALA:H	2.19	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: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:D:82:ASP:CG	1:D:179:PRO:HD3	2.40	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
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:C:270:ARG:HG3	2:C:353:HOH:O	2.21	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%)	34	22
1	C	226/252 (90%)	219 (97%)	5 (2%)	2 (1%)	17	8
1	D	226/252 (90%)	209 (92%)	16 (7%)	1 (0%)	34	22
All	All	904/1008 (90%)	865 (96%)	35 (4%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	253	PRO
1	C	83	GLY
1	C	68	PRO
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%)	162 (95%)	8 (5%)	26	13
1	B	170/186 (91%)	163 (96%)	7 (4%)	30	18
1	C	170/186 (91%)	164 (96%)	6 (4%)	36	24
1	D	170/186 (91%)	166 (98%)	4 (2%)	49	40
All	All	680/744 (91%)	655 (96%)	25 (4%)	34	22

All (25) 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	229	TYR
1	A	249	SER
1	A	251	SER
1	A	264	ARG
1	B	49	LEU
1	B	70	PHE
1	B	199	ASP
1	B	216	LYS
1	B	229	TYR
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	229	TYR
1	C	248	MET
1	D	199	ASP
1	D	212	ASP
1	D	217	SER
1	D	229	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	D	120	GLN
1	D	151	GLN
1	D	189	HIS
1	D	193	ASN

### 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	C	208	1	3,6,7	0.62	0	0,6,8	-	-
1	CSO	A	208	1	3,6,7	0.89	0	0,6,8	-	-
1	CSO	D	208	1	3,6,7	0.56	0	0,6,8	-	-
1	CSO	B	208	1	3,6,7	1.33	0	0,6,8	-	-

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	C	208	1	-	1/1/5/7	-
1	CSO	A	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	228/252 (90%)	0.14	4 (1%) 68 76	13, 22, 39, 101	0
1	B	228/252 (90%)	0.11	5 (2%) 62 70	14, 21, 38, 78	0
1	C	228/252 (90%)	0.11	2 (0%) 84 89	14, 22, 39, 92	0
1	D	228/252 (90%)	0.43	10 (4%) 34 44	14, 24, 54, 135	0
All	All	912/1008 (90%)	0.20	21 (2%) 60 69	13, 23, 45, 135	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	PRO	12.2
1	D	69	GLY	11.2
1	D	70	PHE	7.5
1	A	68	PRO	6.1
1	D	269	LEU	6.0
1	A	70	PHE	5.8
1	D	67	MET	4.3
1	C	70	PHE	4.2
1	A	67	MET	3.8
1	B	70	PHE	3.6
1	B	67	MET	3.5
1	A	42	GLY	3.1
1	D	224	ALA	2.6
1	B	71	GLY	2.4
1	B	68	PRO	2.3
1	C	68	PRO	2.2
1	B	42	GLY	2.2
1	D	66	ASP	2.1
1	D	219	GLY	2.1
1	D	257	ALA	2.1
1	D	42	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSO	C	208	7/8	0.83	0.18	26,30,42,44	0
1	CSO	D	208	7/8	0.87	0.20	34,37,40,43	0
1	CSO	A	208	7/8	0.91	0.14	22,26,38,43	0
1	CSO	B	208	7/8	0.92	0.13	22,23,40,40	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.