



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:38 PM EDT

PDB ID : 3WRZ  
Title : N288Q-N321Q mutant BETA-LACTAMASE DERIVED FROM CHROMOHALOBACTER SP.560 (without soaking)  
Authors : Arai, S.; Yonezawa, Y.; Okazaki, N.; Matsumoto, F.; Shimizu, R.; Yamada, M.; Adachi, M.; Tamada, T.; Tokunaga, H.; Ishibashi, M.; Tokunaga, M.; Kuroki, R.  
Deposited on : 2014-02-27  
Resolution : 1.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

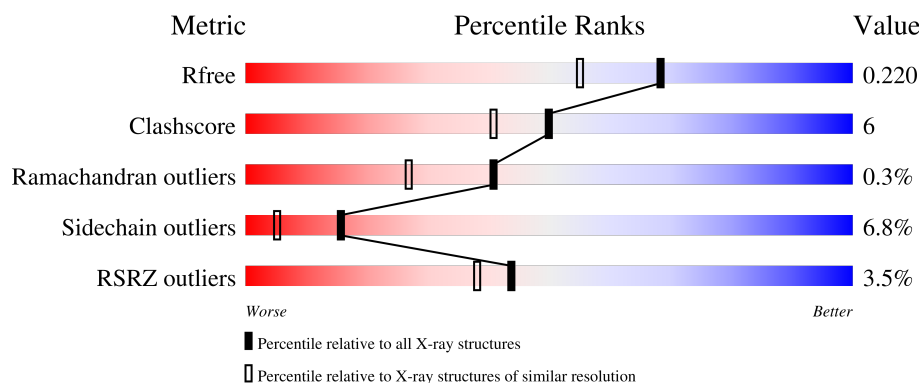
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	367	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	367	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>...</div> </div> </div>
1	C	367	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>...</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8957 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	357	Total	C	N	O	S	0	0	0
			2704	1698	454	541	11			
1	B	357	Total	C	N	O	S	0	0	0
			2707	1698	457	541	11			
1	C	356	Total	C	N	O	S	0	0	0
			2696	1692	452	541	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	GLN	ASN	engineered mutation	UNP Q76LX5
A	321	GLN	ASN	engineered mutation	UNP Q76LX5
B	288	GLN	ASN	engineered mutation	UNP Q76LX5
B	321	GLN	ASN	engineered mutation	UNP Q76LX5
C	288	GLN	ASN	engineered mutation	UNP Q76LX5
C	321	GLN	ASN	engineered mutation	UNP Q76LX5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		
2	B	2	Total	Ca	0	0
			2	2		
2	C	4	Total	Ca	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0

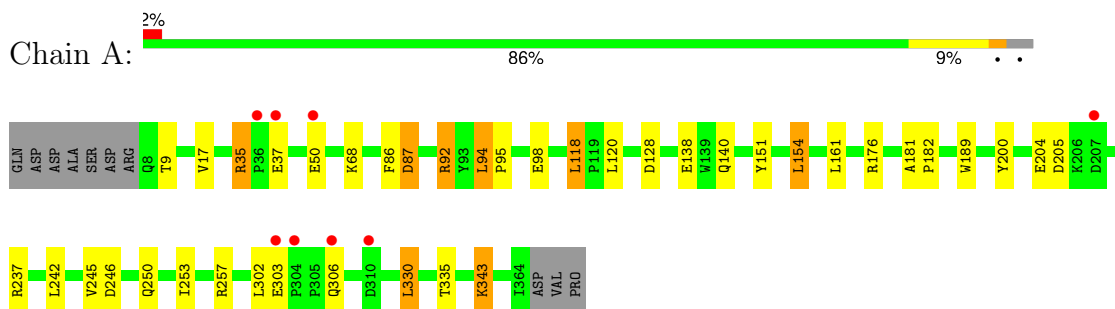
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	311	Total 311	O 311	0	0
4	B	227	Total 227	O 227	0	0
4	C	298	Total 298	O 298	0	0

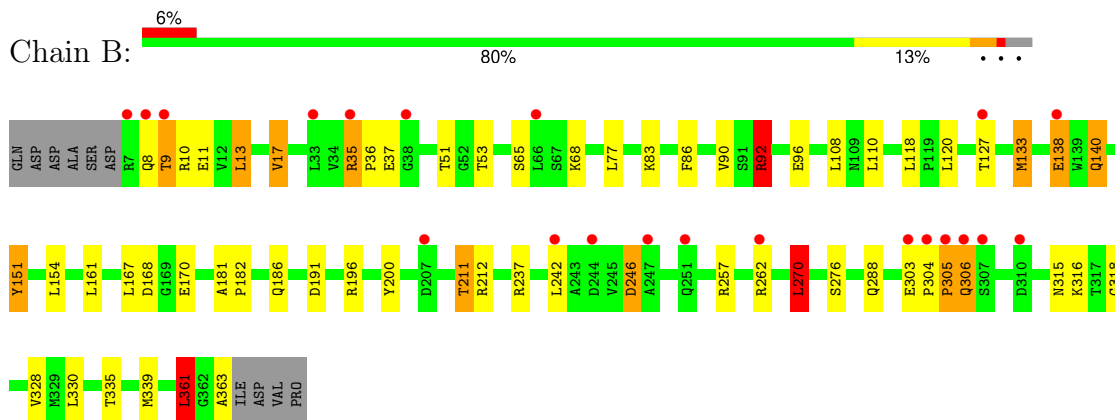
### 3 Residue-property plots [i](#)

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.

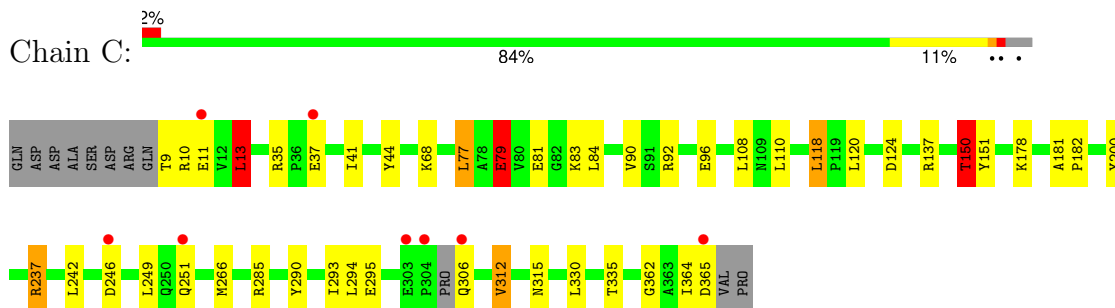
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.93Å 114.93Å 67.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.12 – 1.80 29.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.12-1.80) 100.0 (29.12-1.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.30 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.172 , 0.221 0.195 , 0.220	Depositor DCC
$R_{free}$ test set	4609 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.020 for H, K, L 0.372 for -K, -H, -L 0.020 for -h,-k,l 0.588 for K, H, -L	Depositor
Outliers	0 of 92603 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: CL, CA

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	0.64	1/2760 (0.0%)	0.86	9/3764 (0.2%)
1	B	0.55	0/2763	0.89	8/3767 (0.2%)
1	C	0.65	0/2750	0.92	8/3748 (0.2%)
All	All	0.61	1/8273 (0.0%)	0.89	25/11279 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	THR	C-O	-5.49	1.12	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	94	LEU	CB-CG-CD1	6.46	121.98	111.00
1	C	124	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	87	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	B	339	MET	CG-SD-CE	6.04	109.87	100.20
1	C	312	VAL	N-CA-CB	-5.97	98.36	111.50
1	B	270	LEU	CA-CB-CG	5.67	128.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	LEU	CA-CB-CG	5.62	128.24	115.30
1	C	237	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	128	ASP	CB-CG-OD2	5.61	123.34	118.30
1	C	246	ASP	CB-CA-C	5.47	121.35	110.40
1	B	133	MET	CG-SD-CE	5.43	108.89	100.20
1	B	92	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	191	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	79	GLU	CA-CB-CG	5.29	125.04	113.40
1	C	118	LEU	CB-CG-CD2	5.23	119.89	111.00
1	A	154	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	35	ARG	CG-CD-NE	5.14	122.60	111.80
1	A	257	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	246	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	330	LEU	CB-CG-CD1	5.08	119.63	111.00
1	C	150	THR	N-CA-CB	5.06	119.91	110.30
1	A	118	LEU	CB-CG-CD2	5.05	119.58	111.00
1	B	361	LEU	N-CA-C	5.03	124.59	111.00
1	A	205	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLU	Peptide
1	A	37	GLU	Peptide
1	B	303	GLU	Peptide
1	B	305	PRO	Peptide
1	B	361	LEU	Peptide
1	B	8	GLN	Peptide

## 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	2704	0	2636	19	0
1	B	2707	0	2638	38	0
1	C	2696	0	2624	37	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	311	0	0	5	0
4	B	227	0	0	8	0
4	C	298	0	0	15	1
All	All	8957	0	7898	93	1

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 6.

All (93) 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:266:MET:HG2	4:C:653:HOH:O	1.27	1.34
1:B:212:ARG:HG2	4:B:713:HOH:O	1.69	0.92
1:C:150:THR:HG21	4:C:797:HOH:O	1.75	0.85
1:C:266:MET:CE	4:C:653:HOH:O	2.24	0.83
1:C:77:LEU:HG	4:C:763:HOH:O	1.79	0.80
1:A:250:GLN:HA	4:A:747:HOH:O	1.84	0.78
1:C:150:THR:HG23	4:C:593:HOH:O	1.87	0.74
1:B:304:PRO:HB2	1:B:305:PRO:C	2.07	0.74
1:A:253:ILE:HD12	4:A:747:HOH:O	1.90	0.71
1:A:68:LYS:NZ	1:A:151:TYR:HE1	1.89	0.70
1:C:77:LEU:CD1	4:C:763:HOH:O	2.41	0.69
1:C:68:LYS:NZ	1:C:151:TYR:HE1	1.90	0.69
1:A:68:LYS:NZ	1:A:151:TYR:CE1	2.62	0.68
1:C:9:THR:HG22	1:C:35:ARG:NH1	2.09	0.67
1:C:266:MET:CG	4:C:653:HOH:O	2.05	0.67
1:B:68:LYS:NZ	1:B:151:TYR:HE1	1.92	0.67
1:C:96:GLU:CG	1:C:137:ARG:NH1	2.58	0.67
1:B:68:LYS:HZ3	1:B:151:TYR:HE1	1.40	0.66
1:B:92:ARG:HH11	1:B:92:ARG:HG3	1.61	0.66
1:B:363:ALA:O	4:B:634:HOH:O	2.14	0.65
1:C:68:LYS:NZ	1:C:151:TYR:CE1	2.65	0.65
1:C:10:ARG:NH2	1:C:41:ILE:O	2.31	0.64
1:C:77:LEU:CG	4:C:763:HOH:O	2.40	0.64
1:B:68:LYS:NZ	1:B:151:TYR:CE1	2.67	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HZ2	1:A:151:TYR:HE1	1.47	0.63
1:C:81:GLU:OE1	4:C:556:HOH:O	2.16	0.63
1:C:68:LYS:HZ2	1:C:151:TYR:HE1	1.50	0.60
1:B:9:THR:HG23	1:B:361:LEU:HD11	1.85	0.59
1:A:138:GLU:HG3	4:A:706:HOH:O	2.03	0.58
1:A:95:PRO:O	1:A:98:GLU:HG3	2.02	0.58
1:C:77:LEU:HD12	4:C:763:HOH:O	2.03	0.57
1:B:138:GLU:O	1:B:140:GLN:NE2	2.37	0.57
1:B:262:ARG:HG3	4:B:722:HOH:O	2.06	0.56
1:C:266:MET:SD	4:C:653:HOH:O	2.58	0.56
1:B:257:ARG:NH1	4:B:519:HOH:O	2.17	0.56
1:B:305:PRO:CA	1:B:306:GLN:HB3	2.36	0.56
1:C:364:ILE:O	1:C:365:ASP:C	2.44	0.55
1:B:65:SER:OG	1:B:318:GLY:HA2	2.06	0.54
1:B:305:PRO:HA	1:B:306:GLN:HB3	1.89	0.54
1:C:96:GLU:HG3	1:C:137:ARG:NH1	2.22	0.53
1:C:96:GLU:CG	1:C:137:ARG:HH12	2.21	0.53
1:A:9:THR:OG1	1:A:35:ARG:NH1	2.36	0.53
1:C:251:GLN:HA	1:C:251:GLN:OE1	2.09	0.53
1:A:140:GLN:NE2	4:A:574:HOH:O	2.42	0.52
1:B:51:THR:OG1	1:B:53:THR:HG22	2.08	0.52
1:C:120:LEU:HD11	1:C:151:TYR:CE2	2.45	0.52
1:B:9:THR:HA	4:B:698:HOH:O	2.10	0.51
1:A:120:LEU:HD11	1:A:151:TYR:CE2	2.46	0.51
1:B:13:LEU:HD12	1:B:17:VAL:CG1	2.40	0.51
1:B:196:ARG:NH2	4:B:530:HOH:O	2.43	0.51
1:B:288:GLN:NE2	4:B:504:HOH:O	2.41	0.50
1:C:9:THR:N	4:C:769:HOH:O	2.44	0.50
1:B:9:THR:O	1:B:11:GLU:N	2.46	0.49
1:B:305:PRO:HB3	1:B:306:GLN:HB3	1.94	0.49
1:B:35:ARG:HH11	1:B:35:ARG:HB3	1.77	0.49
1:C:285:ARG:CZ	4:C:638:HOH:O	2.60	0.49
1:B:37:GLU:OE1	1:B:37:GLU:N	2.34	0.48
1:A:204:GLU:OE2	1:A:343:LYS:HE3	2.14	0.48
1:C:79:GLU:HB2	1:C:84:LEU:O	2.14	0.47
1:A:181:ALA:HB3	1:A:182:PRO:HD3	1.97	0.47
1:B:305:PRO:CB	1:B:306:GLN:HB3	2.45	0.47
1:B:237:ARG:HG2	1:B:242:LEU:HB2	1.97	0.47
1:C:13:LEU:HD13	1:C:44:TYR:OH	2.15	0.47
1:C:96:GLU:HG2	1:C:137:ARG:NH1	2.29	0.47
1:C:237:ARG:HG2	1:C:242:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:CZ	1:B:270:LEU:HD11	2.50	0.46
1:C:293:ILE:HG13	1:C:294:LEU:HG	1.97	0.46
1:C:90:VAL:HG11	1:C:110:LEU:HD11	1.98	0.46
1:A:176:ARG:NH1	1:A:189:TRP:CE3	2.85	0.45
1:B:120:LEU:HD11	1:B:151:TYR:CE2	2.51	0.45
1:C:120:LEU:CD1	1:C:151:TYR:CE2	3.00	0.45
1:B:96:GLU:CG	1:B:133:MET:HE3	2.47	0.45
1:B:211:THR:HG22	4:B:693:HOH:O	2.16	0.45
1:B:83:LYS:HD3	1:B:167:LEU:HD23	1.98	0.44
1:B:181:ALA:HB3	1:B:182:PRO:HD3	1.99	0.44
1:A:92:ARG:HG2	1:B:186:GLN:OE1	2.18	0.44
1:B:305:PRO:HA	1:B:306:GLN:CB	2.48	0.44
1:C:181:ALA:HB3	1:C:182:PRO:HD3	2.00	0.44
1:C:9:THR:N	4:C:773:HOH:O	2.50	0.44
1:A:204:GLU:O	1:A:343:LYS:HD3	2.18	0.44
1:B:96:GLU:CG	1:B:133:MET:CE	2.96	0.44
1:C:68:LYS:HZ3	1:C:151:TYR:HE1	1.67	0.43
1:A:237:ARG:HG2	1:A:242:LEU:HB2	1.99	0.43
1:A:237:ARG:HD2	4:A:801:HOH:O	2.18	0.43
1:B:92:ARG:HG3	1:B:92:ARG:NH1	2.28	0.43
1:C:77:LEU:CD1	1:C:178:LYS:HE3	2.49	0.43
1:B:90:VAL:HG11	1:B:110:LEU:HD11	2.01	0.42
1:A:120:LEU:CD1	1:A:151:TYR:CE2	3.02	0.42
1:B:9:THR:C	1:B:11:GLU:N	2.73	0.42
1:B:36:PRO:HD2	1:B:37:GLU:OE1	2.20	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.88	0.41
1:C:266:MET:HE2	4:C:653:HOH:O	2.03	0.41
1:C:290:TYR:HE1	1:C:295:GLU:OE1	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:GLY:O	4:C:739:HOH:O[3_554]	1.91	0.29

## 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	355/367 (97%)	346 (98%)	9 (2%)	0	100	100
1	B	355/367 (97%)	343 (97%)	9 (2%)	3 (1%)	19	7
1	C	352/367 (96%)	345 (98%)	7 (2%)	0	100	100
All	All	1062/1101 (96%)	1034 (97%)	25 (2%)	3 (0%)	41	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	10	ARG
1	B	306	GLN
1	B	9	THR

### 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	283/292 (97%)	268 (95%)	15 (5%)	22	9
1	B	283/292 (97%)	257 (91%)	26 (9%)	9	2
1	C	282/292 (97%)	265 (94%)	17 (6%)	19	7
All	All	848/876 (97%)	790 (93%)	58 (7%)	16	5

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	50	GLU
1	A	86	PHE
1	A	87	ASP
1	A	92	ARG
1	A	94	LEU
1	A	118	LEU
1	A	154	LEU
1	A	161	LEU
1	A	200	TYR
1	A	245	VAL
1	A	246	ASP
1	A	306	GLN
1	A	330	LEU
1	A	343	LYS
1	B	13	LEU
1	B	17	VAL
1	B	35	ARG
1	B	77	LEU
1	B	92	ARG
1	B	108	LEU
1	B	118	LEU
1	B	127	THR
1	B	138	GLU
1	B	140	GLN
1	B	151	TYR
1	B	154	LEU
1	B	161	LEU
1	B	168	ASP
1	B	170	GLU
1	B	200	TYR
1	B	211	THR
1	B	246	ASP
1	B	270	LEU
1	B	276	SER
1	B	315	ASN
1	B	316	LYS
1	B	328	VAL
1	B	330	LEU
1	B	335	THR
1	B	361	LEU
1	C	11	GLU
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	37	GLU
1	C	77	LEU
1	C	79	GLU
1	C	83	LYS
1	C	92	ARG
1	C	108	LEU
1	C	118	LEU
1	C	150	THR
1	C	200	TYR
1	C	249	LEU
1	C	306	GLN
1	C	312	VAL
1	C	315	ASN
1	C	330	LEU
1	C	335	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	140	GLN
1	A	186	GLN
1	A	334	HIS
1	B	25	GLN
1	B	140	GLN
1	B	209	GLN
1	C	209	GLN
1	C	241	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	357/367 (97%)	0.01	8 (2%) 62 57	8, 15, 33, 63	0
1	B	357/367 (97%)	0.33	21 (5%) 22 17	11, 22, 41, 74	0
1	C	356/367 (97%)	0.03	8 (2%) 62 57	8, 15, 29, 53	0
All	All	1070/1101 (97%)	0.12	37 (3%) 44 38	8, 17, 36, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	PRO	9.1
1	A	304	PRO	7.8
1	C	304	PRO	7.0
1	A	303	GLU	6.0
1	B	303	GLU	5.6
1	A	37	GLU	5.4
1	B	9	THR	5.0
1	B	305	PRO	4.0
1	C	303	GLU	3.7
1	B	244	ASP	3.7
1	B	8	GLN	3.4
1	B	310	ASP	3.2
1	B	306	GLN	3.2
1	C	306	GLN	3.2
1	B	38	GLY	3.0
1	B	262	ARG	2.9
1	B	207	ASP	2.8
1	B	138	GLU	2.6
1	A	310	ASP	2.5
1	B	307	SER	2.4
1	A	50	GLU	2.3
1	B	7	ARG	2.3
1	C	37	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	306	GLN	2.2
1	A	36	PRO	2.2
1	C	365	ASP	2.2
1	C	251	GLN	2.2
1	C	246	ASP	2.2
1	C	11	GLU	2.2
1	B	242	LEU	2.1
1	B	247	ALA	2.1
1	B	33	LEU	2.1
1	B	35	ARG	2.1
1	B	127	THR	2.1
1	B	251	GLN	2.1
1	B	66	LEU	2.1
1	A	207	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [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
2	CA	C	403	1/1	0.96	0.23	51,51,51,51	0
2	CA	B	401	1/1	0.97	0.04	25,25,25,25	0
2	CA	A	403	1/1	0.97	0.28	35,35,35,35	0
2	CA	B	402	1/1	0.98	0.04	24,24,24,24	0
3	CL	A	406	1/1	0.98	0.06	20,20,20,20	0
3	CL	C	405	1/1	0.98	0.07	17,17,17,17	0
2	CA	C	402	1/1	0.99	0.08	30,30,30,30	0
2	CA	A	402	1/1	0.99	0.04	16,16,16,16	0
2	CA	C	404	1/1	0.99	0.06	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	401	1/1	0.99	0.11	33,33,33,33	0
3	CL	B	403	1/1	0.99	0.09	27,27,27,27	0
2	CA	C	401	1/1	0.99	0.07	18,18,18,18	0
2	CA	A	405	1/1	1.00	0.05	15,15,15,15	0
2	CA	A	404	1/1	1.00	0.05	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.