Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:06 PM UTC

PDB ID	:	3WS1 / pdb_00003ws1
Title	:	N288Q-N321Q mutant BETA-LACTAMASE DERIVED FROM CHROMOHALOBACTER SP.560 (Condition-1B)
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

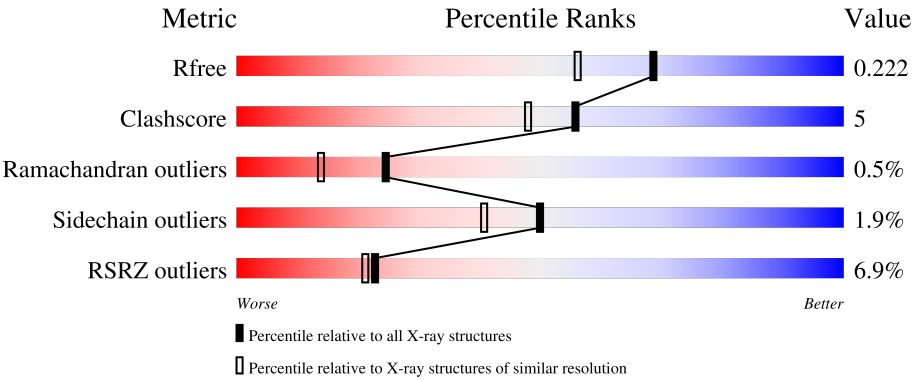
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 >=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 <=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	3% 90% 6%
1	B	367	15% 85% 10%
1	C	367	3% 90% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8801 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	360	Total	C	N	O	S	0	2	0
			2742	1722	463	546	11			
1	B	360	Total	C	N	O	S	0	0	0
			2730	1713	460	546	11			
1	C	360	Total	C	N	O	S	0	1	0
			2736	1717	460	548	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 CESIUM ION (CCD ID: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cs	0	0
			1	1		
2	C	1	Total	Cs	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	B	3	Total	Ca	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	3	Total Ca 3 3	0	0

- Molecule 4 is water.

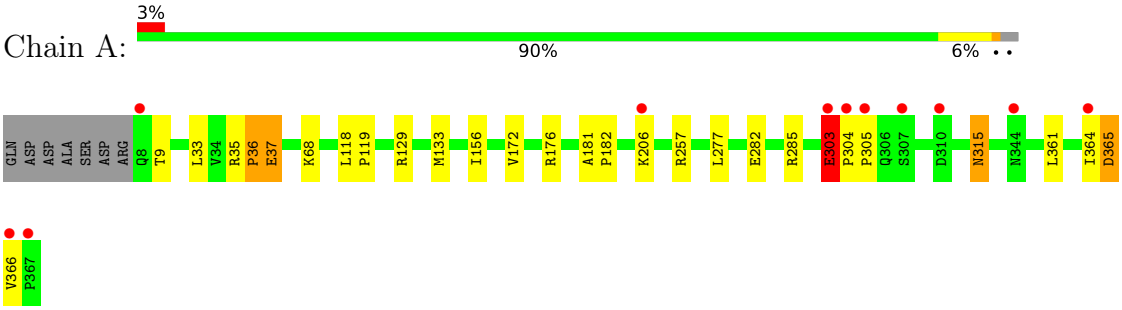
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	221	Total O 221 221	0	0
4	B	115	Total O 115 115	0	0
4	C	245	Total O 245 245	0	0

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.

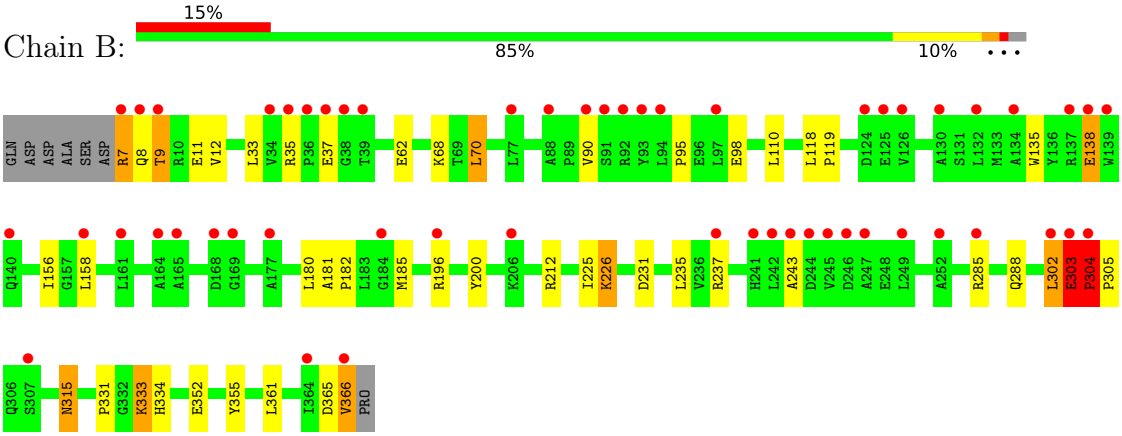
• Molecule 1: Beta-lactamase

Chain A:



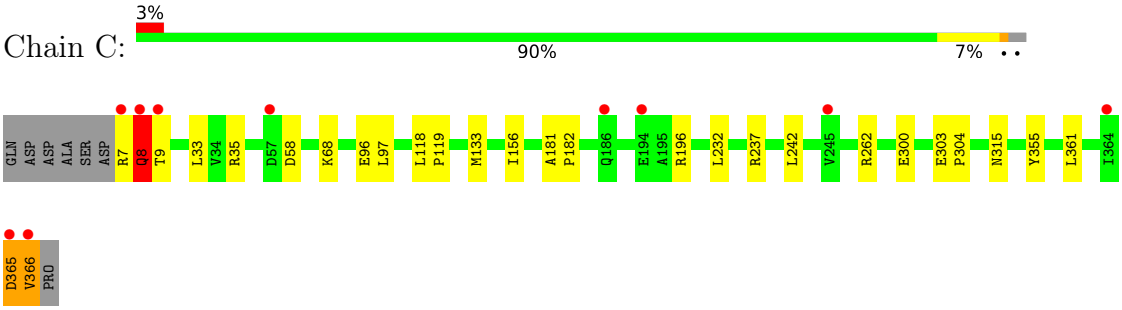
• Molecule 1: Beta-lactamase

Chain B:



• Molecule 1: Beta-lactamase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	115.12Å 115.12Å 67.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.68 – 1.80 37.68 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.68-1.80) 99.8 (37.68-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.61 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.211 (Not available) , 0.222	Depositor DCC
R_{free} test set	4618 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.025 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8801	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CS, 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	0.80	0/2805	0.94	6/3825 (0.2%)
1	B	0.70	1/2786 (0.0%)	0.96	11/3799 (0.3%)
1	C	0.81	0/2795	0.88	3/3811 (0.1%)
All	All	0.77	1/8386 (0.0%)	0.92	20/11435 (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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	THR	CA-C	6.47	1.60	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	GLU	CA-C-N	-12.77	107.23	120.38
1	A	303	GLU	C-N-CA	-12.77	107.23	120.38
1	B	333	LYS	N-CA-C	-11.88	91.29	109.94
1	B	303	GLU	CA-C-N	-11.00	109.05	120.38
1	B	303	GLU	C-N-CA	-11.00	109.05	120.38
1	B	9	THR	N-CA-C	8.46	121.29	107.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	PRO	CA-C-N	-8.36	110.28	119.98
1	A	304	PRO	C-N-CA	-8.36	110.28	119.98
1	C	304	PRO	CA-C-N	-7.36	112.42	119.85
1	C	304	PRO	C-N-CA	-7.36	112.42	119.85
1	A	315	ASN	N-CA-C	6.30	118.65	109.07
1	B	333	LYS	CA-C-N	-6.14	109.81	121.54
1	B	333	LYS	C-N-CA	-6.14	109.81	121.54
1	B	334	HIS	N-CA-C	-5.97	98.08	110.80
1	B	315	ASN	N-CA-C	5.74	117.80	109.07
1	A	36	PRO	N-CA-C	-5.62	101.68	110.50
1	B	288	GLN	CB-CG-CD	-5.50	103.24	112.60
1	B	302	LEU	N-CA-C	5.32	117.89	111.40
1	B	304	PRO	CB-CA-C	5.28	117.37	110.92
1	C	315	ASN	N-CA-C	5.17	116.92	109.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLU	Peptide
1	B	303	GLU	Peptide
1	C	7	ARG	Peptide

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	2742	0	2681	15	0
1	B	2730	0	2662	43	0
1	C	2736	0	2668	17	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	1	0
4	A	221	0	0	2	1
4	B	115	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	245	0	0	4	0
All	All	8801	0	8011	76	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 5.

All (76) 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:196:ARG:NH2	4:C:601:HOH:O	1.75	1.15
1:B:185:MET:HE1	1:B:235:LEU:HB2	1.37	1.06
1:C:262:ARG:NH1	1:C:300:GLU:OE1	2.02	0.92
1:B:304:PRO:HB2	1:B:305:PRO:O	1.72	0.88
1:B:196:ARG:NH1	4:B:611:HOH:O	2.08	0.87
1:B:7:ARG:HA	1:B:8:GLN:HB2	1.63	0.80
1:B:304:PRO:HB2	1:B:305:PRO:C	2.07	0.78
1:A:68:LYS:HE3	1:A:156:ILE:HG21	1.68	0.75
3:C:402:CA:CA	4:C:743:HOH:O	1.65	0.74
1:A:257[A]:ARG:NH1	4:A:602:HOH:O	2.24	0.71
1:C:58:ASP:OD2	4:C:743:HOH:O	2.09	0.71
1:B:7:ARG:HD3	4:B:613:HOH:O	1.91	0.70
1:A:303:GLU:O	1:A:305:PRO:HD3	1.93	0.69
1:B:185:MET:HE1	1:B:235:LEU:CB	2.20	0.69
1:B:95:PRO:O	1:B:98:GLU:HG2	1.92	0.68
1:B:185:MET:HE2	1:B:231:ASP:O	1.99	0.63
1:B:158:LEU:HD23	1:B:158:LEU:O	1.99	0.63
1:C:237:ARG:HG3	1:C:242:LEU:HB2	1.81	0.62
1:B:90:VAL:HG11	1:B:158:LEU:HD21	1.83	0.58
1:B:33:LEU:HD21	1:B:35:ARG:HH11	1.68	0.58
1:B:62:GLU:HG2	1:B:226:LYS:HD2	1.85	0.58
1:B:285:ARG:NH2	1:B:352:GLU:HB2	2.19	0.58
1:B:135:TRP:O	1:B:138:GLU:OE1	2.22	0.57
1:B:355:TYR:OH	1:B:366:VAL:HG13	2.06	0.55
1:A:9:THR:OG1	1:A:35:ARG:NH2	2.41	0.53
1:A:277:LEU:O	4:A:659:HOH:O	2.19	0.52
1:B:33:LEU:CD2	1:B:35:ARG:HH11	2.22	0.52
1:C:9:THR:OG1	1:C:35:ARG:NH2	2.43	0.52
1:C:355:TYR:OH	1:C:366:VAL:HG13	2.09	0.51
1:B:7:ARG:HA	1:B:8:GLN:CB	2.31	0.51
1:B:237:ARG:CD	1:B:243:ALA:HB2	2.40	0.51
1:B:226:LYS:N	1:B:226:LYS:HD3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ARG:CZ	4:C:601:HOH:O	2.35	0.49
1:A:282:GLU:OE1	1:A:285:ARG:NH2	2.37	0.47
1:B:302:LEU:HB3	1:B:304:PRO:HD2	1.97	0.47
1:B:185:MET:CE	1:B:235:LEU:N	2.78	0.47
1:A:36:PRO:O	1:A:37:GLU:CB	2.63	0.46
1:B:70:LEU:HD22	1:B:180:LEU:HD21	1.97	0.46
1:B:110:LEU:HD11	1:B:158:LEU:HD22	1.97	0.46
1:B:181:ALA:HB3	1:B:182:PRO:HD3	1.97	0.46
1:C:181:ALA:HB3	1:C:182:PRO:HD3	1.98	0.45
1:B:200:TYR:O	1:B:212:ARG:NH2	2.49	0.45
1:A:129:ARG:NH1	1:A:133:MET:HE3	2.31	0.45
1:A:303:GLU:C	1:A:305:PRO:HD3	2.42	0.45
1:B:33:LEU:HD21	1:B:361:LEU:HD13	1.97	0.45
1:B:135:TRP:HA	1:B:138:GLU:OE1	2.17	0.45
1:A:181:ALA:HB3	1:A:182:PRO:HD3	1.99	0.45
1:B:90:VAL:HG11	1:B:158:LEU:CD2	2.47	0.44
1:A:33:LEU:HD21	1:A:361:LEU:HD13	1.99	0.44
1:C:97:LEU:HD21	1:C:133:MET:HE3	1.98	0.44
1:C:96[B]:GLU:OE1	1:C:133:MET:HE2	2.17	0.44
1:B:9:THR:HG22	1:B:12:VAL:H	1.82	0.44
1:C:33:LEU:HD21	1:C:361:LEU:HD13	2.00	0.44
1:B:285:ARG:HH21	1:B:352:GLU:HB2	1.80	0.43
1:B:68:LYS:HE2	1:B:156:ILE:HG21	2.00	0.43
1:B:331:PRO:O	1:B:333:LYS:O	2.36	0.43
1:C:8:GLN:CG	1:C:9:THR:H	2.32	0.43
1:C:8:GLN:CG	1:C:9:THR:N	2.82	0.43
1:A:172:VAL:O	1:A:176:ARG:HG3	2.19	0.42
1:A:364:ILE:HG22	1:A:365:ASP:N	2.34	0.42
1:C:365:ASP:O	1:C:366:VAL:C	2.61	0.42
1:C:68:LYS:HE2	1:C:156:ILE:HG21	2.02	0.42
1:B:237:ARG:HD3	1:B:243:ALA:HB2	2.02	0.42
1:B:302:LEU:C	1:B:304:PRO:CD	2.93	0.42
1:A:36:PRO:O	1:A:37:GLU:HB3	2.20	0.41
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.95	0.41
1:C:118:LEU:HA	1:C:119:PRO:HD3	1.94	0.41
1:B:7:ARG:NE	1:B:8:GLN:O	2.53	0.41
1:B:90:VAL:CG1	1:B:158:LEU:HD21	2.49	0.41
1:B:158:LEU:HD23	1:B:158:LEU:C	2.45	0.41
1:B:225:ILE:C	1:B:226:LYS:HD3	2.46	0.41
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.91	0.41
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HD2	4:B:578:HOH:O	2.19	0.40
1:B:9:THR:CG2	1:B:11:GLU:HB2	2.51	0.40
1:B:118:LEU:HA	1:B:119:PRO:HD3	1.96	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)
4:A:659:HOH:O	4:A:721:HOH:O[3_454]	2.17	0.03

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	360/367 (98%)	348 (97%)	11 (3%)	1 (0%)	36 25
1	B	358/367 (98%)	345 (96%)	10 (3%)	3 (1%)	16 6
1	C	359/367 (98%)	348 (97%)	10 (3%)	1 (0%)	36 25
All	All	1077/1101 (98%)	1041 (97%)	31 (3%)	5 (0%)	24 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	B	37	GLU
1	C	8	GLN
1	B	303	GLU
1	B	304	PRO

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	288/292 (99%)	283 (98%)	5 (2%)	53	45
1	B	286/292 (98%)	279 (98%)	7 (2%)	43	31
1	C	287/292 (98%)	283 (99%)	4 (1%)	59	52
All	All	861/876 (98%)	845 (98%)	16 (2%)	50	41

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

Mol	Chain	Res	Type
1	A	206	LYS
1	A	303	GLU
1	A	315	ASN
1	A	365	ASP
1	A	366	VAL
1	B	7	ARG
1	B	70	LEU
1	B	138	GLU
1	B	226	LYS
1	B	315	ASN
1	B	365	ASP
1	B	366	VAL
1	C	8	GLN
1	C	303	GLU
1	C	365	ASP
1	C	366	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	HIS
1	A	288	GLN
1	B	43	HIS
1	B	140	GLN
1	B	241	HIS

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Mol	Chain	Res	Type
1	C	258	GLN
1	C	315	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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^{th} 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	360/367 (98%)	0.07	11 (3%) 51 51	12, 25, 48, 64	2 (0%)
1	B	360/367 (98%)	0.89	54 (15%) 5 4	21, 37, 70, 88	0
1	C	360/367 (98%)	0.00	10 (2%) 55 55	12, 23, 43, 81	1 (0%)
All	All	1080/1101 (98%)	0.32	75 (6%) 23 21	12, 28, 62, 88	3 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	VAL	8.1
1	B	366	VAL	6.2
1	B	304	PRO	6.0
1	B	9	THR	5.8
1	A	304	PRO	5.4
1	A	367	PRO	4.9
1	B	36	PRO	4.6
1	B	8	GLN	4.5
1	A	366	VAL	4.3
1	A	303	GLU	4.1
1	A	305	PRO	4.0
1	B	38	GLY	3.8
1	B	97	LEU	3.8
1	A	8	GLN	3.7
1	B	242	LEU	3.7
1	C	7	ARG	3.5
1	B	243	ALA	3.4
1	B	7	ARG	3.4
1	B	364	ILE	3.3
1	B	246	ASP	3.3
1	B	168	ASP	3.2
1	B	169	GLY	3.2
1	B	252	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	302	LEU	3.1
1	A	310	ASP	3.1
1	B	241	HIS	3.1
1	B	247	ALA	3.0
1	B	307	SER	2.9
1	B	138	GLU	2.9
1	B	303	GLU	2.9
1	A	307	SER	2.8
1	B	94	LEU	2.8
1	B	92	ARG	2.7
1	B	165	ALA	2.7
1	B	77	LEU	2.7
1	B	237	ARG	2.6
1	B	244	ASP	2.6
1	B	39	THR	2.6
1	B	206	LYS	2.6
1	B	177	ALA	2.6
1	B	164	ALA	2.5
1	C	9	THR	2.5
1	B	140	GLN	2.5
1	B	184	GLY	2.5
1	B	90	VAL	2.5
1	B	35	ARG	2.5
1	B	139	TRP	2.5
1	B	34	VAL	2.5
1	A	206	LYS	2.5
1	B	124	ASP	2.5
1	A	364	ILE	2.4
1	B	196	ARG	2.4
1	B	137	ARG	2.4
1	A	344	ASN	2.3
1	B	285	ARG	2.3
1	B	126	VAL	2.3
1	B	130	ALA	2.2
1	B	134	ALA	2.2
1	B	132	LEU	2.2
1	B	249	LEU	2.2
1	B	245	VAL	2.2
1	B	37	GLU	2.2
1	C	57	ASP	2.2
1	C	186	GLN	2.2
1	B	88	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	8	GLN	2.1
1	C	194	GLU	2.1
1	B	91	SER	2.1
1	C	245	VAL	2.1
1	B	158	LEU	2.1
1	C	365	ASP	2.1
1	B	125	GLU	2.0
1	B	93	TYR	2.0
1	B	161	LEU	2.0
1	C	364	ILE	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)

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^{th} 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
2	CS	C	401	1/1	0.84	0.15	50,50,50,50	1
3	CA	C	403	1/1	0.91	0.19	47,47,47,47	0
3	CA	B	402	1/1	0.92	0.08	51,51,51,51	0
3	CA	A	402	1/1	0.92	0.10	30,30,30,30	0
3	CA	C	404	1/1	0.92	0.11	25,25,25,25	0
3	CA	A	403	1/1	0.93	0.19	42,42,42,42	0
2	CS	A	401	1/1	0.94	0.11	40,40,40,40	1
3	CA	B	403	1/1	0.96	0.05	36,36,36,36	0
3	CA	B	401	1/1	0.97	0.09	35,35,35,35	0
3	CA	C	402	1/1	0.97	0.22	35,35,35,35	0
3	CA	A	404	1/1	0.99	0.03	25,25,25,25	0
3	CA	A	405	1/1	0.99	0.05	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.