



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:18 PM GMT

PDB ID : 3WS4
Title : N288Q-N321Q mutant BETA-LACTAMASE DERIVED FROM CHROMOHALOBACTER SP.560 (Condition-2A)
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 : 2014-02-28
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

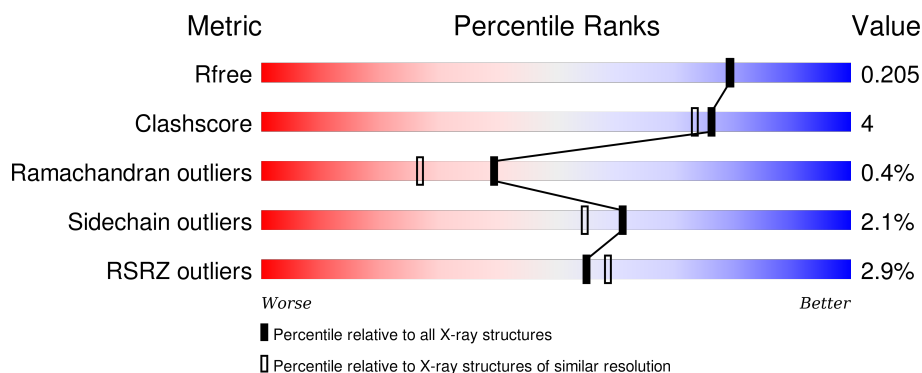
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>4%</div> <div>89%</div> <div>7% ..</div> </div>
1	B	367	<div> <div>3%</div> <div>91%</div> <div>5% ..</div> </div>
1	C	367	<div> <div>2%</div> <div>88%</div> <div>9% ..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8710 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	3	0
			2722	1709	457	545	11			
1	B	359	Total	C	N	O	S	0	3	0
			2737	1718	459	549	11			
1	C	358	Total	C	N	O	S	0	2	0
			2732	1713	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 STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Sr	0	0
			2	2		
2	A	3	Total	Sr	0	0
			3	3		
2	C	3	Total	Sr	0	0
			3	3		

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

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

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

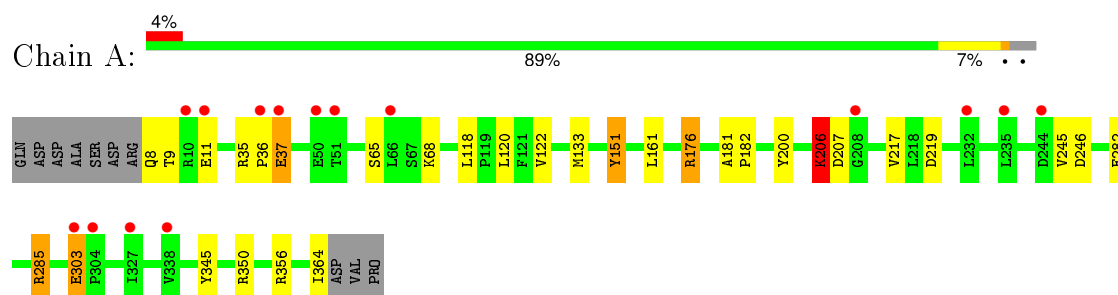
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	157	Total	O	0	0
			157	157		
4	C	192	Total	O	0	0
			192	192		

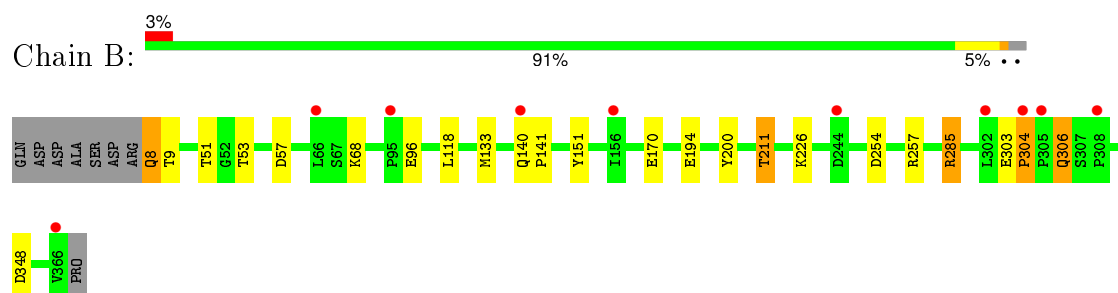
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

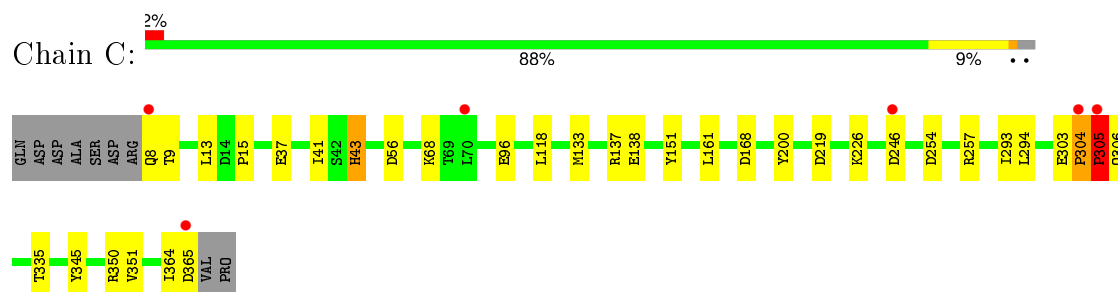
• Molecule 1: Beta-lactamase



• 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, α , β , γ	115.02Å 115.02Å 67.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.02 – 1.90 28.02 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.02-1.90) 99.9 (28.02-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.20 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.182 , 0.216 0.177 , 0.205	Depositor DCC
R_{free} test set	4015 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.5	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 78897 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8710	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 2.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SR, CL

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	0.74	1/2787 (0.0%)	0.87	9/3800 (0.2%)
1	B	0.76	0/2802	0.84	3/3822 (0.1%)
1	C	0.78	0/2788	0.85	1/3801 (0.0%)
All	All	0.76	1/8377 (0.0%)	0.85	13/11423 (0.1%)

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	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	TYR	CG-CD1	-5.49	1.32	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285[A]	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	285[B]	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	285[A]	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	285[B]	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	206	LYS	CD-CE-NZ	8.26	130.69	111.70
1	B	285	ARG	NE-CZ-NH2	-6.53	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	B	304	PRO	C-N-CD	-6.35	106.64	120.60
1	A	219	ASP	CB-CG-OD1	6.03	123.73	118.30
1	C	219	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	285	ARG	CB-CG-CD	5.58	126.11	111.60
1	A	356	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	176	ARG	NE-CZ-NH2	5.36	122.98	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	GLU	Peptide
1	B	303	GLU	Peptide
1	C	304	PRO	Peptide
1	C	305	PRO	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	2722	0	2657	17	0
1	B	2737	0	2670	16	0
1	C	2732	0	2658	28	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	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	159	0	0	1	0
4	B	157	0	0	2	0
4	C	192	0	0	3	0
All	All	8710	0	7985	61	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 4.

All (61) 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:37:GLU:HG2	4:C:542:HOH:O	1.42	1.14
1:A:282:GLU:OE1	1:A:285[A]:ARG:NH2	1.91	1.03
1:C:137[B]:ARG:NH1	1:C:138[B]:GLU:OE2	2.04	0.89
1:C:305:PRO:HB2	1:C:306:GLN:HA	1.56	0.86
1:C:304:PRO:N	1:C:305:PRO:HD3	1.92	0.85
1:A:364:ILE:HD11	4:A:567:HOH:O	1.76	0.84
1:C:293:ILE:HG13	1:C:294:LEU:HG	1.63	0.79
1:B:140:GLN:NE2	1:B:141:PRO:O	2.14	0.75
1:C:41:ILE:HG22	1:C:43:HIS:CE1	2.24	0.72
1:C:41:ILE:HG22	1:C:43:HIS:HE1	1.60	0.66
1:B:8:GLN:HE21	1:B:8:GLN:HA	1.62	0.64
1:C:8:GLN:HG3	1:C:9:THR:H	1.63	0.64
1:B:304:PRO:HG2	1:B:306:GLN:N	2.14	0.63
1:C:68:LYS:NZ	1:C:151:TYR:CE1	2.68	0.62
1:B:211:THR:HG22	4:B:640:HOH:O	1.99	0.61
1:C:8:GLN:HG3	1:C:9:THR:N	2.20	0.57
1:A:8:GLN:O	1:A:11:GLU:HG2	2.04	0.57
1:C:68:LYS:NZ	1:C:151:TYR:HE1	2.03	0.56
1:A:206:LYS:HE2	1:A:207:ASP:OD1	2.06	0.56
1:C:305:PRO:HB2	1:C:306:GLN:CA	2.33	0.54
1:A:68:LYS:HZ1	1:A:151:TYR:HE1	1.54	0.54
1:C:41:ILE:CG2	1:C:43:HIS:HE1	2.20	0.54
1:A:68:LYS:NZ	1:A:151:TYR:HE1	2.06	0.53
1:B:68:LYS:NZ	1:B:151:TYR:HE1	2.07	0.53
1:A:36:PRO:O	1:A:37:GLU:CB	2.58	0.52
1:C:168:ASP:HB3	4:C:675:HOH:O	2.09	0.52
1:A:345:TYR:CZ	1:A:350:ARG:HG2	2.47	0.50
1:A:120:LEU:HD11	1:A:151:TYR:CE2	2.47	0.49
1:C:254:ASP:OD1	1:C:257:ARG:NH2	2.44	0.49
1:B:254:ASP:OD1	1:B:257:ARG:NH2	2.45	0.49
1:C:305:PRO:HG2	1:C:306:GLN:HG3	1.95	0.49
1:B:68:LYS:HZ1	1:B:151:TYR:HE1	1.58	0.48
1:C:133:MET:CE	1:C:161:LEU:HD13	2.44	0.48
1:C:305:PRO:CB	1:C:306:GLN:HA	2.37	0.48
1:A:36:PRO:O	1:A:37:GLU:HB3	2.15	0.47
1:B:8:GLN:NE2	1:B:9:THR:H	2.12	0.47
1:A:68:LYS:NZ	1:A:151:TYR:CE1	2.82	0.47
1:C:43:HIS:HD2	1:C:56:ASP:HA	1.80	0.47
1:A:9:THR:OG1	1:A:35:ARG:NH1	2.32	0.46
1:A:133:MET:CE	1:A:161:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:PRO:CD	1:C:305:PRO:HD3	2.46	0.46
1:C:304:PRO:N	1:C:305:PRO:CD	2.72	0.45
1:C:303:GLU:C	1:C:305:PRO:HD3	2.38	0.45
1:A:245:VAL:HG12	1:A:246:ASP:O	2.17	0.45
1:B:285:ARG:HD2	1:B:348:ASP:HA	1.99	0.44
1:B:226:LYS:HD2	1:B:226:LYS:N	2.33	0.44
1:A:122:VAL:HG11	1:A:217:VAL:HG22	2.00	0.43
1:B:51:THR:OG1	1:B:53:THR:HG22	2.18	0.43
1:B:96:GLU:HG3	1:B:133:MET:HE3	2.01	0.43
1:B:194:GLU:OE2	4:B:639:HOH:O	2.22	0.42
1:C:364:ILE:O	1:C:365:ASP:HB2	2.18	0.42
1:C:226:LYS:N	1:C:226:LYS:HD3	2.34	0.42
1:A:133:MET:HE1	1:A:161:LEU:HD13	2.02	0.41
1:C:137[B]:ARG:NH2	4:C:661:HOH:O	2.53	0.41
1:C:43:HIS:CD2	1:C:56:ASP:HA	2.55	0.41
1:A:181:ALA:HB3	1:A:182:PRO:HD3	2.02	0.41
1:C:345:TYR:CZ	1:C:350:ARG:HG2	2.55	0.41
1:C:133:MET:HE2	1:C:161:LEU:HD13	2.03	0.40
1:B:68:LYS:NZ	1:B:151:TYR:CE1	2.83	0.40
1:B:170:GLU:OE1	1:B:170:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/367 (98%)	348 (97%)	8 (2%)	2 (1%)	30	17
1	B	360/367 (98%)	350 (97%)	9 (2%)	1 (0%)	46	35
1	C	358/367 (98%)	349 (98%)	8 (2%)	1 (0%)	46	35
All	All	1076/1101 (98%)	1047 (97%)	25 (2%)	4 (0%)	39	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	305	PRO
1	A	37	GLU
1	B	306	GLN
1	A	303	GLU

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	286/292 (98%)	281 (98%)	5 (2%)	68	64
1	B	288/292 (99%)	284 (99%)	4 (1%)	74	71
1	C	286/292 (98%)	277 (97%)	9 (3%)	47	37
All	All	860/876 (98%)	842 (98%)	18 (2%)	61	55

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	SER
1	A	118	LEU
1	A	176	ARG
1	A	200	TYR
1	A	206	LYS
1	B	8	GLN
1	B	118	LEU
1	B	200	TYR
1	B	211	THR
1	C	13	LEU
1	C	15	PRO
1	C	43	HIS
1	C	96	GLU
1	C	118	LEU
1	C	200	TYR
1	C	246	ASP
1	C	335	THR

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Mol	Chain	Res	Type
1	C	351	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	B	8	GLN
1	B	315	ASN
1	C	43	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 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 [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	357/367 (97%)	0.15	15 (4%)	40 44	18, 32, 55, 94	0
1	B	359/367 (97%)	0.09	10 (2%)	56 60	19, 29, 48, 95	0
1	C	358/367 (97%)	0.03	6 (1%)	73 76	19, 28, 49, 81	0
All	All	1074/1101 (97%)	0.09	31 (2%)	55 59	18, 29, 51, 95	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	PRO	8.4
1	C	305	PRO	6.6
1	A	303	GLU	5.1
1	C	365	ASP	4.8
1	B	366	VAL	4.6
1	A	50	GLU	4.5
1	A	304	PRO	4.2
1	B	305	PRO	3.8
1	B	244	ASP	3.6
1	A	37	GLU	3.6
1	A	327	ILE	3.3
1	A	232	LEU	3.2
1	A	11	GLU	2.9
1	B	95	PRO	2.9
1	B	66	LEU	2.9
1	A	66	LEU	2.8
1	C	8	GLN	2.8
1	A	51	THR	2.7
1	A	244	ASP	2.5
1	A	338	VAL	2.5
1	A	235	LEU	2.4
1	B	302	LEU	2.3
1	A	208	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	304	PRO	2.2
1	B	308	PRO	2.2
1	B	156	ILE	2.2
1	C	246	ASP	2.2
1	C	70	LEU	2.1
1	B	140	GLN	2.1
1	A	36	PRO	2.1
1	A	10	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SR	B	402	1/1	1.00	0.06	-1.46	22,22,22,22	0
2	SR	A	401	1/1	0.99	0.08	-1.91	35,35,35,35	0
2	SR	A	403	1/1	1.00	0.04	-2.71	21,21,21,21	0
2	SR	C	403	1/1	1.00	0.04	-6.64	21,21,21,21	0
2	SR	C	401	1/1	0.98	0.14	-	48,48,48,48	0
3	CL	B	403	1/1	0.94	0.14	-	39,39,39,39	0
2	SR	A	402	1/1	1.00	0.03	-	28,28,28,28	0
3	CL	A	404	1/1	0.99	0.05	-	39,39,39,39	0
3	CL	C	404	1/1	0.99	0.07	-	32,32,32,32	0
2	SR	B	401	1/1	1.00	0.06	-	30,30,30,30	0
2	SR	C	402	1/1	0.99	0.07	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.