



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:54 AM UTC

PDB ID : 3I46 / pdb_00003i46
Title : Crystal structure of beta toxin from Staphylococcus aureus F277A, P278A mutant with bound calcium ions
Authors : Huseby, M.; Shi, K.; Kruse, A.C.; Ohlendorf, D.H.
Deposited on : 2009-07-01
Resolution : 2.60 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

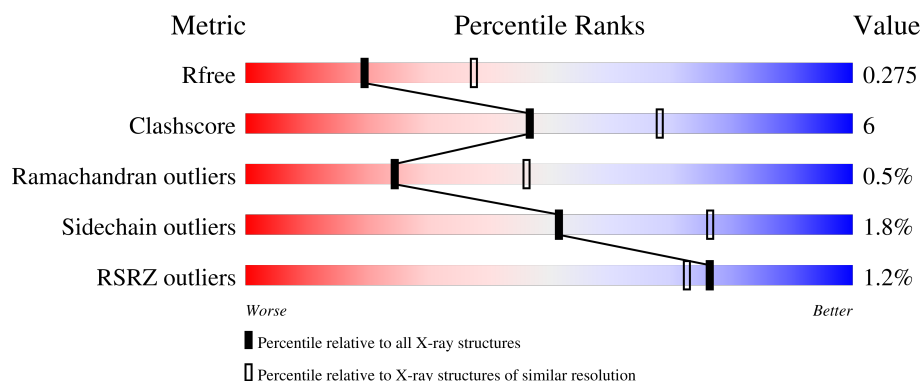
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	317	
1	B	317	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4685 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-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2322	1473	392	452	5			
1	B	289	Total	C	N	O	S	0	0	0
			2322	1473	392	452	5			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A7LAI8
A	-18	ARG	-	expression tag	UNP A7LAI8
A	-17	SER	-	expression tag	UNP A7LAI8
A	-16	SER	-	expression tag	UNP A7LAI8
A	-15	HIS	-	expression tag	UNP A7LAI8
A	-14	HIS	-	expression tag	UNP A7LAI8
A	-13	HIS	-	expression tag	UNP A7LAI8
A	-12	HIS	-	expression tag	UNP A7LAI8
A	-11	HIS	-	expression tag	UNP A7LAI8
A	-10	HIS	-	expression tag	UNP A7LAI8
A	-9	SER	-	expression tag	UNP A7LAI8
A	-8	SER	-	expression tag	UNP A7LAI8
A	-7	GLY	-	expression tag	UNP A7LAI8
A	-6	LEU	-	expression tag	UNP A7LAI8
A	-5	VAL	-	expression tag	UNP A7LAI8
A	-4	PRO	-	expression tag	UNP A7LAI8
A	-3	ARG	-	expression tag	UNP A7LAI8
A	-2	GLY	-	expression tag	UNP A7LAI8
A	-1	SER	-	expression tag	UNP A7LAI8
A	0	HIS	-	expression tag	UNP A7LAI8
A	1	MET	-	expression tag	UNP A7LAI8
A	277	ALA	PHE	engineered mutation	UNP A7LAI8
A	278	ALA	PRO	engineered mutation	UNP A7LAI8
B	-19	MET	-	expression tag	UNP A7LAI8
B	-18	ARG	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP A7LAI8
B	-16	SER	-	expression tag	UNP A7LAI8
B	-15	HIS	-	expression tag	UNP A7LAI8
B	-14	HIS	-	expression tag	UNP A7LAI8
B	-13	HIS	-	expression tag	UNP A7LAI8
B	-12	HIS	-	expression tag	UNP A7LAI8
B	-11	HIS	-	expression tag	UNP A7LAI8
B	-10	HIS	-	expression tag	UNP A7LAI8
B	-9	SER	-	expression tag	UNP A7LAI8
B	-8	SER	-	expression tag	UNP A7LAI8
B	-7	GLY	-	expression tag	UNP A7LAI8
B	-6	LEU	-	expression tag	UNP A7LAI8
B	-5	VAL	-	expression tag	UNP A7LAI8
B	-4	PRO	-	expression tag	UNP A7LAI8
B	-3	ARG	-	expression tag	UNP A7LAI8
B	-2	GLY	-	expression tag	UNP A7LAI8
B	-1	SER	-	expression tag	UNP A7LAI8
B	0	HIS	-	expression tag	UNP A7LAI8
B	1	MET	-	expression tag	UNP A7LAI8
B	277	ALA	PHE	engineered mutation	UNP A7LAI8
B	278	ALA	PRO	engineered mutation	UNP A7LAI8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	13	Total O 13 13	0	0

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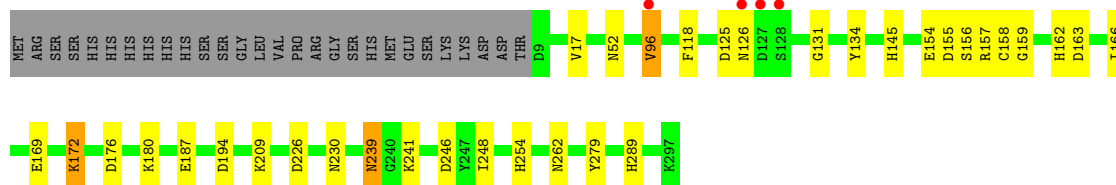
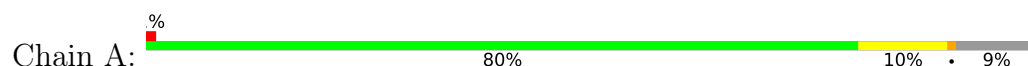
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	22	Total	O	0	0
			22	22		

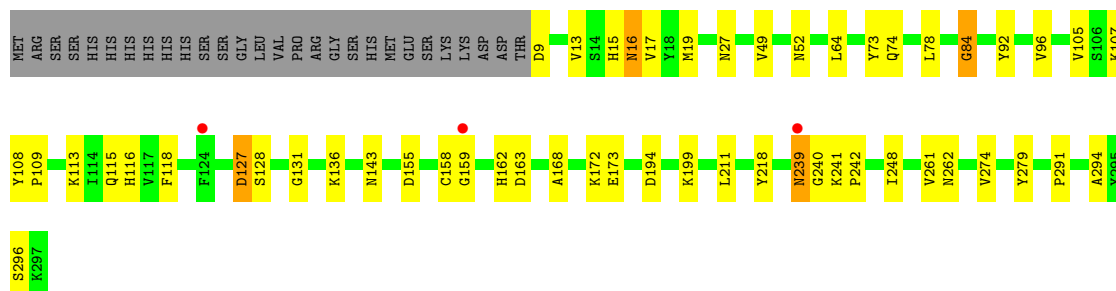
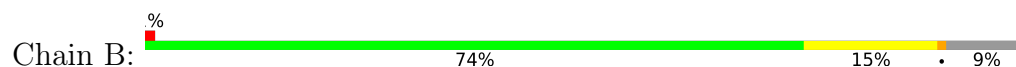
3 Residue-property plots [i](#)

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-hemolysin



• Molecule 1: Beta-hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.09Å 70.19Å 129.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.04 – 2.60 34.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.04-2.60) 98.8 (34.04-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.275 0.220 , 0.275	Depositor DCC
R_{free} test set	1000 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 20.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.65	0/2381	0.94	5/3221 (0.2%)
1	B	0.65	0/2381	0.93	3/3221 (0.1%)
All	All	0.65	0/4762	0.94	8/6442 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	VAL	N-CA-C	6.97	118.78	109.37
1	A	241	LYS	CA-C-N	5.97	126.28	119.83
1	A	241	LYS	C-N-CA	5.97	126.28	119.83
1	B	279	TYR	N-CA-C	5.97	116.29	107.88
1	B	84	GLY	N-CA-C	-5.79	107.68	115.21
1	B	16	ASN	N-CA-C	-5.63	99.94	108.67
1	A	17	VAL	N-CA-C	5.34	118.12	112.83
1	A	279	TYR	N-CA-C	5.10	118.32	110.42

There are no chirality outliers.

There are no planarity outliers.

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	2322	0	2240	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2322	0	2240	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	0	0
4	A	13	0	0	0	0
4	B	22	0	0	2	0
All	All	4685	0	4480	52	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 6.

All (52) 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:A:248:ILE:H	1:A:262:ASN:HD21	1.30	0.79
1:A:134:TYR:OH	1:A:145:HIS:HD2	1.66	0.78
1:A:176:ASP:O	1:A:180:LYS:HG2	1.89	0.71
1:B:116:HIS:HE1	1:B:173:GLU:OE1	1.74	0.71
1:A:159:GLY:HA3	1:A:162:HIS:ND1	2.11	0.65
1:B:155:ASP:HB3	1:B:158:CYS:SG	2.38	0.64
1:A:162:HIS:O	1:A:166:ILE:HG13	1.99	0.62
1:B:248:ILE:H	1:B:262:ASN:HD21	1.49	0.60
1:A:52:ASN:HD21	1:A:194:ASP:H	1.51	0.59
1:B:17:VAL:HG23	1:B:19:MET:HG2	1.85	0.57
1:A:154:GLU:O	1:A:156:SER:N	2.38	0.57
1:A:145:HIS:HE1	1:A:187:GLU:OE1	1.88	0.56
1:B:159:GLY:O	1:B:162:HIS:HB2	2.05	0.56
1:A:134:TYR:OH	1:A:145:HIS:CD2	2.53	0.55
1:B:74:GLN:HG2	1:B:105:VAL:HG12	1.89	0.54
1:B:16:ASN:HA	1:B:52:ASN:HB2	1.89	0.54
1:B:136:LYS:HE2	1:B:143:ASN:OD1	2.09	0.53
1:A:239:ASN:ND2	1:A:239:ASN:H	2.07	0.53
1:B:168:ALA:O	1:B:172:LYS:HG2	2.11	0.51
1:A:156:SER:O	1:A:157:ARG:HB3	2.12	0.50
1:B:261:VAL:O	1:B:294:ALA:HA	2.12	0.50
1:B:15:HIS:CG	1:B:291:PRO:HB3	2.48	0.49
1:A:118:PHE:CD2	1:A:131:GLY:HA2	2.48	0.48
1:B:13:VAL:HB	1:B:49:VAL:HG22	1.95	0.48
1:B:96:VAL:HB	1:B:127:ASP:O	2.14	0.48
1:A:246:ASP:OD1	1:A:289:HIS:HD2	1.97	0.47
1:B:239:ASN:H	1:B:239:ASN:HD22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASP:O	1:A:230:ASN:HB3	2.16	0.46
1:A:118:PHE:CE2	1:A:131:GLY:HA2	2.51	0.46
1:A:209:LYS:HB2	1:A:209:LYS:HE2	1.60	0.46
1:A:156:SER:OG	1:A:157:ARG:N	2.50	0.45
1:B:9:ASP:HB2	4:B:302:HOH:O	2.17	0.45
1:B:52:ASN:ND2	1:B:194:ASP:H	2.14	0.45
1:A:52:ASN:ND2	1:A:194:ASP:H	2.13	0.45
1:A:156:SER:HB3	1:A:163:ASP:OD1	2.17	0.44
1:A:156:SER:HB2	1:A:158:CYS:H	1.81	0.44
1:B:92:TYR:CD2	1:B:92:TYR:C	2.96	0.43
1:B:27:ASN:HB2	4:B:315:HOH:O	2.18	0.43
1:B:118:PHE:CD2	1:B:131:GLY:HA2	2.54	0.43
1:B:64:LEU:HB3	1:B:74:GLN:HE22	1.84	0.43
1:B:241:LYS:HA	1:B:242:PRO:HD3	1.89	0.43
1:B:84:GLY:O	1:B:113:LYS:HD2	2.18	0.42
1:A:125:ASP:OD1	1:A:126:ASN:N	2.51	0.42
1:B:73:TYR:CG	1:B:109:PRO:HA	2.55	0.42
1:B:78:LEU:HD12	1:B:115:GLN:HB2	2.01	0.42
1:A:172:LYS:HE2	1:A:172:LYS:HB3	1.82	0.42
1:B:107:LYS:HD2	1:B:108:TYR:CE2	2.55	0.42
1:A:187:GLU:O	1:A:254:HIS:HB3	2.20	0.42
1:B:199:LYS:HE3	1:B:218:TYR:CZ	2.55	0.42
1:B:73:TYR:CD1	1:B:109:PRO:HA	2.55	0.41
1:B:78:LEU:CD1	1:B:115:GLN:HB2	2.51	0.40
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.93	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	287/317 (90%)	266 (93%)	20 (7%)	1 (0%)	36 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	287/317 (90%)	274 (96%)	11 (4%)	2 (1%)	18	38
All	All	574/634 (90%)	540 (94%)	31 (5%)	3 (0%)	24	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
1	B	128	SER
1	B	240	GLY

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	256/282 (91%)	252 (98%)	4 (2%)	55	79
1	B	256/282 (91%)	251 (98%)	5 (2%)	48	74
All	All	512/564 (91%)	503 (98%)	9 (2%)	51	76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	169	GLU
1	A	172	LYS
1	A	239	ASN
1	B	127	ASP
1	B	163	ASP
1	B	239	ASN
1	B	274	VAL
1	B	296	SER

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	45	ASN
1	A	52	ASN
1	A	74	GLN
1	A	116	HIS
1	A	145	HIS
1	A	239	ASN
1	A	256	GLN
1	A	262	ASN
1	A	289	HIS
1	B	52	ASN
1	B	74	GLN
1	B	116	HIS
1	B	145	HIS
1	B	221	HIS
1	B	239	ASN
1	B	244	HIS
1	B	256	GLN
1	B	262	ASN
1	B	289	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	289/317 (91%)	0.11	4 (1%) 73 69	39, 57, 72, 84	0
1	B	289/317 (91%)	0.11	3 (1%) 79 76	39, 58, 76, 82	0
All	All	578/634 (91%)	0.11	7 (1%) 76 73	39, 57, 75, 84	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	ASP	3.9
1	B	239	ASN	3.3
1	A	96	VAL	2.7
1	A	128	SER	2.3
1	B	124	PHE	2.3
1	B	159	GLY	2.1
1	A	126	ASN	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, 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($\text{\AA}^2$)	Q<0.9
2	CA	B	404	1/1	0.80	0.22	111,111,111,111	0
2	CA	B	403	1/1	0.86	0.12	94,94,94,94	0
2	CA	A	401	1/1	0.87	0.21	80,80,80,80	0
3	CL	A	406	1/1	0.92	0.24	78,78,78,78	0
3	CL	A	405	1/1	0.95	0.17	62,62,62,62	0
2	CA	A	402	1/1	0.95	0.15	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.