



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:34 AM UTC

PDB ID : 2NYD / pdb_00002nyd
Title : Crystal structure of Staphylococcus aureus hypothetical protein SA1388
Authors : Singh, K.S.; Zhang, X.; Zhang, H.
Deposited on : 2006-11-20
Resolution : 2.00 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

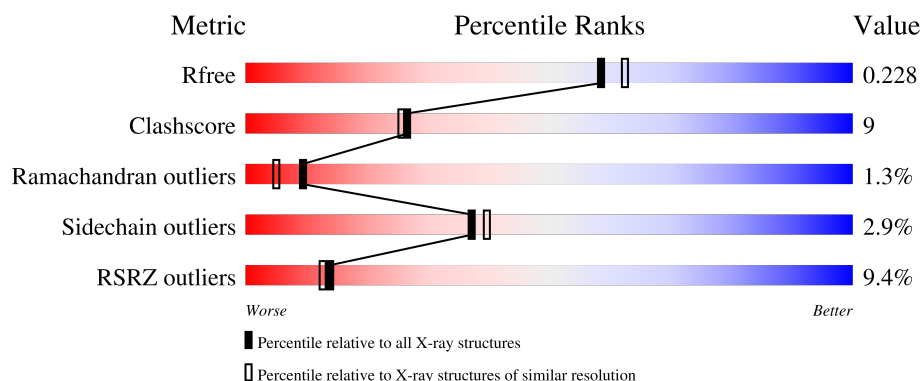
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	370	5% 68% 11% • 19%
1	B	370	12% 78% 15% •• 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5932 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 UPF0135 protein SA1388.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2361	1507	388	454	12			
1	B	348	Total	C	N	O	S	0	0	0
			2718	1739	441	524	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	cloning artifact	UNP P67273
A	-2	MET	-	cloning artifact	UNP P67273
A	-1	ASP	-	cloning artifact	UNP P67273
A	0	PRO	-	cloning artifact	UNP P67273
A	32	GLU	GLY	SEE REMARK 999	UNP P67273
A	115	VAL	ALA	SEE REMARK 999	UNP P67273
B	-3	ALA	-	cloning artifact	UNP P67273
B	-2	MET	-	cloning artifact	UNP P67273
B	-1	ASP	-	cloning artifact	UNP P67273
B	0	PRO	-	cloning artifact	UNP P67273
B	32	GLU	GLY	SEE REMARK 999	UNP P67273
B	115	VAL	ALA	SEE REMARK 999	UNP P67273

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

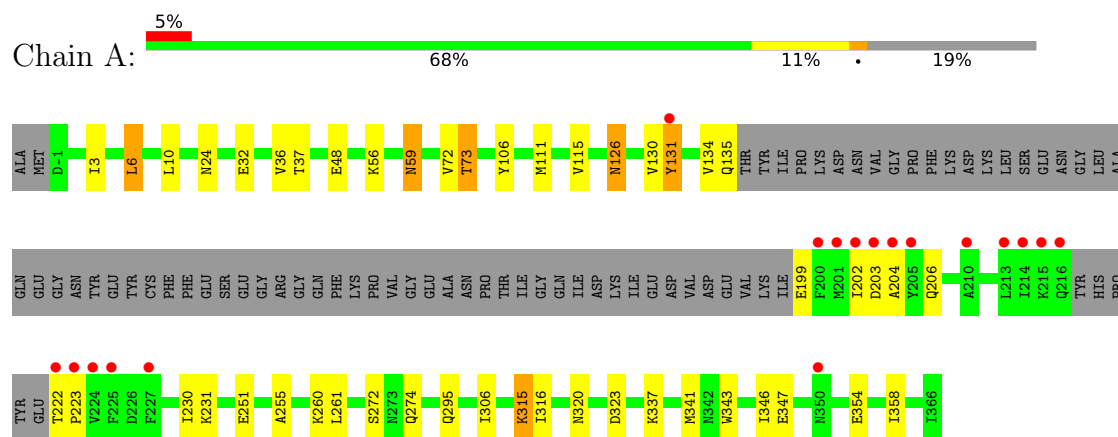
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	419	Total 419	O 419	0	0
3	B	430	Total 430	O 430	0	0

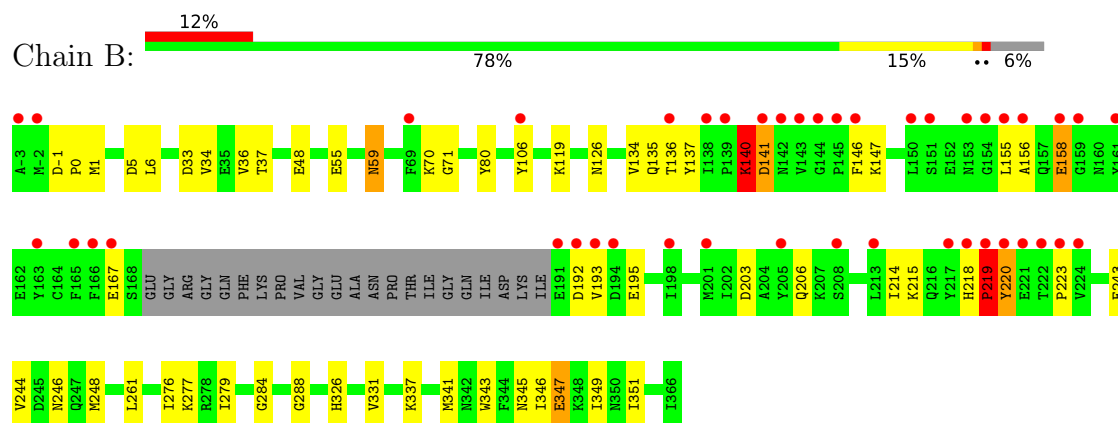
3 Residue-property plots [i](#)

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: UPF0135 protein SA1388



• Molecule 1: UPF0135 protein SA1388



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	132.55Å 132.55Å 125.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.51 – 2.00 84.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (84.51-2.00) 95.0 (84.51-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.231 0.172 , 0.228	Depositor DCC
R_{free} test set	2675 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5932	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 4.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.98	1/2401 (0.0%)	0.97	3/3250 (0.1%)
1	B	0.97	2/2769 (0.1%)	0.95	2/3751 (0.1%)
All	All	0.98	3/5170 (0.1%)	0.96	5/7001 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	276	ILE	CA-CB	6.60	1.62	1.54
1	A	255	ALA	CA-CB	6.56	1.63	1.53
1	B	34	VAL	CA-CB	5.10	1.60	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	GLY	N-CA-C	-6.18	106.96	113.58
1	A	73	THR	CB-CA-C	5.22	118.37	109.24
1	B	193	VAL	N-CA-C	5.10	114.64	106.88
1	A	222	THR	CA-C-N	5.03	126.13	119.84
1	A	222	THR	C-N-CA	5.03	126.13	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	219	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	2361	0	2343	44	0
1	B	2718	0	2668	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	419	0	0	18	0
3	B	430	0	0	17	0
All	All	5932	0	5011	94	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 9.

All (94) 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:346:ILE:HD13	3:A:678:HOH:O	1.10	1.23
1:B:346:ILE:CD1	3:B:832:HOH:O	1.87	1.18
1:B:346:ILE:HD13	3:B:832:HOH:O	1.46	1.06
1:B:33:ASP:HB3	3:B:698:HOH:O	1.59	1.03
1:B:55:GLU:HB3	3:B:689:HOH:O	1.58	1.02
1:B:167:GLU:HB2	1:B:195:GLU:OE1	1.67	0.93
1:A:315:LYS:HE2	3:A:496:HOH:O	1.74	0.88
1:B:0:PRO:HD2	3:B:581:HOH:O	1.79	0.83
1:A:316:ILE:HD11	3:A:451:HOH:O	1.81	0.80
1:B:1:MET:HE2	1:B:351:ILE:HD13	1.62	0.79
1:A:316:ILE:HD13	1:B:80:TYR:CE2	2.18	0.78
1:B:156:ALA:HB2	3:B:799:HOH:O	1.84	0.77
1:B:1:MET:HE2	1:B:351:ILE:CD1	2.16	0.75
1:B:140:LYS:HG3	1:B:141:ASP:H	1.52	0.72
1:B:140:LYS:HG3	1:B:141:ASP:N	2.07	0.69
1:B:203:ASP:H	1:B:206:GLN:HE21	1.42	0.66
1:B:126:ASN:HD22	1:B:126:ASN:H	1.43	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLU:HG3	3:B:439:HOH:O	1.98	0.63
1:B:244:VAL:HG13	1:B:279:ILE:HD11	1.79	0.62
1:A:106:TYR:HD2	3:A:544:HOH:O	1.82	0.62
1:A:111:MET:O	1:A:115:VAL:HG23	1.99	0.62
1:B:218:HIS:HB3	3:B:734:HOH:O	2.00	0.60
1:B:203:ASP:H	1:B:206:GLN:NE2	2.00	0.60
1:A:316:ILE:CD1	1:B:80:TYR:CE2	2.85	0.60
1:A:204:ALA:HA	3:A:790:HOH:O	2.01	0.59
1:B:106:TYR:HE1	3:B:503:HOH:O	1.84	0.59
1:A:135:GLN:NE2	3:A:773:HOH:O	2.36	0.59
1:A:316:ILE:CD1	3:A:451:HOH:O	2.44	0.59
1:B:218:HIS:CG	1:B:219:PRO:HD3	2.37	0.59
1:B:347:GLU:HB3	1:B:349:ILE:HD12	1.84	0.58
1:A:295[B]:GLN:HE21	1:A:295[B]:GLN:HA	1.69	0.58
1:B:243:GLU:OE1	1:B:277:LYS:HE3	2.02	0.58
1:B:218:HIS:CG	1:B:219:PRO:CD	2.87	0.57
1:A:126:ASN:H	1:A:126:ASN:HD22	1.53	0.57
1:B:214:ILE:O	1:B:218:HIS:HB2	2.05	0.56
1:A:337:LYS:HD3	3:A:516:HOH:O	2.05	0.56
1:A:48:GLU:HB3	1:A:358:ILE:HD13	1.89	0.55
1:B:218:HIS:CD2	1:B:219:PRO:HD2	2.44	0.53
1:A:316:ILE:HG13	3:A:607:HOH:O	2.07	0.53
1:B:37:THR:H	1:B:59:ASN:ND2	2.07	0.52
1:B:135:GLN:HB2	3:B:765:HOH:O	2.10	0.52
1:A:202:ILE:HB	1:A:206:GLN:HB2	1.91	0.52
1:B:246:ASN:O	1:B:248:MET:HG3	2.09	0.51
1:A:56:LYS:HE3	1:A:354:GLU:OE1	2.11	0.51
1:A:37:THR:H	1:A:59:ASN:ND2	2.08	0.51
1:A:316:ILE:HD12	1:B:80:TYR:CZ	2.45	0.51
1:B:220:TYR:O	1:B:223:PRO:HD3	2.10	0.51
1:A:3:ILE:HB	1:A:32:GLU:HA	1.93	0.51
1:A:343:TRP:HA	1:A:346:ILE:HD12	1.92	0.51
1:A:295[B]:GLN:HA	1:A:295[B]:GLN:NE2	2.25	0.50
1:A:274:GLN:HE21	1:A:320:ASN:HD21	1.60	0.50
1:A:131:TYR:C	3:A:786:HOH:O	2.55	0.49
1:B:346:ILE:HG13	3:B:558:HOH:O	2.11	0.49
1:A:251:GLU:HB2	1:A:272:SER:HB2	1.94	0.49
1:A:72:VAL:HG13	3:A:772:HOH:O	2.14	0.48
1:A:24:ASN:ND2	3:A:797:HOH:O	2.42	0.48
1:A:316:ILE:CD1	1:B:80:TYR:CZ	2.97	0.47
1:B:70:LYS:O	1:B:71:GLY:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG22	1:A:231:LYS:HD3	1.96	0.47
1:A:115:VAL:HG11	1:A:261:LEU:HD23	1.95	0.47
1:A:306:ILE:HD12	1:A:323:ASP:HB2	1.97	0.46
1:B:48:GLU:HG3	3:B:521:HOH:O	2.14	0.46
1:A:36:VAL:HA	1:A:59:ASN:HD21	1.81	0.46
1:B:126:ASN:H	1:B:126:ASN:ND2	2.11	0.46
1:B:215:LYS:HA	3:B:734:HOH:O	2.15	0.46
1:B:146:PHE:HD1	3:B:709:HOH:O	1.98	0.45
1:B:345:ASN:O	1:B:346:ILE:C	2.60	0.45
1:B:55:GLU:HG3	3:B:508:HOH:O	2.16	0.45
1:B:218:HIS:CD2	1:B:219:PRO:CD	3.01	0.44
1:A:346:ILE:HG12	3:A:817:HOH:O	2.16	0.44
1:B:218:HIS:HD2	1:B:223:PRO:CB	2.31	0.44
1:A:315:LYS:CE	3:A:496:HOH:O	2.46	0.44
1:B:36:VAL:HA	1:B:59:ASN:HD21	1.84	0.43
1:A:316:ILE:HD12	1:B:80:TYR:OH	2.18	0.43
1:B:-1:ASP:OD2	1:B:-1:ASP:N	2.51	0.43
1:B:337:LYS:HE3	1:B:341:MET:SD	2.58	0.43
1:A:134:VAL:O	1:A:199:GLU:HA	2.19	0.43
1:A:316:ILE:CG1	3:A:451:HOH:O	2.67	0.42
1:A:260:LYS:NZ	3:A:689:HOH:O	2.53	0.42
1:A:6:LEU:HD22	1:A:10:LEU:HG	2.01	0.42
1:A:72:VAL:CG1	3:A:772:HOH:O	2.66	0.42
1:A:316:ILE:HG12	3:A:451:HOH:O	2.20	0.42
1:B:343:TRP:HA	1:B:346:ILE:HD12	2.01	0.42
1:B:244:VAL:HG13	1:B:279:ILE:CD1	2.46	0.42
1:B:1:MET:HE2	1:B:351:ILE:HD12	2.01	0.41
1:B:137:TYR:HE1	3:B:765:HOH:O	2.00	0.41
1:B:140:LYS:CG	1:B:141:ASP:H	2.20	0.41
1:B:119:LYS:HB3	3:B:706:HOH:O	2.21	0.41
1:B:1:MET:HG3	1:B:5:ASP:HB2	2.03	0.41
1:A:295[B]:GLN:HE21	1:A:295[B]:GLN:CA	2.32	0.41
1:B:261:LEU:CD2	1:B:331:VAL:HG11	2.50	0.41
1:B:284:GLY:HA2	1:B:326:HIS:CD2	2.56	0.40
1:A:202:ILE:HD12	1:A:203:ASP:O	2.22	0.40
1:A:341:MET:HE2	1:A:341:MET:HB3	1.90	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	295/370 (80%)	285 (97%)	9 (3%)	1 (0%)	36	35
1	B	344/370 (93%)	322 (94%)	15 (4%)	7 (2%)	6	2
All	All	639/740 (86%)	607 (95%)	24 (4%)	8 (1%)	9	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	LYS
1	B	219	PRO
1	B	141	ASP
1	B	155	LEU
1	B	192	ASP
1	B	158	GLU
1	A	223	PRO
1	B	220	TYR

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	259/322 (80%)	251 (97%)	8 (3%)	35	37
1	B	294/322 (91%)	286 (97%)	8 (3%)	39	42
All	All	553/644 (86%)	537 (97%)	16 (3%)	37	40

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

Mol	Chain	Res	Type
1	A	6	LEU
1	A	59	ASN
1	A	73	THR
1	A	126	ASN
1	A	131	TYR
1	A	230	ILE
1	A	315	LYS
1	A	347	GLU
1	B	6	LEU
1	B	59	ASN
1	B	134	VAL
1	B	136	THR
1	B	140	LYS
1	B	147	LYS
1	B	158	GLU
1	B	347	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	59	ASN
1	A	126	ASN
1	A	128	GLN
1	A	206	GLN
1	A	262	ASN
1	A	274	GLN
1	A	317	HIS
1	B	24	ASN
1	B	59	ASN
1	B	78	ASN
1	B	126	ASN
1	B	135	GLN
1	B	160	ASN
1	B	206	GLN
1	B	212	GLN
1	B	218	HIS
1	B	320	ASN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 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	300/370 (81%)	-0.11	18 (6%) 27 26	12, 21, 80, 80	1 (0%)
1	B	348/370 (94%)	0.11	43 (12%) 8 7	11, 21, 76, 80	0
All	All	648/740 (87%)	0.01	61 (9%) 14 13	11, 21, 78, 80	1 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	220	TYR	6.9
1	A	131	TYR	5.5
1	B	-3	ALA	5.0
1	A	224	VAL	4.9
1	B	222	THR	4.8
1	B	142	ASN	4.5
1	A	223	PRO	4.3
1	A	213	LEU	4.1
1	B	150	LEU	4.0
1	B	143	VAL	4.0
1	B	219	PRO	3.9
1	A	214	ILE	3.8
1	B	191	GLU	3.8
1	A	202	ILE	3.8
1	B	154	GLY	3.7
1	B	221	GLU	3.7
1	B	158	GLU	3.5
1	B	193	VAL	3.5
1	B	156	ALA	3.4
1	B	163	TYR	3.3
1	A	200	PHE	3.3
1	B	192	ASP	3.3
1	B	213	LEU	3.2
1	B	166	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	204	ALA	3.1
1	B	145	PRO	3.1
1	B	155	LEU	3.1
1	A	210	ALA	3.1
1	B	167	GLU	3.0
1	B	141	ASP	2.9
1	B	146	PHE	2.9
1	A	201	MET	2.9
1	A	222	THR	2.9
1	B	194	ASP	2.8
1	B	159	GLY	2.8
1	B	139	PRO	2.7
1	A	216	GLN	2.7
1	A	225	PHE	2.6
1	A	203	ASP	2.4
1	B	136	THR	2.4
1	A	205	TYR	2.4
1	B	198	ILE	2.4
1	B	161	TYR	2.3
1	A	215	LYS	2.3
1	A	350	ASN	2.3
1	B	217	TYR	2.2
1	B	151	SER	2.2
1	B	208	SER	2.2
1	B	-2	MET	2.2
1	B	138	ILE	2.2
1	B	144	GLY	2.2
1	B	218	HIS	2.2
1	B	106	TYR	2.2
1	B	165	PHE	2.1
1	B	201	MET	2.1
1	B	205	TYR	2.1
1	B	223	PRO	2.1
1	B	69	PHE	2.1
1	B	224	VAL	2.1
1	A	227	PHE	2.1
1	B	153	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	ZN	A	401	1/1	0.97	0.14	50,50,50,50	0
2	ZN	B	402	1/1	0.97	0.17	47,47,47,47	0
2	ZN	B	401	1/1	0.98	0.14	41,41,41,41	0
2	ZN	A	402	1/1	0.98	0.14	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.