Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 09:35 AM EDT

PDB ID	:	4F1Z
Title	:	Crystal structures reveal the multi-ligand binding mechanism of the Staphylococcus aureus ClfB
Authors	:	Yang, M.J.; Xiang, H.; Wang, J.W.; Liu, B.; Chen, Y.G.; Liu, L.; Deng, X.M.; Feng, Y.
Deposited on	:	2012-05-07
Resolution	:	2.30 Å(reported)

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

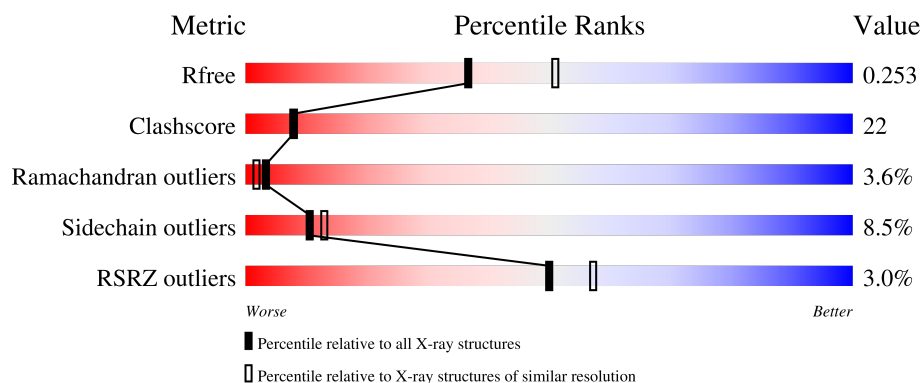|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
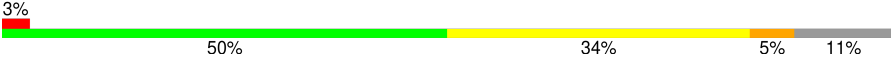*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		22
Ramachandran outliers		3.6%
Sidechain outliers		8.5%
RSRZ outliers		3.0%

Worse　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	363	3% / 50% / 34% / 5% / 11%
2	Q	14	100%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 2594 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 Clumping factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total 2510	C 1575	N 412	O 520	S 3	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	MET	-	expression tag	UNP Q6GDH2
A	181	ARG	-	expression tag	UNP Q6GDH2
A	182	GLY	-	expression tag	UNP Q6GDH2
A	183	SER	-	expression tag	UNP Q6GDH2
A	184	HIS	-	expression tag	UNP Q6GDH2
A	185	HIS	-	expression tag	UNP Q6GDH2
A	186	HIS	-	expression tag	UNP Q6GDH2
A	187	HIS	-	expression tag	UNP Q6GDH2
A	188	HIS	-	expression tag	UNP Q6GDH2
A	189	HIS	-	expression tag	UNP Q6GDH2
A	190	GLU	-	expression tag	UNP Q6GDH2
A	191	ASN	-	expression tag	UNP Q6GDH2
A	192	LEU	-	expression tag	UNP Q6GDH2
A	193	TYR	-	expression tag	UNP Q6GDH2
A	194	PHE	-	expression tag	UNP Q6GDH2
A	195	GLN	-	expression tag	UNP Q6GDH2
A	196	GLY	-	expression tag	UNP Q6GDH2

- Molecule 2 is a protein called peptide from Keratin, type I cytoskeletal 10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	14	Total 72	C 39	N 14	O 19	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total 9	O 9	0	0
4	Q	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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: Clumping factor B
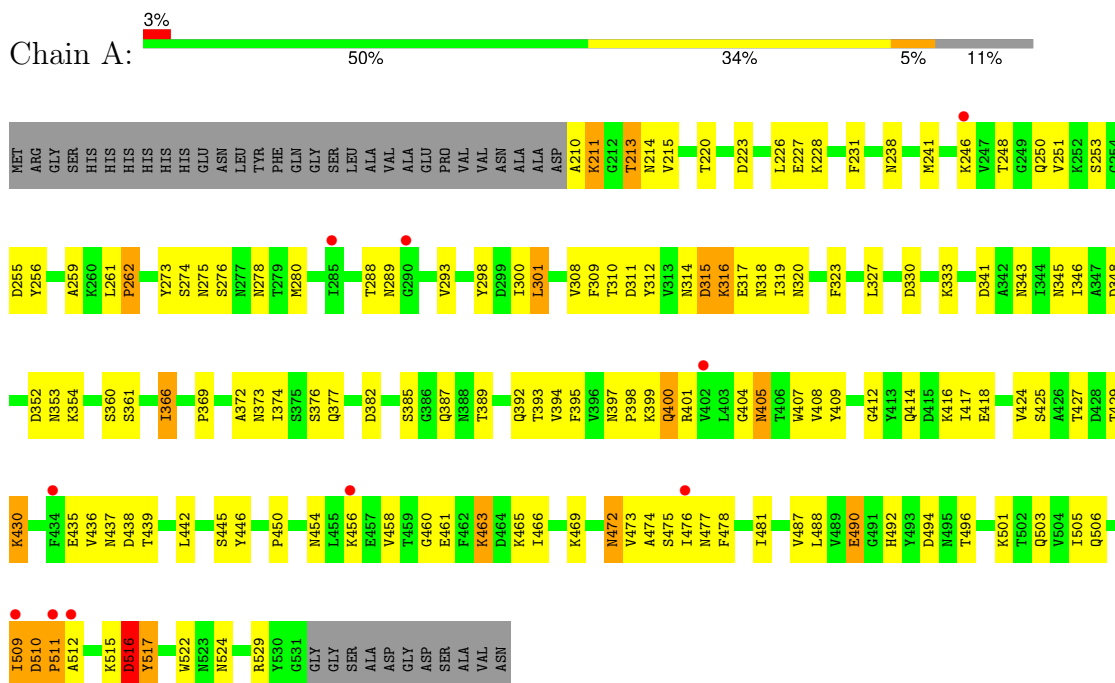
Chain A:

• Molecule 2: peptide from Keratin, type I cytoskeletal 10

Chain Q:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	70.33Å 70.33Å 177.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.19 – 2.30 60.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	77.6 (50.19-2.30) 81.0 (60.91-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.247 , 0.251 0.252 , 0.253	Depositor DCC
R_{free} test set	948 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 56.5	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2594	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG

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	0.42	0/2558	0.60	0/3471
2	Q	0.41	0/72	0.51	0/92
All	All	0.42	0/2630	0.60	0/3563

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2510	0	2410	109	0
2	Q	72	0	55	0	0
3	A	1	0	0	0	0
4	A	9	0	0	0	0
4	Q	2	0	0	0	0
All	All	2594	0	2465	109	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 22.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ASP:HB3	1:A:511:PRO:HA	1.25	1.16
1:A:463:LYS:HD2	1:A:463:LYS:H	1.25	0.98
1:A:238:ASN:HD21	1:A:529:ARG:HE	1.12	0.92
1:A:404:GLY:HA3	1:A:510:ASP:HB2	1.51	0.92
1:A:510:ASP:HB3	1:A:511:PRO:CA	2.01	0.89
1:A:262:PRO:HG3	1:A:343:ASN:O	1.78	0.83
1:A:317:GLU:HG2	1:A:318:ASN:H	1.46	0.81
1:A:389:THR:HG22	1:A:492:HIS:CD2	2.19	0.78
1:A:463:LYS:H	1:A:463:LYS:CD	1.95	0.76
1:A:509:ILE:HG22	1:A:510:ASP:H	1.51	0.76
1:A:210:ALA:O	1:A:211:LYS:HB2	1.86	0.76
1:A:437:ASN:HB3	1:A:454:ASN:ND2	2.00	0.75
1:A:437:ASN:HB3	1:A:454:ASN:HD22	1.52	0.73
1:A:445:SER:O	1:A:446:TYR:HB2	1.86	0.73
1:A:317:GLU:HG2	1:A:318:ASN:N	2.03	0.72
1:A:253:SER:H	1:A:314:ASN:HD21	1.39	0.70
1:A:438:ASP:H	1:A:454:ASN:HD21	1.39	0.69
1:A:475:SER:C	1:A:476:ILE:HD13	2.13	0.69
1:A:392:GLN:HE21	1:A:524:ASN:HD22	1.41	0.68
1:A:460:GLY:HA2	1:A:463:LYS:HE3	1.75	0.67
1:A:430:LYS:HG2	1:A:490:GLU:HG3	1.77	0.66
1:A:238:ASN:ND2	1:A:529:ARG:HE	1.91	0.65
1:A:366:ILE:HG12	1:A:372:ALA:O	1.96	0.65
1:A:314:ASN:O	1:A:315:ASP:HB3	1.98	0.63
1:A:430:LYS:HD3	1:A:490:GLU:HG3	1.80	0.63
1:A:476:ILE:HD13	1:A:476:ILE:N	2.12	0.63
1:A:424:VAL:H	1:A:472:ASN:ND2	1.96	0.63
1:A:273:TYR:CZ	1:A:280:MET:HG3	2.36	0.60
1:A:374:ILE:HG13	1:A:395:PHE:O	2.03	0.59
1:A:509:ILE:HG22	1:A:510:ASP:N	2.17	0.59
1:A:466:ILE:HA	1:A:475:SER:O	2.03	0.59
1:A:345:ASN:HD21	1:A:348:ASP:HA	1.67	0.58
1:A:369:PRO:O	1:A:401:ARG:HD3	2.02	0.58
1:A:214:ASN:OD1	1:A:214:ASN:C	2.42	0.58
1:A:227:GLU:OE1	1:A:228:LYS:HG2	2.04	0.57
1:A:215:VAL:HG22	1:A:256:TYR:O	2.06	0.56
1:A:465:LYS:HE2	1:A:477:ASN:O	2.06	0.56
1:A:298:TYR:CE2	1:A:300:ILE:HD13	2.41	0.55
1:A:314:ASN:O	1:A:315:ASP:CB	2.56	0.54
1:A:438:ASP:N	1:A:454:ASN:HD21	2.07	0.52
1:A:275:ASN:HB2	1:A:382:ASP:OD2	2.10	0.52
1:A:315:ASP:C	1:A:316:LYS:HG2	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:HD21	1:A:529:ARG:NE	1.93	0.52
1:A:430:LYS:CD	1:A:490:GLU:HG3	2.40	0.52
1:A:463:LYS:HD2	1:A:463:LYS:N	2.09	0.52
1:A:389:THR:HG22	1:A:492:HIS:NE2	2.25	0.51
1:A:251:VAL:HB	1:A:255:ASP:OD2	2.11	0.51
1:A:517:TYR:CD2	1:A:517:TYR:C	2.84	0.50
1:A:220:THR:O	1:A:246:LYS:HG2	2.12	0.50
1:A:430:LYS:CG	1:A:490:GLU:HG3	2.42	0.50
1:A:510:ASP:CB	1:A:511:PRO:CA	2.83	0.50
1:A:310:THR:C	1:A:312:TYR:H	2.15	0.49
1:A:494:ASP:OD2	1:A:496:THR:HG23	2.12	0.49
1:A:214:ASN:HB2	1:A:256:TYR:CZ	2.47	0.49
1:A:330:ASP:OD2	1:A:333:LYS:HG2	2.13	0.49
1:A:215:VAL:CG1	1:A:255:ASP:HB3	2.43	0.49
1:A:418:GLU:H	1:A:418:GLU:CD	2.16	0.48
1:A:407:TRP:O	1:A:506:GLN:HA	2.14	0.48
1:A:226:LEU:O	1:A:227:GLU:C	2.51	0.48
1:A:450:PRO:HG3	1:A:488:LEU:HD11	1.95	0.48
1:A:323:PHE:HZ	1:A:346:ILE:HD13	1.79	0.48
1:A:213:THR:O	1:A:256:TYR:CD2	2.67	0.47
1:A:456:LYS:O	1:A:458:VAL:HG13	2.13	0.47
1:A:408:VAL:O	1:A:475:SER:HA	2.15	0.47
1:A:414:GLN:OE1	1:A:501:LYS:HE2	2.14	0.47
1:A:404:GLY:O	1:A:405:ASN:C	2.52	0.47
1:A:250:GLN:HG2	1:A:251:VAL:N	2.30	0.47
1:A:436:VAL:HG21	1:A:442:LEU:HD11	1.96	0.47
1:A:503:GLN:HA	1:A:522:TRP:O	2.15	0.47
1:A:343:ASN:OD1	1:A:352:ASP:OD2	2.33	0.47
1:A:320:ASN:OD1	1:A:320:ASN:N	2.46	0.46
1:A:425:SER:O	1:A:429:THR:HB	2.15	0.46
1:A:416:LYS:HB3	1:A:418:GLU:OE2	2.16	0.46
1:A:424:VAL:H	1:A:472:ASN:HD22	1.63	0.46
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.68	0.46
1:A:450:PRO:HG3	1:A:488:LEU:CD1	2.46	0.46
1:A:274:SER:HA	1:A:278:ASN:ND2	2.31	0.46
1:A:515:LYS:O	1:A:516:ASP:C	2.54	0.45
1:A:397:ASN:N	1:A:398:PRO:CD	2.80	0.45
1:A:259:ALA:HA	1:A:345:ASN:O	2.16	0.45
1:A:511:PRO:O	1:A:512:ALA:HB3	2.16	0.45
1:A:385:SER:OG	1:A:387:GLN:HB2	2.17	0.45
1:A:210:ALA:O	1:A:211:LYS:CB	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:SER:HA	1:A:393:THR:O	2.18	0.44
1:A:494:ASP:CG	1:A:496:THR:HG23	2.39	0.44
1:A:315:ASP:OD1	1:A:316:LYS:HG2	2.17	0.43
1:A:298:TYR:HE2	1:A:300:ILE:CD1	2.31	0.43
1:A:308:VAL:O	1:A:308:VAL:HG13	2.19	0.42
1:A:409:TYR:HA	1:A:474:ALA:O	2.19	0.42
1:A:439:THR:HA	1:A:442:LEU:HD12	2.01	0.42
1:A:473:VAL:HG22	1:A:474:ALA:N	2.34	0.42
1:A:394:VAL:HB	1:A:487:VAL:HB	2.01	0.42
1:A:424:VAL:N	1:A:472:ASN:ND2	2.64	0.42
1:A:341:ASP:OD1	1:A:354:LYS:NZ	2.48	0.42
1:A:377:GLN:O	1:A:392:GLN:HG3	2.20	0.42
1:A:215:VAL:HG11	1:A:255:ASP:HB3	2.01	0.42
1:A:412:GLY:HA3	1:A:472:ASN:ND2	2.34	0.42
1:A:478:PHE:HB3	1:A:481:ILE:HG21	2.02	0.42
1:A:298:TYR:CE2	1:A:300:ILE:CD1	3.03	0.42
1:A:360:SER:O	1:A:361:SER:C	2.57	0.42
1:A:460:GLY:O	1:A:463:LYS:HD3	2.20	0.41
1:A:463:LYS:HB3	1:A:463:LYS:HE2	1.65	0.41
1:A:241:MET:HB3	1:A:327:LEU:HD11	2.03	0.41
1:A:231:PHE:CE1	1:A:238:ASN:HA	2.55	0.41
1:A:399:LYS:C	1:A:400:GLN:HG3	2.41	0.41
1:A:445:SER:O	1:A:446:TYR:CB	2.60	0.41
1:A:392:GLN:HE21	1:A:524:ASN:ND2	2.13	0.41
1:A:330:ASP:CG	1:A:333:LYS:HB2	2.41	0.41
1:A:293:VAL:HG22	1:A:312:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

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	320/363 (88%)	276 (86%)	32 (10%)	12 (4%)	3	1
2	Q	12/14 (86%)	12 (100%)	0	0	100	100
All	All	332/377 (88%)	288 (87%)	32 (10%)	12 (4%)	3	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	LYS
1	A	315	ASP
1	A	510	ASP
1	A	248	THR
1	A	311	ASP
1	A	405	ASN
1	A	516	ASP
1	A	469	LYS
1	A	509	ILE
1	A	309	PHE
1	A	262	PRO
1	A	511	PRO

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	279/309 (90%)	255 (91%)	24 (9%)	10	12
2	Q	5/5 (100%)	5 (100%)	0	100	100
All	All	284/314 (90%)	260 (92%)	24 (8%)	10	13

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	THR
1	A	223	ASP
1	A	261	LEU
1	A	276	SER

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Mol	Chain	Res	Type
1	A	288	THR
1	A	289	ASN
1	A	301	LEU
1	A	316	LYS
1	A	319	ILE
1	A	353	ASN
1	A	366	ILE
1	A	373	ASN
1	A	400	GLN
1	A	417	ILE
1	A	427	THR
1	A	430	LYS
1	A	435	GLU
1	A	461	GLU
1	A	463	LYS
1	A	472	ASN
1	A	490	GLU
1	A	505	ILE
1	A	516	ASP
1	A	517	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	244	ASN
1	A	314	ASN
1	A	345	ASN
1	A	451	ASN
1	A	454	ASN
1	A	472	ASN
1	A	524	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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	322/363 (88%)	0.46	10 (3%)	49	56	49, 87, 139, 178	0
2	Q	14/14 (100%)	0.20	0	100	100	55, 71, 114, 124	0
All	All	336/377 (89%)	0.45	10 (2%)	50	57	49, 87, 139, 178	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	ALA	3.9
1	A	246	LYS	3.6
1	A	509	ILE	3.5
1	A	434	PHE	2.6
1	A	511	PRO	2.3
1	A	290	GLY	2.1
1	A	285	ILE	2.1
1	A	456	LYS	2.0
1	A	402	VAL	2.0
1	A	476	ILE	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 ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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(Å^2)	Q<0.9
3	MG	A	601	1/1	0.75	0.12	72,72,72,72	0

6.5   Other polymers ⓘ

There are no such residues in this entry.