



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:36 am BST

PDB ID : 6HC6  
Title : The structure of BSAP, a zinc aminopeptidase from *Bacillus subtilis*  
Authors : Rogoulenko, E.; Lansky, S.; Faygenboim, R.; Cohen, T.; Alhadeff, R.; Shoham, Y.; Shoham, G.  
Deposited on : 2018-08-14  
Resolution : 1.77 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

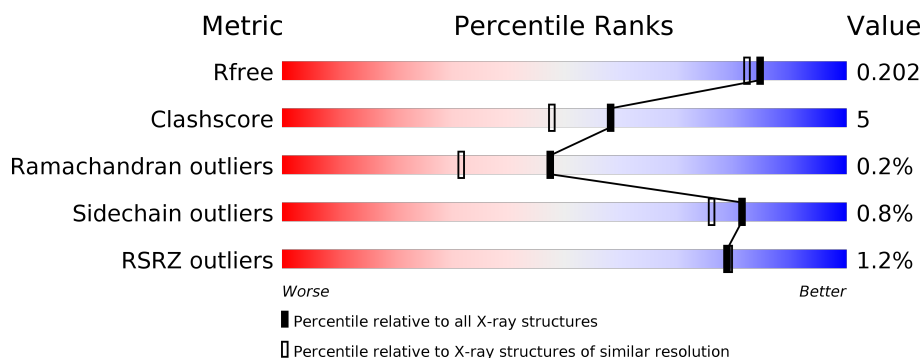
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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))
$R_{free}$	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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  $\geq 3$ , 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	455	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>8%</span> <span>11%</span> </div> </div>
1	B	455	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>8%</span> <span>11%</span> </div> </div>
1	C	455	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">3%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>78%</span> <span>11%</span> <span>10%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	505	-	-	X	X
3	ACT	B	503	-	-	X	-
4	GOL	C	511	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10584 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 Aminopeptidase YwaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3129	1972	531	621	5			
1	B	407	Total	C	N	O	S	0	2	0
			3135	1977	532	621	5			
1	C	408	Total	C	N	O	S	0	10	0
			3185	2014	535	629	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

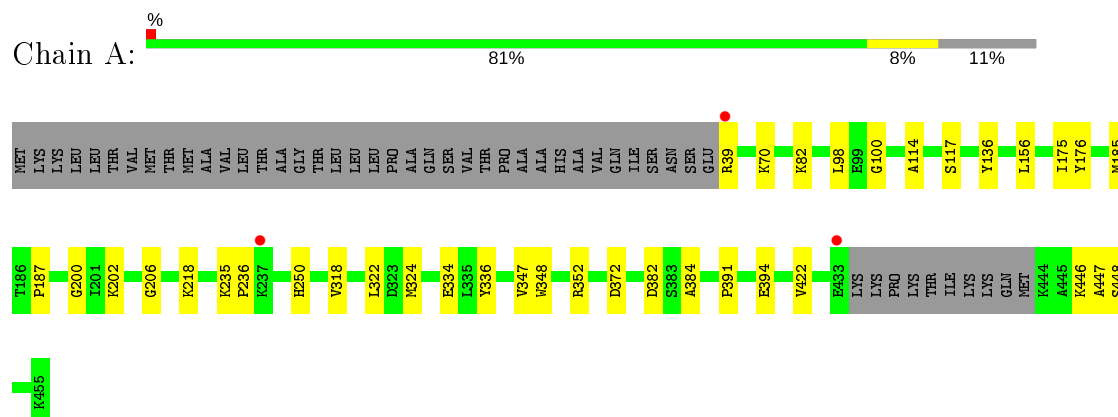
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	333	Total	O	0	0
			333	333		
5	B	377	Total	O	0	0
			377	377		
5	C	337	Total	O	0	0
			337	337		

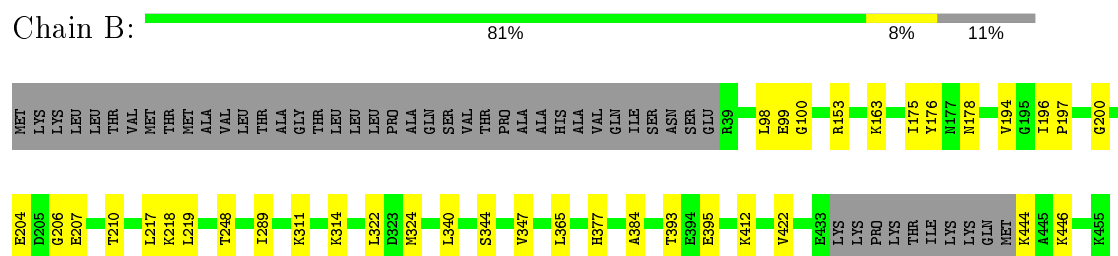
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

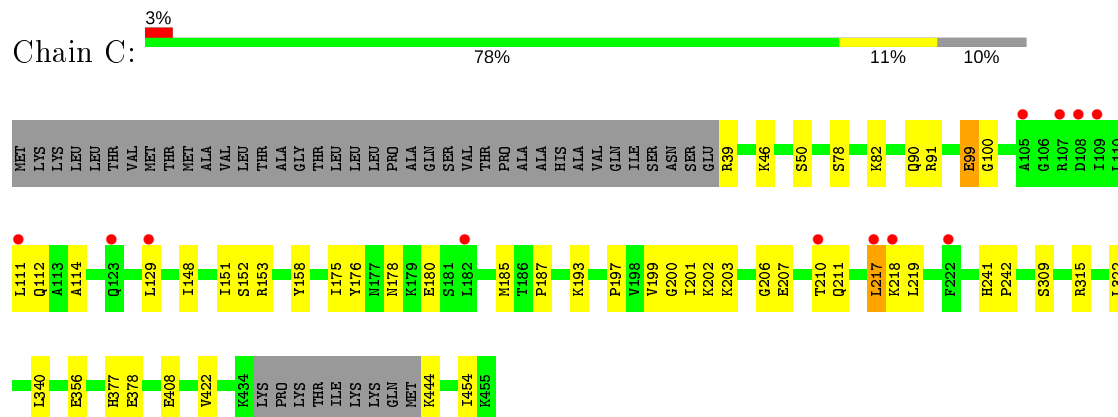
#### • Molecule 1: Aminopeptidase YwaD



#### • Molecule 1: Aminopeptidase YwaD



#### • Molecule 1: Aminopeptidase YwaD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.92Å 224.92Å 42.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.70 – 1.77 48.70 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.70-1.77) 100.0 (48.70-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.165 , 0.203 0.165 , 0.202	Depositor DCC
$R_{free}$ test set	2902 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10584	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, ACT

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	0.37	0/3189	0.53	0/4308
1	B	0.42	0/3198	0.55	0/4319
1	C	0.50	0/3270	0.57	0/4415
All	All	0.44	0/9657	0.55	0/13042

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	3129	0	3119	28	0
1	B	3135	0	3133	26	0
1	C	3185	0	3202	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	16	0	12	3	0
3	B	8	0	6	3	0
3	C	16	0	12	1	0
4	B	12	0	16	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	30	0	40	7	0
5	A	333	0	0	2	0
5	B	377	0	0	2	0
5	C	337	0	0	8	0
All	All	10584	0	9540	92	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 5.

All (92) 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:B:322:LEU:HD21	1:B:422[A]:VAL:HG11	1.64	0.79
1:C:322:LEU:HD21	1:C:422[A]:VAL:HG11	1.68	0.73
1:A:446:LYS:HD3	1:A:448:SER:H	1.55	0.72
1:A:322:LEU:HD21	1:A:422[A]:VAL:HG11	1.77	0.67
1:C:153:ARG:NH1	1:C:158:TYR:OH	2.26	0.67
1:C:378[A]:GLU:OE1	1:C:444:LYS:N	2.31	0.63
1:A:136:TYR:CE1	1:A:156:LEU:HD21	2.34	0.63
1:A:39:ARG:NH2	1:B:412:LYS:H	1.97	0.62
1:A:202:LYS:NZ	5:A:603:HOH:O	2.34	0.61
1:B:207:GLU:O	1:B:210:THR:HG22	2.01	0.60
1:C:90:GLN:HE21	4:C:511:GOL:H2	1.66	0.60
1:A:39:ARG:HH22	1:B:412:LYS:H	1.49	0.59
1:A:114:ALA:HB2	1:A:187:PRO:HG2	1.85	0.58
1:C:152:SER:HB2	1:C:176:TYR:CZ	2.39	0.58
1:A:318:VAL:HG23	1:A:347:VAL:HG22	1.85	0.57
1:C:39:ARG:NH1	5:C:605:HOH:O	2.33	0.56
1:B:197:PRO:HB3	1:B:219:LEU:HD12	1.87	0.56
1:B:217:LEU:HD11	1:B:219:LEU:HG	1.87	0.55
1:C:241:HIS:HB3	1:C:315:ARG:HD3	1.88	0.55
1:A:336:TYR:CZ	1:A:394:GLU:HG2	2.41	0.55
1:C:100:GLY:HA3	1:C:218:LYS:O	2.05	0.55
1:C:111:LEU:HD23	1:C:201:ILE:HG22	1.89	0.54
1:A:348:TRP:HE1	3:A:505:ACT:C	2.21	0.54
1:B:153:ARG:HD3	1:B:178:ASN:OD1	2.08	0.54
1:B:340:LEU:HD23	1:B:377:HIS:CD2	2.44	0.53
1:A:318:VAL:CG2	1:A:347:VAL:HG22	2.40	0.53
3:B:504:ACT:H3	1:C:50:SER:OG	2.08	0.52
1:C:153:ARG:HD2	1:C:158:TYR:OH	2.09	0.52
1:C:112:GLN:HG3	5:C:692:HOH:O	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:HA	1:C:99:GLU:OE1	2.09	0.52
1:C:309:SER:OG	4:C:510:GOL:H2	2.10	0.51
1:A:235:LYS:HG3	1:A:236:PRO:HD2	1.93	0.51
1:A:347:VAL:HG11	1:A:384:ALA:HB3	1.92	0.51
1:B:347:VAL:HG11	1:B:384:ALA:HB3	1.92	0.50
1:B:365:LEU:HD23	4:B:506:GOL:H31	1.93	0.50
1:C:114:ALA:HB2	1:C:187:PRO:HG2	1.94	0.50
1:C:111:LEU:HD22	1:C:199:VAL:HB	1.93	0.50
1:C:197:PRO:HB3	1:C:219:LEU:HD12	1.94	0.48
1:C:210:THR:OG1	1:C:211:GLN:HG3	2.13	0.48
1:B:344:SER:H	4:B:506:GOL:H12	1.78	0.48
1:C:151:ILE:O	1:C:175:ILE:HA	2.14	0.48
1:C:46:LYS:HE3	4:C:507:GOL:H12	1.96	0.48
1:B:393:THR:HB	1:B:395:GLU:HG2	1.96	0.48
1:C:203:LYS:HE2	1:C:207:GLU:OE2	2.13	0.47
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.68	0.47
1:C:175:ILE:O	1:C:200:GLY:HA2	2.15	0.47
1:A:352:ARG:HD3	3:A:505:ACT:OXT	2.14	0.46
1:C:129:LEU:HD23	1:C:148:ILE:HB	1.96	0.46
1:A:98:LEU:HD11	1:A:117:SER:O	2.14	0.46
1:B:393:THR:CB	1:B:395:GLU:HG2	2.45	0.46
1:C:340:LEU:HD23	1:C:377:HIS:CD2	2.51	0.46
1:A:446:LYS:HE3	1:A:448:SER:HB3	1.98	0.46
1:A:82:LYS:HB3	1:A:82:LYS:HE2	1.88	0.46
1:B:100:GLY:HA3	1:B:218:LYS:O	2.17	0.45
1:C:454[A]:ILE:HG12	5:C:821:HOH:O	2.15	0.45
1:C:90:GLN:HE21	4:C:511:GOL:C2	2.29	0.45
1:C:46:LYS:CE	4:C:507:GOL:H12	2.47	0.45
1:C:176:TYR:CG	1:C:206:GLY:HA3	2.51	0.45
1:A:446:LYS:HZ2	1:A:447:ALA:HB3	1.83	0.44
1:B:175:ILE:O	1:B:200:GLY:HA2	2.17	0.44
1:B:446:LYS:HE3	1:B:446:LYS:HB2	1.76	0.44
1:A:250:HIS:HB3	1:A:372:ASP:OD1	2.18	0.44
1:A:39:ARG:HH22	1:B:412:LYS:N	2.15	0.44
1:A:446:LYS:CD	1:A:448:SER:H	2.29	0.44
1:A:100:GLY:HA3	1:A:218:LYS:O	2.18	0.43
1:C:90:GLN:HG3	4:C:511:GOL:H2	2.00	0.43
1:B:248:THR:HG22	1:B:289:ILE:HB	1.99	0.43
1:C:202:LYS:HG3	5:C:610:HOH:O	2.18	0.43
1:A:446:LYS:HD3	1:A:448:SER:N	2.29	0.43
1:A:70:LYS:HE2	5:A:608:HOH:O	2.19	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:THR:OG1	1:B:395:GLU:HG2	2.19	0.43
1:B:204:GLU:HB3	5:B:646:HOH:O	2.18	0.42
1:C:193:LYS:NZ	5:C:630:HOH:O	2.52	0.42
1:B:311:LYS:HD2	3:B:503:ACT:H1	2.01	0.42
1:C:242:PRO:O	1:C:315:ARG:HD2	2.19	0.42
1:C:180:GLU:N	5:C:618:HOH:O	2.44	0.42
1:C:153:ARG:HG2	1:C:178:ASN:OD1	2.19	0.42
1:C:217:LEU:HD22	1:C:219:LEU:HG	2.00	0.42
1:C:356:GLU:HG3	5:C:756:HOH:O	2.19	0.42
1:C:78:SER:O	1:C:82:LYS:HG3	2.20	0.42
1:B:176:TYR:CG	1:B:206:GLY:HA3	2.54	0.42
1:A:175:ILE:O	1:A:200:GLY:HA2	2.20	0.41
1:B:163:LYS:HE2	5:B:938:HOH:O	2.20	0.41
1:B:98:LEU:C	1:B:99:GLU:HG2	2.40	0.41
1:A:176:TYR:CG	1:A:206:GLY:HA3	2.56	0.41
1:C:91:ARG:NH2	3:C:504:ACT:O	2.53	0.41
1:A:334:GLU:HB2	1:A:391:PRO:HB3	2.02	0.41
1:C:207:GLU:HA	1:C:210:THR:HG23	2.03	0.40
1:A:352:ARG:HD3	3:A:505:ACT:C	2.51	0.40
1:B:311:LYS:HD2	3:B:503:ACT:CH3	2.52	0.40
4:C:511:GOL:H12	5:C:682:HOH:O	2.20	0.40
1:B:194:VAL:HG12	1:B:196:ILE:H	1.85	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	404/455 (89%)	397 (98%)	6 (2%)	1 (0%)	47	32
1	B	405/455 (89%)	396 (98%)	8 (2%)	1 (0%)	47	32
1	C	414/455 (91%)	403 (97%)	11 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1223/1365 (90%)	1196 (98%)	25 (2%)	2 (0%)	47 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	MET
1	B	324	MET

### 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	336/376 (89%)	334 (99%)	2 (1%)	86 82
1	B	337/376 (90%)	335 (99%)	2 (1%)	86 82
1	C	346/376 (92%)	340 (98%)	6 (2%)	60 48
All	All	1019/1128 (90%)	1009 (99%)	10 (1%)	81 68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	MET
1	A	382	ASP
1	B	314	LYS
1	B	444	LYS
1	C	99	GLU
1	C	185[A]	MET
1	C	185[B]	MET
1	C	217	LEU
1	C	408[A]	GLU
1	C	408[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	A	504	-	1,3,3	5.70	1 (100%)	0,3,3	0.00	-
4	GOL	B	506	-	5,5,5	0.96	0	5,5,5	0.98	0
3	ACT	C	504	-	1,3,3	7.14	1 (100%)	0,3,3	0.00	-
3	ACT	C	503	-	1,3,3	5.93	1 (100%)	0,3,3	0.00	-
4	GOL	B	505	-	5,5,5	0.88	0	5,5,5	0.99	0
3	ACT	A	505	1	1,3,3	7.13	1 (100%)	0,3,3	0.00	-
4	GOL	C	508	-	5,5,5	0.90	0	5,5,5	0.98	0
3	ACT	C	505	-	1,3,3	7.03	1 (100%)	0,3,3	0.00	-
4	GOL	C	511	-	5,5,5	0.99	0	5,5,5	0.86	0
3	ACT	C	506	-	1,3,3	6.65	1 (100%)	0,3,3	0.00	-
3	ACT	B	504	-	1,3,3	7.13	1 (100%)	0,3,3	0.00	-
3	ACT	A	506	-	1,3,3	1.17	0	0,3,3	0.00	-
4	GOL	C	509	-	5,5,5	0.87	0	5,5,5	1.01	0
3	ACT	B	503	-	1,3,3	5.15	1 (100%)	0,3,3	0.00	-
3	ACT	A	503	-	1,3,3	7.01	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	C	510	-	5,5,5	0.89	0	5,5,5	0.94	0
4	GOL	C	507	-	5,5,5	1.00	0	5,5,5	1.06	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	506	-	-	0/4/4/4	-
4	GOL	B	505	-	-	0/4/4/4	-
4	GOL	C	508	-	-	0/4/4/4	-
4	GOL	C	511	-	-	2/4/4/4	-
4	GOL	C	509	-	-	4/4/4/4	-
4	GOL	C	510	-	-	3/4/4/4	-
4	GOL	C	507	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	504	ACT	CH3-C	7.14	1.57	1.48
3	B	504	ACT	CH3-C	7.13	1.57	1.48
3	A	505	ACT	CH3-C	7.13	1.57	1.48
3	C	505	ACT	CH3-C	7.03	1.57	1.48
3	A	503	ACT	CH3-C	7.01	1.57	1.48
3	C	506	ACT	CH3-C	6.65	1.57	1.48
3	C	503	ACT	CH3-C	5.93	1.56	1.48
3	A	504	ACT	CH3-C	5.70	1.56	1.48
3	B	503	ACT	CH3-C	5.15	1.55	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	507	GOL	C3-C2-C1	-2.07	103.65	111.70

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	511	GOL	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	C	507	GOL	C1-C2-C3-O3
4	C	510	GOL	O2-C2-C3-O3
4	C	507	GOL	O2-C2-C3-O3
4	C	510	GOL	C1-C2-C3-O3
4	C	509	GOL	O1-C1-C2-C3
4	C	511	GOL	O2-C2-C3-O3
4	C	510	GOL	O1-C1-C2-O2
4	C	509	GOL	O2-C2-C3-O3
4	C	509	GOL	O1-C1-C2-O2
4	C	509	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	506	GOL	2	0
3	C	504	ACT	1	0
3	A	505	ACT	3	0
4	C	511	GOL	4	0
3	B	504	ACT	1	0
3	B	503	ACT	2	0
4	C	510	GOL	1	0
4	C	507	GOL	2	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/455 (89%)	-0.37	3 (0%) 87 88	14, 30, 52, 89	0
1	B	407/455 (89%)	-0.30	0 100 100	14, 29, 51, 79	0
1	C	408/455 (89%)	-0.09	12 (2%) 51 50	15, 28, 66, 89	0
All	All	1222/1365 (89%)	-0.25	15 (1%) 79 79	14, 29, 59, 89	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	LEU	3.6
1	A	39	ARG	3.4
1	C	109	ILE	3.4
1	C	111	LEU	3.2
1	C	129	LEU	3.0
1	C	108	ASP	3.0
1	C	107	ARG	2.9
1	C	123	GLN	2.9
1	A	433	GLU	2.8
1	C	182	LEU	2.5
1	C	210	THR	2.2
1	C	218	LYS	2.2
1	C	222	PHE	2.1
1	C	105	ALA	2.1
1	A	237	LYS	2.1

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
3	ACT	A	505	4/4	0.21	0.40	53,62,63,65	0
4	GOL	B	506	6/6	0.65	0.30	51,58,66,71	0
3	ACT	A	506	4/4	0.71	0.34	20,20,20,20	0
4	GOL	C	508	6/6	0.76	0.21	65,68,69,71	0
4	GOL	C	509	6/6	0.77	0.13	68,68,71,73	0
4	GOL	B	505	6/6	0.80	0.21	58,75,80,83	0
4	GOL	C	510	6/6	0.81	0.16	61,64,65,70	0
4	GOL	C	511	6/6	0.84	0.22	49,57,63,69	0
3	ACT	B	504	4/4	0.85	0.15	37,47,47,62	0
3	ACT	C	505	4/4	0.86	0.15	50,52,55,62	0
3	ACT	A	503	4/4	0.87	0.13	56,59,60,61	0
3	ACT	C	504	4/4	0.88	0.19	34,36,45,46	0
3	ACT	B	503	4/4	0.90	0.14	37,38,45,53	0
3	ACT	C	506	4/4	0.91	0.10	62,63,63,66	0
4	GOL	C	507	6/6	0.91	0.14	42,52,61,65	0
3	ACT	A	504	4/4	0.94	0.08	51,54,57,60	0
3	ACT	C	503	4/4	0.98	0.12	30,37,50,52	0
2	ZN	C	501	1/1	0.99	0.05	19,19,19,19	0
2	ZN	B	501	1/1	0.99	0.06	18,18,18,18	0
2	ZN	A	501	1/1	0.99	0.04	19,19,19,19	0
2	ZN	C	502	1/1	0.99	0.04	21,21,21,21	0
2	ZN	A	502	1/1	1.00	0.04	21,21,21,21	0
2	ZN	B	502	1/1	1.00	0.05	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.