



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:25 PM BST

PDB ID : 4FN6  
Title : Structural Characterization of Thiaminase type II TenA from *Staphylococcus aureus*  
Authors : Begum, A.; Drebes, J.; Perbandt, M.; Wrenger, C.; Betzel, C.  
Deposited on : 2012-06-19  
Resolution : 2.69 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.

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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	:	2.13
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)	:	2.13

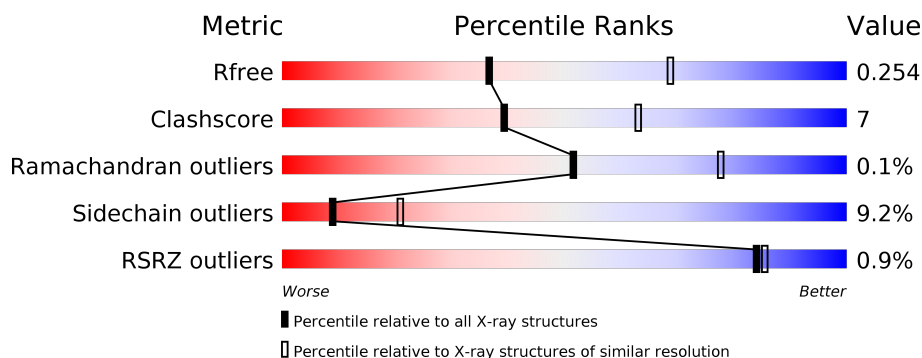
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	229	<div> <div>79%</div> <div>18%</div> <div>..</div> </div>
1	B	229	<div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	C	229	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	D	229	<div> <div>3%</div> <div>72%</div> <div>23%</div> <div>..</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CME	B	137	-	-	-	X
2	ACT	A	301	-	-	-	X
2	ACT	C	304	-	-	-	X

## 2 Entry composition [i](#)

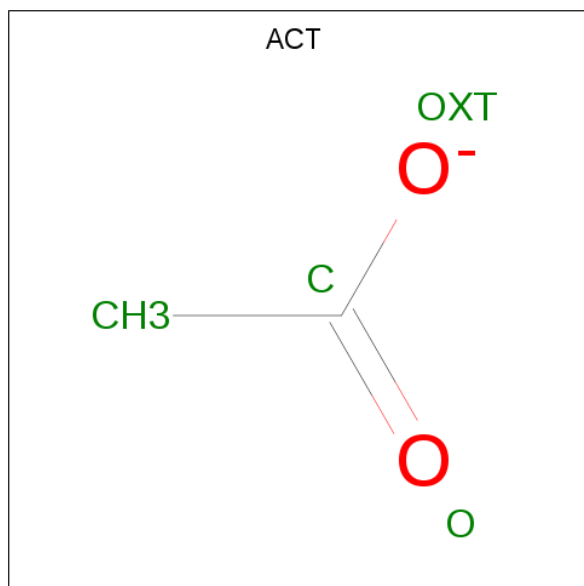
There are 4 unique types of molecules in this entry. The entry contains 7598 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 thiaminase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	4	2	0
			1875	1209	299	352	15			
1	B	225	Total	C	N	O	S	20	1	0
			1864	1200	299	350	15			
1	C	224	Total	C	N	O	S	30	0	0
			1854	1193	297	349	15			
1	D	225	Total	C	N	O	S	29	1	0
			1864	1199	298	352	15			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

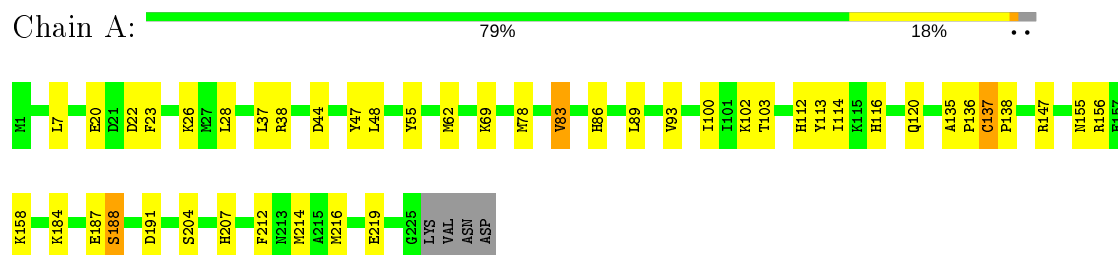
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total 32	O 32	0	0
4	B	16	Total 16	O 16	0	0
4	C	16	Total 16	O 16	0	0
4	D	17	Total 17	O 17	0	0

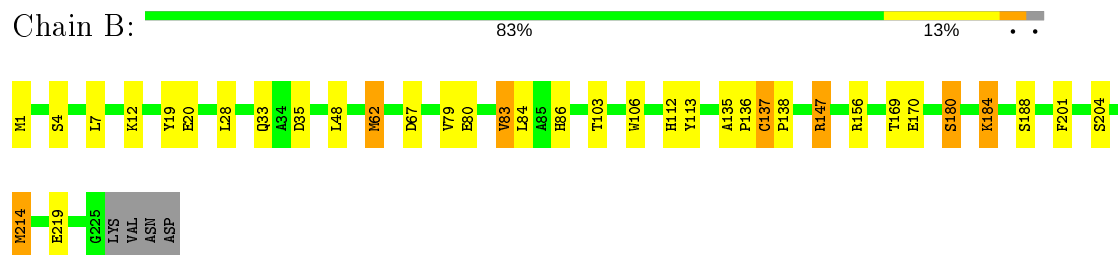
### 3 Residue-property plots [i](#)

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.

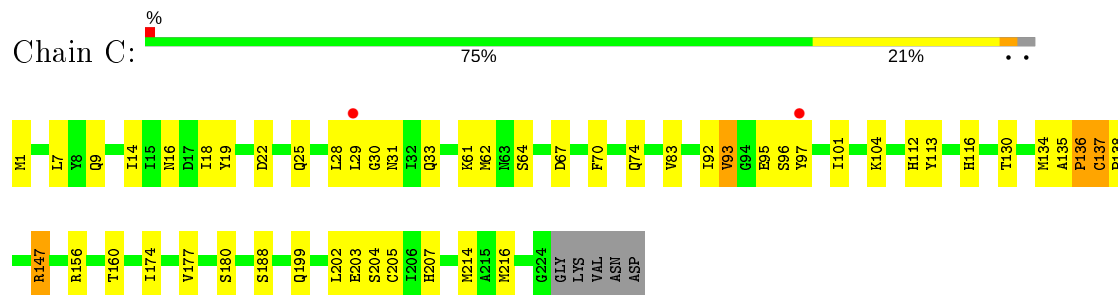
- Molecule 1: thiaminase-2



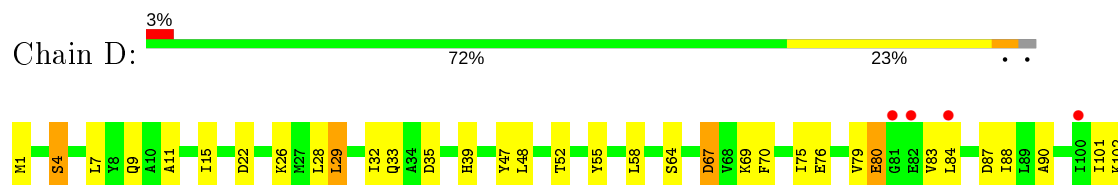
- Molecule 1: thiaminase-2



- Molecule 1: thiaminase-2



- Molecule 1: thiaminase-2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.28Å 104.06Å 109.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.69 29.87 – 2.69	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.87-2.69) 90.8 (29.87-2.69)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.49 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.213 , 0.258 0.211 , 0.254	Depositor DCC
$R_{free}$ test set	2002 reflections (6.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 36.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CME, 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	0.53	0/1911	0.58	0/2575
1	B	0.52	0/1899	0.56	0/2558
1	C	0.48	0/1886	0.57	0/2541
1	D	0.49	0/1899	0.54	0/2558
All	All	0.50	0/7595	0.57	0/10232

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 [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	1875	0	1827	28	0
1	B	1864	0	1820	20	0
1	C	1854	0	1805	23	0
1	D	1864	0	1813	41	0
2	A	8	0	6	2	0
2	B	8	0	6	0	0
2	C	8	0	6	1	0
2	D	12	0	9	0	0
3	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	1	0
3	C	12	0	16	0	0
4	A	32	0	0	4	0
4	B	16	0	0	0	0
4	C	16	0	0	0	0
4	D	17	0	0	0	0
All	All	7598	0	7324	108	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 7.

All (108) 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:137:CME:HB2	1:B:138:PRO:HD3	1.29	1.09
1:D:136:PRO:HG2	1:D:204:SER:HB3	1.37	1.03
1:D:138:PRO:HB3	1:D:171:MET:SD	2.04	0.98
1:B:137:CME:CB	1:B:138:PRO:HD3	1.92	0.95
1:D:138:PRO:CB	1:D:171:MET:SD	2.72	0.77
1:B:137:CME:HB2	1:B:138:PRO:CD	2.17	0.67
1:A:136:PRO:HG2	1:A:204:SER:HB2	1.75	0.67
1:D:135:ALA:O	1:D:137:CME:N	2.28	0.66
1:B:137:CME:CB	1:B:138:PRO:CD	2.74	0.65
1:C:93:VAL:HG22	1:C:95:GLU:H	1.61	0.64
1:D:138:PRO:HB2	1:D:171:MET:CG	2.28	0.64
1:A:191:ASP:H	2:A:301:ACT:H2	1.65	0.61
1:C:92:ILE:HD13	1:C:160:THR:HG22	1.83	0.61
1:D:136:PRO:HG2	1:D:204:SER:CB	2.23	0.60
1:D:138:PRO:CB	1:D:171:MET:CG	2.79	0.60
1:A:214:MET:HG3	1:A:219:GLU:HB3	1.84	0.60
1:C:135:ALA:O	1:C:138:PRO:HD2	2.03	0.59
1:D:138:PRO:HB2	1:D:171:MET:HG3	1.84	0.58
1:D:75:ILE:O	1:D:79:VAL:HG23	2.03	0.58
1:D:47:TYR:CD1	1:D:114:ILE:HG13	2.39	0.58
1:A:47[B]:TYR:HD2	1:A:114:ILE:HD11	1.68	0.58
1:C:137:CME:HE2	2:C:304:ACT:C	2.33	0.58
1:D:39:HIS:CD2	1:D:218:LEU:HA	2.39	0.57
1:C:14:ILE:HG21	1:C:205:CYS:HB3	1.86	0.57
1:D:39:HIS:CE1	1:D:105:VAL:HG11	2.39	0.57
1:C:130:THR:O	1:C:134:MET:HG3	2.05	0.57
1:D:135:ALA:C	1:D:137:CME:N	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HG2	1:A:204:SER:CB	2.35	0.56
1:A:188:SER:OG	4:A:415:HOH:O	2.18	0.56
1:C:199:GLN:O	1:C:203:GLU:HG3	2.05	0.55
1:C:14:ILE:O	1:C:18:ILE:HG13	2.07	0.55
1:A:22:ASP:N	3:A:303:GOL:O2	2.31	0.55
1:A:44:ASP:O	1:A:47[B]:TYR:HD1	1.90	0.54
1:D:138:PRO:CG	1:D:171:MET:HB3	2.38	0.54
1:D:28:LEU:HD12	1:D:154:LEU:HD12	1.90	0.54
1:D:55:TYR:HA	1:D:58:LEU:HD12	1.90	0.54
1:A:48:LEU:HA	4:A:429:HOH:O	2.08	0.53
1:C:19:TYR:CZ	1:C:147:ARG:HD2	2.44	0.53
1:B:169:THR:OG1	1:B:170:GLU:OE2	2.21	0.52
1:D:70:PHE:HZ	1:D:174:ILE:HG13	1.75	0.52
1:C:25:GLN:HA	1:C:28:LEU:HD12	1.92	0.52
1:C:136:PRO:HG2	1:C:204:SER:HB2	1.91	0.51
1:D:11:ALA:O	1:D:15:ILE:HG13	2.11	0.51
1:C:97:TYR:CE2	1:C:101:ILE:HD13	2.45	0.51
1:C:112:HIS:CE1	1:C:207:HIS:HE1	2.28	0.51
1:D:178:PHE:O	1:D:182:MET:HG3	2.11	0.51
1:D:26:LYS:HB3	1:D:32:ILE:HB	1.91	0.50
1:B:214:MET:HG3	1:B:219:GLU:HB3	1.94	0.50
1:A:47[B]:TYR:OH	2:A:302:ACT:O	2.25	0.49
1:C:29:LEU:HB2	1:C:31:ASN:OD1	2.12	0.49
1:B:136:PRO:HG3	1:B:201:PHE:CE2	2.48	0.48
1:C:16:ASN:OD1	1:C:147:ARG:NH2	2.46	0.48
1:A:26:LYS:HD2	1:A:216:MET:HE1	1.95	0.48
1:D:4:SER:OG	1:D:179:GLU:HG3	2.13	0.48
1:C:112:HIS:HB2	1:D:112:HIS:CE1	2.49	0.48
1:B:19:TYR:CE1	1:B:147:ARG:HB3	2.48	0.48
1:D:138:PRO:HB2	1:D:171:MET:HB3	1.94	0.48
1:A:112:HIS:CE1	1:B:112:HIS:HB2	2.48	0.47
1:A:55:TYR:HE2	1:A:78:MET:HE3	1.78	0.47
1:A:137:CME:HB2	1:A:138:PRO:HD3	1.96	0.47
1:A:137:CME:CB	1:A:138:PRO:HD3	2.45	0.47
1:B:136:PRO:HG3	1:B:201:PHE:CD2	2.50	0.46
1:A:37:LEU:HD22	1:A:89:LEU:HD22	1.96	0.46
1:A:22:ASP:HB2	3:A:303:GOL:H11	1.96	0.46
1:A:44:ASP:O	1:A:47[B]:TYR:CD1	2.69	0.46
1:D:101:ILE:HD12	1:D:104:LYS:HZ1	1.80	0.46
1:D:138:PRO:HB2	1:D:171:MET:CB	2.46	0.46
1:C:116:HIS:HA	1:D:115:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:TYR:CZ	1:B:147:ARG:HD2	2.52	0.45
1:C:30:GLY:HA2	1:C:160:THR:HG21	1.97	0.45
1:D:64:SER:HB3	1:D:67:ASP:OD2	2.16	0.45
1:A:155:ASN:ND2	1:A:158:LYS:HG3	2.32	0.45
1:A:184:LYS:HB3	1:A:184:LYS:HE2	1.84	0.45
1:B:83:VAL:HB	1:B:86:HIS:HB2	1.98	0.45
1:B:12[B]:LYS:HA	1:B:12[B]:LYS:HD2	1.66	0.45
1:D:136:PRO:CG	1:D:204:SER:HB3	2.27	0.45
1:A:83:VAL:HB	1:A:86:HIS:HB2	2.00	0.44
1:D:138:PRO:CB	1:D:171:MET:HB3	2.48	0.44
1:C:202:LEU:O	1:C:205:CYS:HB2	2.18	0.44
1:C:64:SER:HB3	1:C:67:ASP:OD2	2.18	0.44
1:D:135:ALA:N	1:D:136:PRO:CD	2.81	0.43
1:B:180:SER:O	1:B:184:LYS:HB2	2.18	0.43
1:A:47[B]:TYR:CD2	1:A:114:ILE:HD11	2.52	0.43
1:A:116:HIS:O	1:A:120:GLN:HG2	2.19	0.43
1:A:38:ARG:HG2	1:A:100:ILE:HG23	2.01	0.43
1:D:138:PRO:HG3	1:D:171:MET:SD	2.58	0.43
1:D:84:LEU:O	1:D:88:ILE:HG13	2.19	0.42
1:B:79:VAL:HG11	1:D:69:LYS:HG3	2.02	0.42
1:A:188:SER:HB2	4:A:430:HOH:O	2.19	0.42
1:B:135:ALA:N	1:B:136:PRO:CD	2.83	0.42
1:C:70:PHE:CE2	1:C:177:VAL:HG11	2.54	0.42
3:B:303:GOL:O3	1:C:61:LYS:NZ	2.53	0.41
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.82	0.41
1:D:199:GLN:O	1:D:203:GLU:HG3	2.20	0.41
1:A:207:HIS:HD2	4:A:418:HOH:O	2.03	0.41
1:B:135:ALA:HB3	1:B:136:PRO:HD3	2.03	0.41
1:A:135:ALA:N	1:A:136:PRO:CD	2.83	0.41
1:A:23:PHE:CD1	1:A:212:PHE:CD1	3.09	0.41
1:D:102:LYS:HB3	1:D:102:LYS:HE2	1.78	0.41
1:B:136:PRO:HG2	1:B:204:SER:HB2	2.03	0.41
1:B:28:LEU:HD12	1:B:28:LEU:HA	1.95	0.41
1:B:62:MET:HG3	1:B:67:ASP:HB3	2.03	0.41
1:D:135:ALA:N	1:D:136:PRO:HD2	2.35	0.41
1:C:74:GLN:NE2	1:C:174:ILE:HD12	2.35	0.40
1:D:29:LEU:HG	1:D:29:LEU:H	1.77	0.40
1:D:76:GLU:O	1:D:80:GLU:HB2	2.21	0.40
1:D:87:ASP:HA	1:D:90:ALA:HB3	2.04	0.40
1:D:171:MET:O	1:D:175:ILE:HG13	2.22	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	224/229 (98%)	220 (98%)	4 (2%)	0	100	100
1	B	223/229 (97%)	218 (98%)	5 (2%)	0	100	100
1	C	221/229 (96%)	218 (99%)	3 (1%)	0	100	100
1	D	223/229 (97%)	218 (98%)	4 (2%)	1 (0%)	34	60
All	All	891/916 (97%)	874 (98%)	16 (2%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	136	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	200/202 (99%)	186 (93%)	14 (7%)	15	35
1	B	199/202 (98%)	179 (90%)	20 (10%)	7	17
1	C	198/202 (98%)	180 (91%)	18 (9%)	9	21
1	D	199/202 (98%)	178 (89%)	21 (11%)	6	15
All	All	796/808 (98%)	723 (91%)	73 (9%)	9	21

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	20	GLU
1	A	28	LEU
1	A	62	MET
1	A	69	LYS
1	A	83	VAL
1	A	93	VAL
1	A	102	LYS
1	A	103	THR
1	A	113	TYR
1	A	147	ARG
1	A	156	ARG
1	A	187	GLU
1	A	188	SER
1	B	1	MET
1	B	4	SER
1	B	7	LEU
1	B	20	GLU
1	B	33	GLN
1	B	35	ASP
1	B	48	LEU
1	B	62	MET
1	B	80	GLU
1	B	83	VAL
1	B	84	LEU
1	B	103	THR
1	B	106	TRP
1	B	113	TYR
1	B	147	ARG
1	B	156	ARG
1	B	180	SER
1	B	184	LYS
1	B	188	SER
1	B	214	MET
1	C	1	MET
1	C	7	LEU
1	C	9	GLN
1	C	22	ASP
1	C	33	GLN
1	C	62	MET
1	C	83	VAL
1	C	93	VAL
1	C	96	SER

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Mol	Chain	Res	Type
1	C	104	LYS
1	C	113	TYR
1	C	136	PRO
1	C	147	ARG
1	C	156	ARG
1	C	180	SER
1	C	188	SER
1	C	214	MET
1	C	216	MET
1	D	1	MET
1	D	4	SER
1	D	7	LEU
1	D	9	GLN
1	D	22	ASP
1	D	29	LEU
1	D	33	GLN
1	D	35	ASP
1	D	48	LEU
1	D	52	THR
1	D	67	ASP
1	D	80	GLU
1	D	83	VAL
1	D	113	TYR
1	D	147	ARG
1	D	156	ARG
1	D	158	LYS
1	D	173	ASP
1	D	188	SER
1	D	204	SER
1	D	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	74	GLN
1	C	207	HIS
1	D	199	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CME	A	137	1	8,9,10	0.93	0	5,9,11	1.49	1 (20%)
1	CME	C	137	1	8,9,10	1.03	1 (12%)	5,9,11	1.96	1 (20%)
1	CME	B	137	1	8,9,10	0.90	0	5,9,11	1.34	1 (20%)
1	CME	D	137	1	8,9,10	0.92	0	5,9,11	1.13	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
1	CME	A	137	1	-	3/5/8/10	-
1	CME	C	137	1	-	3/5/8/10	-
1	CME	B	137	1	-	3/5/8/10	-
1	CME	D	137	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	CME	CB-SG	-2.08	1.74	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	CME	CA-CB-SG	-3.79	98.34	114.55
1	A	137	CME	CB-SG-SD	3.13	111.94	103.82
1	B	137	CME	CB-SG-SD	2.49	110.27	103.82
1	D	137	CME	CB-SG-SD	2.16	109.42	103.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	137	CME	CE-SD-SG-CB
1	A	137	CME	SD-CE-CZ-OH
1	C	137	CME	N-CA-CB-SG
1	D	137	CME	N-CA-CB-SG
1	B	137	CME	CE-SD-SG-CB
1	C	137	CME	SD-CE-CZ-OH
1	B	137	CME	SD-CE-CZ-OH
1	D	137	CME	SD-CE-CZ-OH
1	A	137	CME	N-CA-CB-SG
1	C	137	CME	CZ-CE-SD-SG
1	B	137	CME	CZ-CE-SD-SG
1	D	137	CME	CZ-CE-SD-SG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	137	CME	2	0
1	C	137	CME	1	0
1	B	137	CME	4	0
1	D	137	CME	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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
2	ACT	D	302	-	1,3,3	1.47	0	0,3,3	0.00	-
2	ACT	B	302	-	1,3,3	1.41	0	0,3,3	0.00	-
2	ACT	D	301	-	1,3,3	1.56	0	0,3,3	0.00	-
3	GOL	A	303	-	5,5,5	0.61	0	5,5,5	0.42	0
2	ACT	D	303	-	1,3,3	1.54	0	0,3,3	0.00	-
2	ACT	C	303	-	1,3,3	1.60	0	0,3,3	0.00	-
3	GOL	B	303	-	5,5,5	0.41	0	5,5,5	0.66	0
2	ACT	A	302	-	1,3,3	1.45	0	0,3,3	0.00	-
3	GOL	C	302	-	5,5,5	0.42	0	5,5,5	0.45	0
3	GOL	C	301	-	5,5,5	0.37	0	5,5,5	0.29	0
2	ACT	A	301	-	1,3,3	1.45	0	0,3,3	0.00	-
2	ACT	B	301	-	1,3,3	1.43	0	0,3,3	0.00	-
2	ACT	C	304	-	1,3,3	1.32	0	0,3,3	0.00	-

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
3	GOL	B	303	-	-	3/4/4/4	-
3	GOL	C	302	-	-	4/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-
3	GOL	C	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	C	302	GOL	O1-C1-C2-C3
3	C	301	GOL	O1-C1-C2-C3
3	C	301	GOL	O1-C1-C2-O2
3	B	303	GOL	O1-C1-C2-C3
3	C	302	GOL	C1-C2-C3-O3
3	C	301	GOL	C1-C2-C3-O3
3	C	302	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	C	301	GOL	O2-C2-C3-O3
3	B	303	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	GOL	2	0
3	B	303	GOL	1	0
2	A	302	ACT	1	0
2	A	301	ACT	1	0
2	C	304	ACT	1	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

### 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, 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	224/229 (97%)	-0.38	0	100 100	32, 49, 78, 101	7 (3%)
1	B	224/229 (97%)	-0.27	0	100 100	32, 57, 85, 116	9 (4%)
1	C	223/229 (97%)	-0.26	2 (0%)	84 85	36, 63, 97, 139	10 (4%)
1	D	224/229 (97%)	-0.05	6 (2%)	54 55	40, 74, 110, 143	10 (4%)
All	All	895/916 (97%)	-0.24	8 (0%)	84 85	32, 59, 99, 143	36 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	GLY	5.3
1	D	82	GLU	5.1
1	D	225	GLY	2.9
1	C	97	TYR	2.5
1	D	100	ILE	2.4
1	D	222	GLU	2.3
1	C	29	LEU	2.1
1	D	84	LEU	2.0

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

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(Å <sup>2</sup> )	Q<0.9
1	CME	B	137	10/11	0.62	0.45	68,70,73,74	0
1	CME	D	137	10/11	0.81	0.33	84,85,90,92	0
1	CME	C	137	10/11	0.85	0.27	64,65,69,71	0
1	CME	A	137	10/11	0.93	0.26	50,51,58,58	0

### 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, 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(Å <sup>2</sup> )	Q<0.9
2	ACT	A	301	4/4	0.29	0.83	112,112,112,112	0
2	ACT	C	304	4/4	0.75	0.72	123,123,123,124	0
3	GOL	A	303	6/6	0.76	0.33	65,66,67,68	0
3	GOL	C	302	6/6	0.81	0.24	87,88,88,88	0
2	ACT	B	301	4/4	0.85	0.41	81,82,82,82	0
2	ACT	C	303	4/4	0.85	0.31	104,104,104,104	0
2	ACT	B	302	4/4	0.87	0.28	91,92,92,92	0
2	ACT	A	302	4/4	0.87	0.81	94,94,94,94	0
2	ACT	D	302	4/4	0.87	0.37	115,115,116,117	0
3	GOL	C	301	6/6	0.92	0.54	101,101,102,102	0
2	ACT	D	303	4/4	0.92	0.17	69,69,69,69	0
2	ACT	D	301	4/4	0.93	0.73	80,81,81,81	0
3	GOL	B	303	6/6	0.93	0.19	71,71,71,71	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.