



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:13 PM GMT

PDB ID : 3TBE  
Title : The crystal structure of the complex of Streptococcus agalactiae sortase C1 and MTSET  
Authors : Khare, B.  
Deposited on : 2011-08-05  
Resolution : 2.85 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

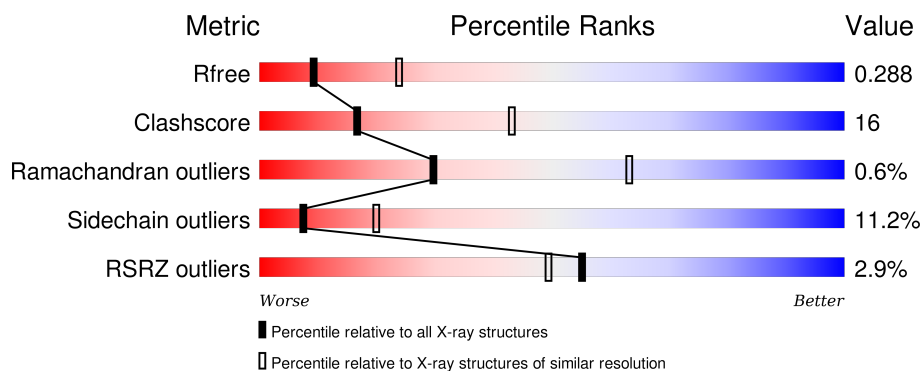
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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. 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	230	<div> <div>5%</div> <div> <div>55%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	230	<div> <div>5%</div> <div> <div>56%</div> <div>24%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	230	<div> <div>5%</div> <div> <div>55%</div> <div>20%</div> <div>7%</div> <div>18%</div> </div> </div>
1	D	230	<div> <div>5%</div> <div> <div>57%</div> <div>23%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	230	<div> <div>4%</div> <div> <div>60%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	230	

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
2	ETM	B	422	-	-	-	X
2	ETM	C	422	-	-	-	X
2	ETM	D	422	-	-	-	X
2	ETM	F	422	-	-	-	X
3	SO4	B	220	-	-	X	-
3	SO4	D	220	-	-	X	-
4	CL	C	220	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9008 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 Sortase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1509	959	266	281	3			
1	B	193	Total	C	N	O	S	0	0	0
			1478	940	261	274	3			
1	C	189	Total	C	N	O	S	0	0	0
			1455	924	255	273	3			
1	D	193	Total	C	N	O	S	0	0	0
			1473	936	262	272	3			
1	E	193	Total	C	N	O	S	0	0	0
			1483	944	261	275	3			
1	F	188	Total	C	N	O	S	0	0	0
			1434	914	253	264	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
A	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
A	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
A	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
A	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
A	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
A	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
B	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
B	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
B	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
B	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
B	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7

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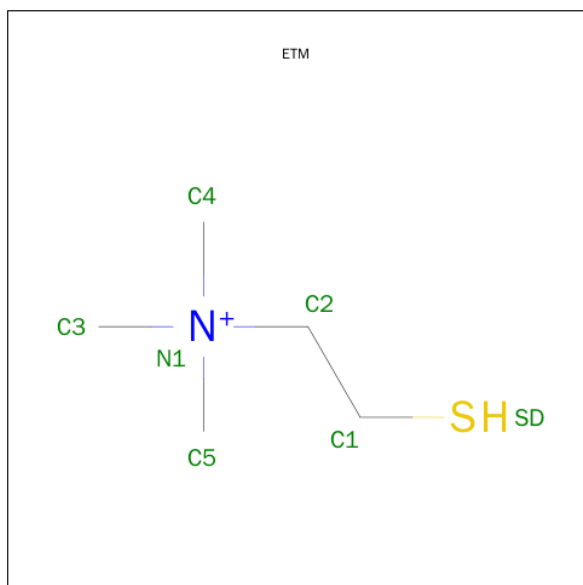
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
B	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
B	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
C	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
C	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
C	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
C	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
C	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
C	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
C	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
C	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
C	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
C	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
C	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
C	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
D	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
D	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
D	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
D	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
D	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
D	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
D	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
D	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
D	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
D	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
D	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
D	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
E	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
E	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
E	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
E	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
E	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
E	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
E	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
E	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
E	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
E	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
E	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	SER	-	EXPRESSION TAG	UNP Q8E0S7
F	-10	MET	-	EXPRESSION TAG	UNP Q8E0S7
F	-9	ARG	-	EXPRESSION TAG	UNP Q8E0S7
F	-8	GLY	-	EXPRESSION TAG	UNP Q8E0S7
F	-7	SER	-	EXPRESSION TAG	UNP Q8E0S7
F	-6	HIS	-	EXPRESSION TAG	UNP Q8E0S7
F	-5	HIS	-	EXPRESSION TAG	UNP Q8E0S7
F	-4	HIS	-	EXPRESSION TAG	UNP Q8E0S7
F	-3	HIS	-	EXPRESSION TAG	UNP Q8E0S7
F	-2	HIS	-	EXPRESSION TAG	UNP Q8E0S7
F	-1	HIS	-	EXPRESSION TAG	UNP Q8E0S7
F	0	GLY	-	EXPRESSION TAG	UNP Q8E0S7
F	1	SER	-	EXPRESSION TAG	UNP Q8E0S7

- Molecule 2 is 2-(TRIMETHYLAMMONIUM)ETHYL THIOL (three-letter code: ETM) (formula: C<sub>5</sub>H<sub>14</sub>NS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			7	5	1	1		
2	B	1	Total	C	N	S	0	0
			7	5	1	1		
2	C	1	Total	C	N	S	0	0
			7	5	1	1		
2	D	1	Total	C	N	S	0	0
			7	5	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	S	0	0
			7	5	1	1		
2	F	1	Total	C	N	S	0	0
			7	5	1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

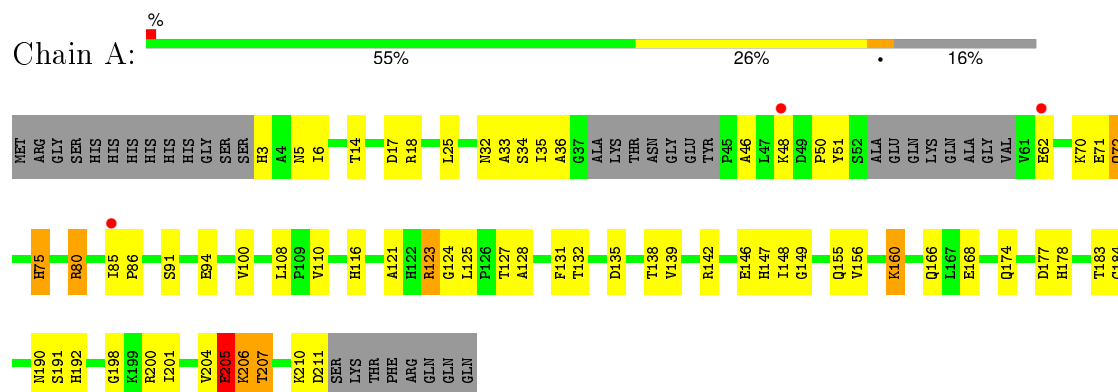
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total 10	O 10	0	0
5	B	17	Total 17	O 17	0	0
5	C	11	Total 11	O 11	0	0
5	D	36	Total 36	O 36	0	0
5	E	19	Total 19	O 19	0	0
5	F	15	Total 15	O 15	0	0



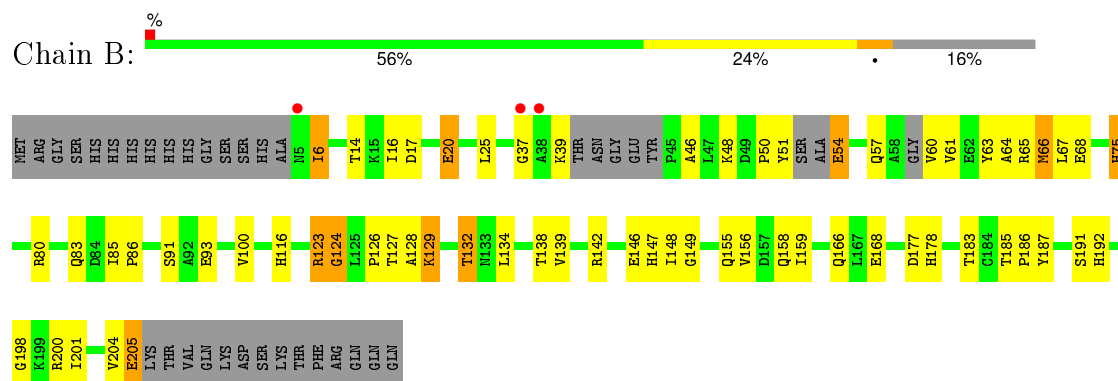
### 3 Residue-property plots [i](#)

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

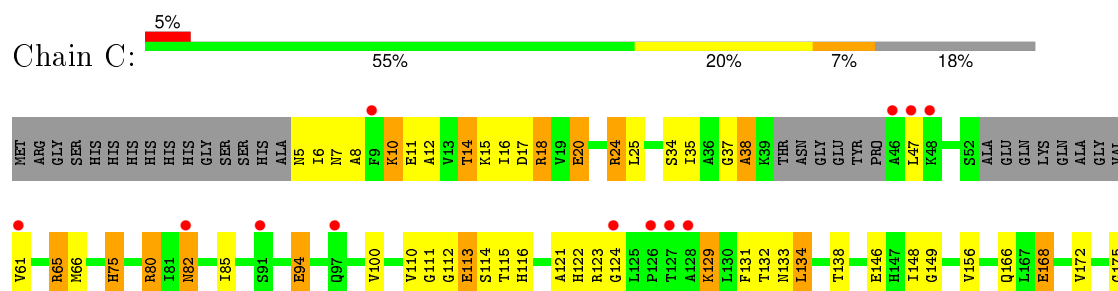
#### • Molecule 1: Sortase family protein

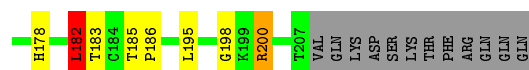


#### • Molecule 1: Sortase family protein



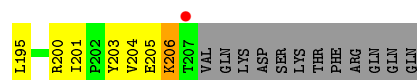
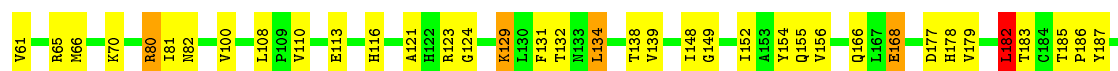
#### • Molecule 1: Sortase family protein





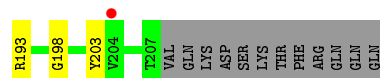
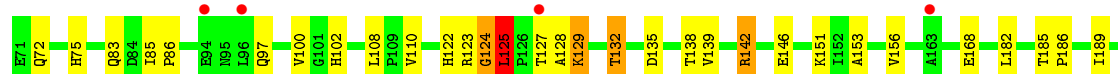
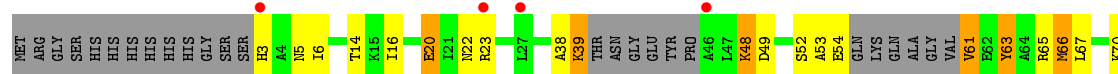
• Molecule 1: Sortase family protein

Chain D: 57% 23% 16%



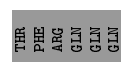
• Molecule 1: Sortase family protein

Chain E: 4% 60% 19% 16%



• Molecule 1: Sortase family protein

Chain F: 2% 63% 17% 18%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.41Å 70.65Å 194.44Å 90.00° 90.43° 90.00°	Depositor
Resolution (Å)	27.71 – 2.85 27.71 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.71-2.85) 97.9 (27.71-2.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.85Å)	Xtriage
Refinement program	CNS, REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.250 , 0.296 0.247 , 0.288	Depositor DCC
$R_{free}$ test set	1956 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 11.7	EDS
Estimated twinning fraction	0.004 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.008 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.448 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.438 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.002 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 38931 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, SO4, ETM

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	0.79	0/1536	0.81	1/2084 (0.0%)
1	B	0.83	1/1503 (0.1%)	0.78	1/2041 (0.0%)
1	C	0.88	0/1480	0.93	6/2010 (0.3%)
1	D	0.87	0/1497	0.92	6/2032 (0.3%)
1	E	0.84	0/1509	0.89	6/2048 (0.3%)
1	F	0.77	0/1460	0.84	5/1987 (0.3%)
All	All	0.83	1/8985 (0.0%)	0.86	25/12202 (0.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	TYR	CE1-CZ	-5.47	1.31	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ARG	NE-CZ-NH1	-11.41	114.59	120.30
1	C	65	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	E	193	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	F	193	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	D	65	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	D	65	ARG	NE-CZ-NH1	-8.19	116.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	F	142	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	F	193	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	E	142	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	D	24	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	C	65	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	E	124	GLY	N-CA-C	-7.29	94.89	113.10
1	C	24	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	E	142	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	F	142	ARG	NE-CZ-NH2	6.99	123.79	120.30
1	A	205	GLU	N-CA-C	-6.54	93.33	111.00
1	C	182	LEU	CA-CB-CG	5.94	128.97	115.30
1	D	23	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	182	LEU	CA-CB-CG	5.81	128.67	115.30
1	F	124	GLY	N-CA-C	5.71	127.38	113.10
1	C	111	GLY	N-CA-C	5.58	127.05	113.10
1	E	125	LEU	N-CA-CB	5.53	121.46	110.40
1	C	82	ASN	N-CA-C	5.25	125.18	111.00
1	B	124	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	ARG	Sidechain

## 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	1509	0	1509	61	0
1	B	1478	0	1459	56	0
1	C	1455	0	1437	57	0
1	D	1473	0	1461	54	0
1	E	1483	0	1468	43	0
1	F	1434	0	1413	26	0
2	A	7	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	7	0	13	0	0
2	C	7	0	14	1	0
2	D	7	0	13	0	0
2	E	7	0	13	2	0
2	F	7	0	13	0	0
3	B	10	0	0	2	0
3	C	5	0	0	0	0
3	D	5	0	0	2	0
3	F	5	0	0	0	0
4	C	1	0	0	2	0
5	A	10	0	0	0	0
5	B	17	0	0	2	0
5	C	11	0	0	0	0
5	D	36	0	0	10	0
5	E	19	0	0	0	0
5	F	15	0	0	0	0
All	All	9008	0	8826	291	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 16.

All (291) 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:E:129:LYS:O	1:E:132:THR:HG22	1.42	1.18
1:B:129:LYS:O	1:B:132:THR:HG22	1.46	1.15
1:A:204:VAL:HG12	1:A:205:GLU:O	1.48	1.11
1:E:123:ARG:HG3	1:E:132:THR:HA	1.36	1.06
1:D:32:ASN:OD1	5:D:241:HOH:O	1.71	1.05
1:B:60:VAL:O	1:B:60:VAL:HG22	1.55	1.03
1:F:61:VAL:HG13	1:F:61:VAL:O	1.55	1.03
1:A:207:THR:O	1:A:207:THR:HG22	1.57	1.02
1:C:110:VAL:O	1:C:110:VAL:HG23	1.57	1.01
1:E:123:ARG:CG	1:E:132:THR:HA	1.95	0.96
1:C:132:THR:HG23	1:C:133:ASN:HD22	1.31	0.95
1:C:7:ASN:HA	1:C:10:LYS:HG3	1.52	0.91
1:E:124:GLY:N	1:E:132:THR:HB	1.84	0.91
1:B:123:ARG:NH2	3:B:220:SO4:O3	2.05	0.89
1:C:123:ARG:HG2	1:C:132:THR:HA	1.55	0.88
1:A:124:GLY:H	1:A:132:THR:HB	1.42	0.84
1:E:16:ILE:CG2	1:E:20:GLU:HG2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:CD2	1:A:146:GLU:HB3	2.14	0.82
1:A:204:VAL:CG1	1:A:205:GLU:O	2.27	0.82
1:E:122:HIS:CE1	2:E:422:ETM:H52	2.16	0.81
1:C:6:ILE:O	1:C:10:LYS:HG2	1.79	0.81
1:A:177:ASP:OD2	1:A:200:ARG:HB2	1.79	0.81
1:B:54:GLU:HG2	1:B:54:GLU:O	1.79	0.81
1:C:113:GLU:O	1:C:114:SER:HB2	1.80	0.81
1:B:75:HIS:CD2	1:B:146:GLU:HB3	2.15	0.81
1:E:61:VAL:CG1	1:E:61:VAL:O	2.30	0.80
1:D:113:GLU:OE1	5:D:244:HOH:O	1.99	0.79
1:E:124:GLY:CA	1:E:132:THR:HB	2.12	0.79
1:C:6:ILE:O	1:C:10:LYS:CG	2.30	0.79
1:B:123:ARG:HG2	1:B:132:THR:HA	1.65	0.78
1:B:60:VAL:CG2	1:B:60:VAL:O	2.30	0.78
1:C:132:THR:HG23	1:C:133:ASN:ND2	1.97	0.78
1:A:166:GLN:HE21	1:A:168:GLU:H	1.29	0.78
1:E:122:HIS:HE1	2:E:422:ETM:H52	1.48	0.78
1:F:39:LYS:O	1:F:40:THR:CB	2.30	0.77
1:C:35:ILE:O	1:C:38:ALA:HB2	1.83	0.77
1:F:61:VAL:O	1:F:62:GLU:CB	2.32	0.77
1:B:129:LYS:O	1:B:132:THR:CG2	2.30	0.76
1:A:205:GLU:O	1:A:206:LYS:CB	2.34	0.76
1:A:124:GLY:N	1:A:132:THR:HB	1.99	0.75
1:E:129:LYS:O	1:E:132:THR:CG2	2.30	0.75
1:C:7:ASN:CA	1:C:10:LYS:HG3	2.16	0.75
1:F:16:ILE:CG2	1:F:20:GLU:HG2	2.16	0.74
1:B:166:GLN:HE21	1:B:168:GLU:H	1.32	0.74
1:E:61:VAL:O	1:E:61:VAL:HG13	1.86	0.73
1:D:9:PHE:CB	5:D:224:HOH:O	2.36	0.72
1:C:112:GLY:O	1:C:115:THR:HG23	1.89	0.72
1:E:61:VAL:HG12	1:E:63:TYR:HB3	1.70	0.72
1:A:205:GLU:O	1:A:206:LYS:HB2	1.89	0.71
1:B:147:HIS:HD2	1:B:149:GLY:H	1.38	0.71
1:A:210:LYS:O	1:A:211:ASP:C	2.27	0.71
1:F:72:GLN:OE1	1:F:86:PRO:HB3	1.91	0.70
1:E:123:ARG:NH2	1:E:135:ASP:HB3	2.06	0.69
1:E:16:ILE:HG23	1:E:20:GLU:HG2	1.73	0.69
1:C:7:ASN:HA	1:C:10:LYS:CG	2.20	0.69
1:E:66:MET:HG2	1:E:67:LEU:N	2.06	0.69
1:A:147:HIS:HD2	1:A:149:GLY:H	1.41	0.69
1:B:129:LYS:HG2	5:B:232:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:GLY:H	1:B:132:THR:HB	1.58	0.68
1:F:61:VAL:CG1	1:F:61:VAL:O	2.29	0.68
1:C:114:SER:O	1:C:172:VAL:CG1	2.41	0.68
1:A:51:TYR:HD2	2:A:422:ETM:SD	2.16	0.67
1:A:123:ARG:NH2	1:A:135:ASP:OD2	2.28	0.67
1:C:7:ASN:HA	1:C:10:LYS:HD3	1.77	0.67
1:A:190:ASN:HD22	2:A:422:ETM:H33	1.60	0.66
1:C:129:LYS:HG2	4:C:220:CL:CL	2.33	0.65
1:D:70:LYS:O	5:D:254:HOH:O	2.14	0.65
1:F:16:ILE:HG23	1:F:20:GLU:HG2	1.79	0.65
1:A:205:GLU:O	1:A:206:LYS:HG3	1.98	0.64
1:D:204:VAL:O	1:D:205:GLU:HB3	1.98	0.63
1:A:35:ILE:HG13	1:A:36:ALA:N	2.13	0.63
1:B:57:GLN:CB	1:B:93:GLU:HB2	2.28	0.63
1:D:123:ARG:HG2	1:D:132:THR:HA	1.80	0.63
1:A:123:ARG:HH22	1:A:135:ASP:HB3	1.65	0.62
1:A:6:ILE:HG23	1:A:86:PRO:HG3	1.82	0.62
1:B:61:VAL:O	1:B:61:VAL:HG23	1.98	0.62
1:C:114:SER:O	1:C:172:VAL:HG13	1.98	0.62
1:B:127:THR:HG23	1:D:34:SER:HB2	1.81	0.62
1:C:12:ALA:HA	1:C:15:LYS:HE3	1.80	0.62
1:A:51:TYR:CD2	2:A:422:ETM:SD	2.93	0.61
1:C:124:GLY:H	1:C:132:THR:HB	1.65	0.61
1:C:110:VAL:O	1:C:110:VAL:CG2	2.30	0.61
1:A:166:GLN:NE2	1:A:168:GLU:H	1.96	0.60
1:B:185:THR:OG1	1:B:186:PRO:HA	2.01	0.60
1:D:123:ARG:NH2	3:D:220:SO4:O1	2.34	0.60
1:D:129:LYS:HD2	5:D:234:HOH:O	2.02	0.60
1:F:185:THR:OG1	1:F:186:PRO:HA	2.02	0.59
1:F:61:VAL:O	1:F:62:GLU:HB2	2.02	0.59
1:A:205:GLU:O	1:A:206:LYS:CG	2.51	0.59
1:C:6:ILE:O	1:C:10:LYS:HG3	2.03	0.59
1:B:139:VAL:HA	1:B:156:VAL:HG12	1.85	0.59
1:B:54:GLU:CG	1:B:54:GLU:O	2.51	0.59
1:C:75:HIS:CE1	1:C:146:GLU:HB3	2.37	0.58
1:B:126:PRO:HG2	1:D:35:ILE:CD1	2.34	0.58
1:C:7:ASN:HA	1:C:10:LYS:CD	2.33	0.58
1:F:83:GLN:HG3	1:F:85:ILE:HD11	1.84	0.57
1:E:123:ARG:HG2	1:E:132:THR:HA	1.80	0.57
1:D:124:GLY:H	1:D:132:THR:HB	1.69	0.57
1:D:185:THR:OG1	1:D:186:PRO:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:HG2	5:D:256:HOH:O	2.04	0.57
1:A:205:GLU:OE1	1:A:205:GLU:HA	2.03	0.57
1:D:166:GLN:HE21	1:D:168:GLU:CG	2.18	0.57
1:B:85:ILE:HG21	1:B:100:VAL:HG23	1.87	0.56
1:B:177:ASP:OD2	1:B:200:ARG:HB2	2.04	0.56
1:A:205:GLU:C	1:A:206:LYS:HG3	2.25	0.56
1:A:50:PRO:C	1:A:51:TYR:HD1	2.09	0.56
1:F:134:LEU:HD23	1:F:183:THR:HG22	1.86	0.56
1:A:124:GLY:CA	1:A:132:THR:HB	2.36	0.56
1:A:207:THR:O	1:A:207:THR:CG2	2.30	0.56
1:A:177:ASP:OD2	1:A:200:ARG:CB	2.53	0.56
1:B:187:TYR:HB2	3:B:220:SO4:O3	2.06	0.56
1:D:203:TYR:HA	5:D:253:HOH:O	2.05	0.56
1:D:80:ARG:HG3	1:D:81:ILE:N	2.16	0.56
1:D:31:TYR:HD2	5:D:241:HOH:O	1.88	0.55
1:A:156:VAL:HA	1:A:198:GLY:HA2	1.88	0.55
1:D:152:ILE:HD12	1:D:154:TYR:HE2	1.71	0.55
1:B:129:LYS:C	1:B:132:THR:HG22	2.25	0.55
1:C:129:LYS:HE3	4:C:220:CL:CL	2.43	0.55
1:C:114:SER:O	1:C:172:VAL:HG11	2.05	0.55
1:C:166:GLN:HE21	1:C:168:GLU:CG	2.19	0.55
1:A:5:ASN:HB3	1:A:72:GLN:HE22	1.71	0.54
1:B:65:ARG:O	1:B:67:LEU:N	2.41	0.54
1:B:57:GLN:CB	1:B:93:GLU:CB	2.84	0.54
1:D:166:GLN:HE21	1:D:168:GLU:HG3	1.73	0.54
1:A:155:GLN:HB2	1:A:201:ILE:HD13	1.90	0.54
1:E:185:THR:OG1	1:E:186:PRO:HA	2.08	0.54
1:F:61:VAL:O	1:F:62:GLU:HB3	2.08	0.54
1:A:123:ARG:HD2	1:A:184:CYS:O	2.08	0.54
1:F:129:LYS:O	1:F:132:THR:HB	2.08	0.54
1:C:121:ALA:HB3	1:C:131:PHE:CD2	2.44	0.53
1:D:110:VAL:HG23	1:D:110:VAL:O	2.08	0.53
1:B:166:GLN:NE2	1:B:168:GLU:H	2.03	0.53
1:D:116:HIS:HA	1:D:178:HIS:O	2.09	0.53
1:D:187:TYR:HB2	3:D:220:SO4:O1	2.09	0.53
1:A:70:LYS:O	1:A:71:GLU:HB2	2.09	0.53
1:C:16:ILE:HG23	1:C:20:GLU:HG2	1.91	0.53
1:F:85:ILE:HG21	1:F:100:VAL:HG23	1.91	0.52
1:A:75:HIS:NE2	1:A:146:GLU:HB3	2.25	0.52
1:A:25:LEU:HD11	1:A:149:GLY:HA3	1.92	0.51
1:B:65:ARG:O	1:B:66:MET:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:HD11	1:C:149:GLY:HA3	1.92	0.51
1:B:127:THR:OG1	1:B:128:ALA:N	2.44	0.51
1:B:50:PRO:C	1:B:51:TYR:HD1	2.14	0.51
1:B:204:VAL:O	1:B:205:GLU:HG3	2.11	0.51
1:E:108:LEU:O	1:E:110:VAL:N	2.43	0.51
1:E:72:GLN:OE1	1:E:86:PRO:HB3	2.10	0.51
1:C:16:ILE:CG2	1:C:20:GLU:HG2	2.40	0.51
1:F:123:ARG:HG3	1:F:183:THR:OG1	2.11	0.50
1:D:134:LEU:HD22	1:D:183:THR:HG22	1.93	0.50
1:E:83:GLN:HG3	1:E:85:ILE:HD11	1.92	0.50
1:D:5:ASN:OD1	1:D:5:ASN:O	2.30	0.50
1:E:16:ILE:HG22	1:E:20:GLU:HG2	1.91	0.49
1:E:127:THR:OG1	1:E:128:ALA:N	2.44	0.49
1:C:85:ILE:HG21	1:C:100:VAL:HG23	1.94	0.49
1:A:123:ARG:HG3	1:A:183:THR:OG1	2.11	0.49
1:F:186:PRO:HG2	1:F:189:ILE:HB	1.95	0.49
1:C:11:GLU:O	1:C:14:THR:OG1	2.29	0.49
1:D:82:ASN:O	1:D:82:ASN:OD1	2.31	0.49
1:D:182:LEU:HD22	1:D:195:LEU:CD2	2.42	0.49
1:B:6:ILE:HG23	1:B:86:PRO:HG3	1.94	0.49
1:C:37:GLY:O	1:C:38:ALA:O	2.30	0.49
1:D:110:VAL:HG23	5:D:225:HOH:O	2.11	0.49
1:D:60:VAL:HG22	1:D:61:VAL:H	1.78	0.49
1:C:185:THR:OG1	1:C:186:PRO:HA	2.13	0.48
1:A:191:SER:OG	1:A:192:HIS:HD2	1.96	0.48
1:C:18:ARG:HG3	1:C:18:ARG:NH1	2.28	0.48
1:B:116:HIS:HA	1:B:178:HIS:O	2.13	0.48
1:B:83:GLN:HE22	1:B:129:LYS:CD	2.27	0.48
1:F:112:GLY:O	1:F:115:THR:HG23	2.14	0.48
1:C:124:GLY:N	1:C:132:THR:HB	2.28	0.48
1:F:108:LEU:O	1:F:110:VAL:N	2.45	0.48
1:A:204:VAL:C	1:A:205:GLU:O	2.40	0.48
1:E:38:ALA:C	1:E:39:LYS:HG3	2.34	0.48
1:A:205:GLU:OE1	1:A:205:GLU:CA	2.59	0.47
1:E:125:LEU:HD23	1:E:125:LEU:HA	1.56	0.47
1:A:100:VAL:HG22	1:A:121:ALA:HB2	1.96	0.47
1:D:121:ALA:HB3	1:D:131:PHE:CD2	2.49	0.47
1:B:155:GLN:HB2	1:B:201:ILE:HD13	1.95	0.47
1:C:200:ARG:CG	1:C:200:ARG:HH11	2.27	0.47
1:C:134:LEU:HD22	1:C:183:THR:HG22	1.95	0.47
1:C:122:HIS:HE1	2:C:422:ETM:H42	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ASN:C	1:C:10:LYS:HG3	2.35	0.47
1:F:63:TYR:HE1	1:F:90:GLY:N	2.12	0.47
1:B:126:PRO:HD2	1:D:34:SER:OG	2.14	0.47
1:B:25:LEU:HD11	1:B:149:GLY:HA3	1.97	0.47
1:C:166:GLN:HE21	1:C:168:GLU:HG3	1.78	0.47
1:E:70:LYS:O	1:E:72:GLN:HG2	2.14	0.47
1:E:85:ILE:HG21	1:E:100:VAL:HG23	1.97	0.46
1:B:16:ILE:CG2	1:B:20:GLU:HG2	2.45	0.46
1:A:108:LEU:O	1:A:110:VAL:N	2.46	0.46
1:B:156:VAL:HA	1:B:198:GLY:HA2	1.98	0.46
1:D:60:VAL:HG22	1:D:61:VAL:N	2.31	0.46
1:E:151:LYS:HD3	1:E:203:TYR:OH	2.16	0.46
1:A:35:ILE:HD13	1:A:174:GLN:OE1	2.15	0.46
1:E:186:PRO:HG2	1:E:189:ILE:HB	1.97	0.46
1:E:63:TYR:OH	1:E:102:HIS:ND1	2.40	0.46
1:D:139:VAL:HA	1:D:156:VAL:HG12	1.99	0.45
1:A:204:VAL:HG12	1:A:206:LYS:HB2	1.98	0.45
1:B:75:HIS:NE2	1:B:146:GLU:HB3	2.32	0.45
1:E:61:VAL:O	1:E:61:VAL:HG12	2.14	0.45
1:F:134:LEU:HA	1:F:134:LEU:HD12	1.81	0.45
1:A:51:TYR:CD1	1:A:51:TYR:N	2.85	0.45
1:D:152:ILE:HG22	1:D:200:ARG:NH2	2.32	0.45
1:C:182:LEU:HD22	1:C:195:LEU:CD2	2.47	0.45
1:B:126:PRO:HG3	1:D:31:TYR:CE1	2.51	0.45
1:D:206:LYS:HA	1:D:206:LYS:HD3	1.65	0.45
1:C:156:VAL:HA	1:C:198:GLY:HA2	1.99	0.45
1:A:33:ALA:HA	1:A:35:ILE:HG23	1.98	0.45
1:A:139:VAL:HA	1:A:156:VAL:HG12	1.99	0.45
1:E:156:VAL:HA	1:E:198:GLY:HA2	1.99	0.45
1:C:94:GLU:CD	1:C:94:GLU:H	2.20	0.45
1:A:85:ILE:HG21	1:A:100:VAL:HG23	1.98	0.44
1:E:49:ASP:O	1:E:52:SER:CB	2.65	0.44
1:E:123:ARG:HG3	1:E:132:THR:CA	2.26	0.44
1:B:129:LYS:HB3	5:B:232:HOH:O	2.17	0.44
1:D:80:ARG:HE	1:D:80:ARG:HB2	1.56	0.44
1:D:35:ILE:N	1:D:35:ILE:CD1	2.80	0.44
1:D:5:ASN:OD1	1:D:5:ASN:C	2.56	0.44
1:D:152:ILE:HD12	1:D:154:TYR:CE2	2.50	0.44
1:E:48:LYS:HE3	1:E:48:LYS:HB3	1.30	0.44
1:E:123:ARG:HH22	1:E:135:ASP:HB3	1.79	0.44
1:E:182:LEU:HD23	1:E:182:LEU:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LEU:HD12	1:D:183:THR:N	2.33	0.43
1:D:31:TYR:O	1:D:35:ILE:HD13	2.18	0.43
1:D:177:ASP:OD2	1:D:200:ARG:HD3	2.17	0.43
1:E:53:ALA:O	1:E:54:GLU:C	2.56	0.43
1:F:121:ALA:HB3	1:F:131:PHE:CD1	2.54	0.43
1:C:80:ARG:HB2	1:C:80:ARG:HE	1.11	0.43
1:C:5:ASN:O	1:C:8:ALA:HB3	2.19	0.43
1:A:124:GLY:HA2	1:A:132:THR:HB	1.99	0.43
1:C:116:HIS:HA	1:C:178:HIS:O	2.18	0.43
1:B:177:ASP:OD2	1:B:200:ARG:CB	2.66	0.43
1:F:139:VAL:HG23	1:F:139:VAL:O	2.18	0.43
1:D:16:ILE:HG23	1:D:20:GLU:HG2	2.00	0.43
1:A:32:ASN:O	1:A:35:ILE:HG23	2.19	0.43
1:A:139:VAL:HG11	1:B:159:ILE:HG22	2.01	0.43
1:D:182:LEU:HD12	1:D:182:LEU:C	2.39	0.43
1:C:113:GLU:HG3	1:C:175:GLY:HA2	2.00	0.43
1:E:139:VAL:HG23	1:E:139:VAL:O	2.19	0.43
1:A:123:ARG:HH22	1:A:135:ASP:CB	2.32	0.43
1:D:168:GLU:H	1:D:168:GLU:HG3	1.53	0.43
1:D:155:GLN:HB2	1:D:201:ILE:HD13	2.01	0.42
1:A:124:GLY:N	1:A:132:THR:CB	2.78	0.42
1:C:35:ILE:O	1:C:38:ALA:CB	2.61	0.42
1:B:61:VAL:CG2	1:B:61:VAL:O	2.67	0.42
1:A:3:HIS:CD2	1:A:5:ASN:H	2.37	0.42
1:F:24:ARG:NE	1:F:66:MET:O	2.42	0.42
1:C:182:LEU:HD12	1:C:182:LEU:C	2.39	0.42
1:D:108:LEU:N	5:D:241:HOH:O	2.50	0.42
1:C:100:VAL:HG22	1:C:121:ALA:HB2	2.00	0.42
1:C:114:SER:OG	1:C:175:GLY:N	2.37	0.42
1:B:75:HIS:HD2	1:B:146:GLU:HB3	1.74	0.42
1:F:66:MET:HG2	1:F:67:LEU:N	2.34	0.42
1:E:3:HIS:O	1:E:6:ILE:CD1	2.68	0.42
1:B:6:ILE:HG21	1:B:75:HIS:HB3	2.02	0.42
1:E:75:HIS:CE1	1:E:146:GLU:HB3	2.55	0.42
1:B:64:ALA:O	1:B:65:ARG:C	2.56	0.41
1:C:18:ARG:NH1	1:C:18:ARG:CG	2.81	0.41
1:C:182:LEU:HD12	1:C:183:THR:N	2.35	0.41
1:D:25:LEU:HD11	1:D:149:GLY:HA3	2.03	0.41
1:C:168:GLU:H	1:C:168:GLU:HG3	1.49	0.41
1:B:83:GLN:HE22	1:B:129:LYS:HD2	1.84	0.41
1:C:18:ARG:HH11	1:C:18:ARG:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:HB3	1:A:131:PHE:CD2	2.55	0.41
1:A:116:HIS:HA	1:A:178:HIS:O	2.20	0.41
1:B:134:LEU:HA	1:B:134:LEU:HD12	1.89	0.41
1:D:121:ALA:HB3	1:D:131:PHE:CG	2.55	0.41
1:B:134:LEU:HD23	1:B:183:THR:HG22	2.03	0.41
1:A:6:ILE:CG2	1:A:86:PRO:HG3	2.49	0.41
1:B:85:ILE:CG2	1:B:100:VAL:HG23	2.50	0.41
1:A:160:LYS:HE2	1:B:158:GLN:OE1	2.20	0.41
1:D:70:LYS:HD3	1:D:70:LYS:HA	1.88	0.41
1:B:191:SER:OG	1:B:192:HIS:HD2	2.04	0.41
1:D:100:VAL:HG22	1:D:121:ALA:HB2	2.03	0.41
1:A:75:HIS:HD2	1:A:146:GLU:HB3	1.80	0.41
1:C:123:ARG:HG2	1:C:132:THR:CA	2.38	0.41
1:B:147:HIS:HD2	1:B:149:GLY:N	2.12	0.41
1:A:80:ARG:HG3	1:A:80:ARG:O	2.17	0.41
1:D:204:VAL:O	1:D:205:GLU:CB	2.64	0.41
1:D:110:VAL:O	1:D:110:VAL:CG2	2.68	0.40
1:B:204:VAL:C	1:B:205:GLU:HG3	2.41	0.40
1:B:37:GLY:C	1:B:39:LYS:H	2.23	0.40
1:F:125:LEU:HA	1:F:126:PRO:HD3	1.94	0.40
1:E:61:VAL:CG1	1:E:63:TYR:HB3	2.47	0.40
1:A:32:ASN:C	1:A:34:SER:H	2.24	0.40
1:A:125:LEU:O	1:A:128:ALA:O	2.39	0.40
1:E:16:ILE:CG2	1:E:20:GLU:CG	2.89	0.40
1:C:113:GLU:HG3	1:C:175:GLY:C	2.42	0.40
1:F:20:GLU:O	1:F:24:ARG:HG2	2.21	0.40
1:E:153:ALA:HB2	1:E:203:TYR:HD2	1.87	0.40
1:D:154:TYR:CZ	1:D:179:VAL:HG23	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	188/230 (82%)	173 (92%)	13 (7%)	2 (1%)	17	47
1	B	185/230 (80%)	171 (92%)	12 (6%)	2 (1%)	17	47
1	C	183/230 (80%)	172 (94%)	10 (6%)	1 (0%)	34	67
1	D	185/230 (80%)	178 (96%)	6 (3%)	1 (0%)	34	67
1	E	187/230 (81%)	178 (95%)	8 (4%)	1 (0%)	34	67
1	F	182/230 (79%)	170 (93%)	12 (7%)	0	100	100
All	All	1110/1380 (80%)	1042 (94%)	61 (6%)	7 (1%)	30	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	ALA
1	E	5	ASN
1	A	46	ALA
1	B	46	ALA
1	A	206	LYS
1	B	66	MET
1	D	37	GLY

### 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	159/193 (82%)	141 (89%)	18 (11%)	7	19
1	B	151/193 (78%)	135 (89%)	16 (11%)	8	22
1	C	150/193 (78%)	127 (85%)	23 (15%)	3	9
1	D	150/193 (78%)	132 (88%)	18 (12%)	6	16
1	E	151/193 (78%)	134 (89%)	17 (11%)	7	19
1	F	146/193 (76%)	136 (93%)	10 (7%)	20	46
All	All	907/1158 (78%)	805 (89%)	102 (11%)	7	20

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	17	ASP
1	A	18	ARG
1	A	48	LYS
1	A	62	GLU
1	A	72	GLN
1	A	75	HIS
1	A	80	ARG
1	A	91	SER
1	A	94	GLU
1	A	123	ARG
1	A	127	THR
1	A	138	THR
1	A	142	ARG
1	A	148	ILE
1	A	160	LYS
1	A	205	GLU
1	A	207	THR
1	B	6	ILE
1	B	14	THR
1	B	17	ASP
1	B	20	GLU
1	B	48	LYS
1	B	54	GLU
1	B	68	GLU
1	B	75	HIS
1	B	80	ARG
1	B	91	SER
1	B	129	LYS
1	B	132	THR
1	B	138	THR
1	B	142	ARG
1	B	148	ILE
1	B	205	GLU
1	C	10	LYS
1	C	14	THR
1	C	17	ASP
1	C	18	ARG
1	C	20	GLU
1	C	24	ARG
1	C	34	SER
1	C	47	LEU
1	C	61	VAL

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Mol	Chain	Res	Type
1	C	65	ARG
1	C	66	MET
1	C	75	HIS
1	C	80	ARG
1	C	82	ASN
1	C	94	GLU
1	C	113	GLU
1	C	129	LYS
1	C	134	LEU
1	C	138	THR
1	C	148	ILE
1	C	168	GLU
1	C	182	LEU
1	C	200	ARG
1	D	14	THR
1	D	17	ASP
1	D	18	ARG
1	D	20	GLU
1	D	23	ARG
1	D	24	ARG
1	D	35	ILE
1	D	47	LEU
1	D	48	LYS
1	D	66	MET
1	D	80	ARG
1	D	129	LYS
1	D	134	LEU
1	D	138	THR
1	D	148	ILE
1	D	168	GLU
1	D	182	LEU
1	D	206	LYS
1	E	14	THR
1	E	20	GLU
1	E	22	ASN
1	E	23	ARG
1	E	39	LYS
1	E	48	LYS
1	E	61	VAL
1	E	63	TYR
1	E	65	ARG
1	E	66	MET

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Mol	Chain	Res	Type
1	E	97	GLN
1	E	125	LEU
1	E	129	LYS
1	E	132	THR
1	E	138	THR
1	E	142	ARG
1	E	168	GLU
1	F	14	THR
1	F	20	GLU
1	F	22	ASN
1	F	66	MET
1	F	127	THR
1	F	129	LYS
1	F	132	THR
1	F	138	THR
1	F	148	ILE
1	F	168	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	72	GLN
1	A	147	HIS
1	A	166	GLN
1	A	190	ASN
1	A	192	HIS
1	B	83	GLN
1	B	147	HIS
1	B	166	GLN
1	B	192	HIS
1	C	97	GLN
1	C	122	HIS
1	C	133	ASN
1	C	166	GLN
1	C	192	HIS
1	D	82	ASN
1	D	97	GLN
1	D	166	GLN
1	D	192	HIS
1	E	7	ASN
1	E	75	HIS

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Mol	Chain	Res	Type
1	E	83	GLN
1	E	122	HIS
1	F	7	ASN
1	F	75	HIS
1	F	122	HIS
1	F	192	HIS

### 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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z  > 2$
2	ETM	A	422	1	6,6,6	0.59	0	6,8,8	0.55	0
3	SO4	B	220	-	4,4,4	0.53	0	6,6,6	0.26	0
3	SO4	B	221	-	4,4,4	0.14	0	6,6,6	0.41	0
2	ETM	B	422	1	6,6,6	0.71	0	6,8,8	0.28	0
3	SO4	C	221	-	4,4,4	0.15	0	6,6,6	0.22	0
2	ETM	C	422	1	6,6,6	0.62	0	6,8,8	0.41	0
3	SO4	D	220	-	4,4,4	0.41	0	6,6,6	0.17	0
2	ETM	D	422	1	6,6,6	0.74	0	6,8,8	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ETM	E	422	1	6,6,6	0.60	0	6,8,8	0.44	0
3	SO4	F	220	-	4,4,4	0.41	0	6,6,6	0.42	0
2	ETM	F	422	1	6,6,6	0.49	0	6,8,8	0.39	0

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
2	ETM	A	422	1	-	0/4/4/4	0/0/0/0
3	SO4	B	220	-	-	0/0/0/0	0/0/0/0
3	SO4	B	221	-	-	0/0/0/0	0/0/0/0
2	ETM	B	422	1	-	0/4/4/4	0/0/0/0
3	SO4	C	221	-	-	0/0/0/0	0/0/0/0
2	ETM	C	422	1	-	0/4/4/4	0/0/0/0
3	SO4	D	220	-	-	0/0/0/0	0/0/0/0
2	ETM	D	422	1	-	0/4/4/4	0/0/0/0
2	ETM	E	422	1	-	0/4/4/4	0/0/0/0
3	SO4	F	220	-	-	0/0/0/0	0/0/0/0
2	ETM	F	422	1	-	0/4/4/4	0/0/0/0

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.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	422	ETM	3	0
3	B	220	SO4	2	0
2	C	422	ETM	1	0
3	D	220	SO4	2	0
2	E	422	ETM	2	0

## 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 ⓘ

### 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	194/230 (84%)	0.22	3 (1%) 76 73	24, 43, 89, 96	0
1	B	193/230 (83%)	0.06	3 (1%) 74 72	25, 43, 85, 122	0
1	C	189/230 (82%)	0.10	12 (6%) 23 17	26, 45, 89, 93	0
1	D	193/230 (83%)	0.15	1 (0%) 91 90	26, 44, 88, 115	0
1	E	193/230 (83%)	0.20	9 (4%) 35 29	28, 49, 95, 106	0
1	F	188/230 (81%)	0.26	5 (2%) 58 52	29, 49, 93, 109	0
All	All	1150/1380 (83%)	0.17	33 (2%) 55 49	24, 46, 90, 122	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	LEU	5.0
1	C	124	GLY	4.5
1	C	126	PRO	3.6
1	C	9	PHE	3.5
1	E	46	ALA	3.4
1	E	96	LEU	3.4
1	F	96	LEU	3.3
1	E	94	GLU	3.3
1	F	27	LEU	3.0
1	B	38	ALA	3.0
1	F	127	THR	3.0
1	E	23	ARG	2.8
1	E	27	LEU	2.7
1	E	127	THR	2.6
1	C	91	SER	2.6
1	C	127	THR	2.5
1	D	207	THR	2.5
1	E	163	ALA	2.4
1	A	62	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	37	GLY	2.4
1	E	3	HIS	2.3
1	F	47	LEU	2.3
1	C	48	LYS	2.3
1	F	99	GLY	2.2
1	E	204	VAL	2.2
1	C	128	ALA	2.2
1	C	97	GLN	2.2
1	A	48	LYS	2.1
1	C	61	VAL	2.1
1	C	46	ALA	2.1
1	C	82	ASN	2.0
1	A	85	ILE	2.0
1	B	5	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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ETM	F	422	7/7	0.54	0.77	5.56	182,184,185,185	0
2	ETM	D	422	7/7	0.79	0.43	5.31	85,85,86,88	0
2	ETM	B	422	7/7	0.87	0.37	3.46	99,99,100,101	0
2	ETM	C	422	7/7	0.60	0.36	2.76	144,146,146,146	0
3	SO4	B	220	5/5	0.96	0.19	-0.28	48,48,49,49	0
3	SO4	F	220	5/5	0.92	0.15	-0.62	55,56,57,57	0
3	SO4	D	220	5/5	0.96	0.18	-0.83	50,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	221	5/5	0.95	0.12	-3.00	93,94,94,95	0
2	ETM	E	422	7/7	0.78	0.40	-	121,123,124,124	0
2	ETM	A	422	7/7	0.62	0.30	-	111,115,116,116	0
3	SO4	B	221	5/5	0.91	0.18	-	89,89,90,90	0
4	CL	C	220	1/1	0.94	0.20	-	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.