



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:28 AM GMT

PDB ID : 3ETC  
Title : 2.1 Å structure of acyl-adenylate synthetase from Methanosarcina acetivorans containing a link between Lys256 and Cys298  
Authors : Shah, M.B.; Gulick, A.M.; Smith, K.S.; Ingram-Smith, C.  
Deposited on : 2008-10-07  
Resolution : 2.10 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

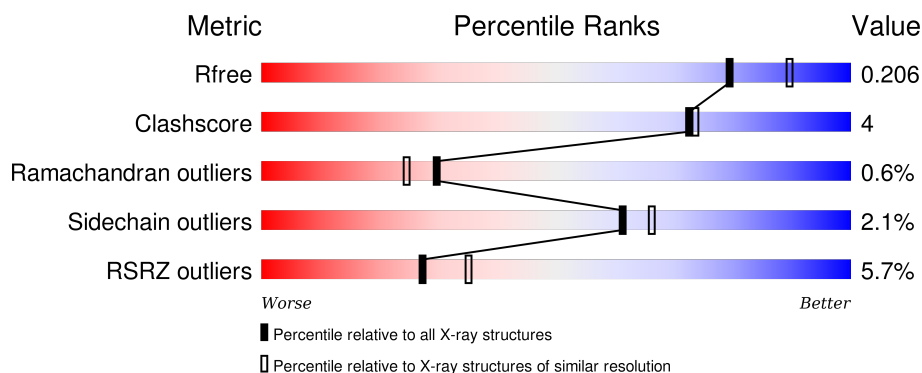
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	580	
1	B	580	

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	FOR	B	999	-	-	X	-
3	PGE	B	993	-	-	-	X
4	1PE	A	994	-	-	-	X
5	EPE	A	997	-	-	-	X
7	NO3	A	1001	-	X	-	-
7	NO3	B	1001	-	X	-	X
8	GOL	A	1002	-	-	-	X
8	GOL	A	1005	-	-	X	X
8	GOL	B	1004	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9016 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 AMP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	3	0
			4191	2719	663	786	23			
1	B	537	Total	C	N	O	S	0	2	0
			4233	2746	668	796	23			

There are 46 discrepancies between the modelled and reference sequences:

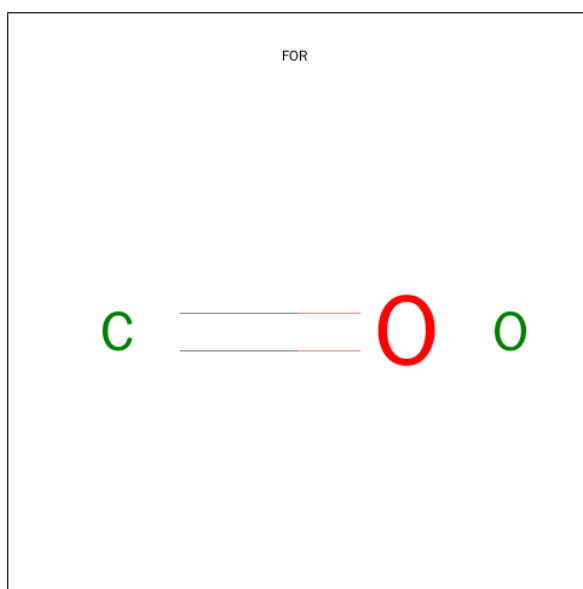
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q8TLW1
A	-21	GLY	-	EXPRESSION TAG	UNP Q8TLW1
A	-20	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-19	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-18	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-17	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-16	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-15	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-14	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-13	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-12	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-11	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-10	SER	-	EXPRESSION TAG	UNP Q8TLW1
A	-9	SER	-	EXPRESSION TAG	UNP Q8TLW1
A	-8	GLY	-	EXPRESSION TAG	UNP Q8TLW1
A	-7	HIS	-	EXPRESSION TAG	UNP Q8TLW1
A	-6	ILE	-	EXPRESSION TAG	UNP Q8TLW1
A	-5	ASP	-	EXPRESSION TAG	UNP Q8TLW1
A	-4	ASP	-	EXPRESSION TAG	UNP Q8TLW1
A	-3	ASP	-	EXPRESSION TAG	UNP Q8TLW1
A	-2	ASP	-	EXPRESSION TAG	UNP Q8TLW1
A	-1	LYS	-	EXPRESSION TAG	UNP Q8TLW1
A	0	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-22	MET	-	EXPRESSION TAG	UNP Q8TLW1
B	-21	GLY	-	EXPRESSION TAG	UNP Q8TLW1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-19	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-18	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-17	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-16	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-15	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-14	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-13	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-12	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-11	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-10	SER	-	EXPRESSION TAG	UNP Q8TLW1
B	-9	SER	-	EXPRESSION TAG	UNP Q8TLW1
B	-8	GLY	-	EXPRESSION TAG	UNP Q8TLW1
B	-7	HIS	-	EXPRESSION TAG	UNP Q8TLW1
B	-6	ILE	-	EXPRESSION TAG	UNP Q8TLW1
B	-5	ASP	-	EXPRESSION TAG	UNP Q8TLW1
B	-4	ASP	-	EXPRESSION TAG	UNP Q8TLW1
B	-3	ASP	-	EXPRESSION TAG	UNP Q8TLW1
B	-2	ASP	-	EXPRESSION TAG	UNP Q8TLW1
B	-1	LYS	-	EXPRESSION TAG	UNP Q8TLW1
B	0	HIS	-	EXPRESSION TAG	UNP Q8TLW1

- Molecule 2 is FORMYL GROUP (three-letter code: FOR) (formula: CH<sub>2</sub>O).



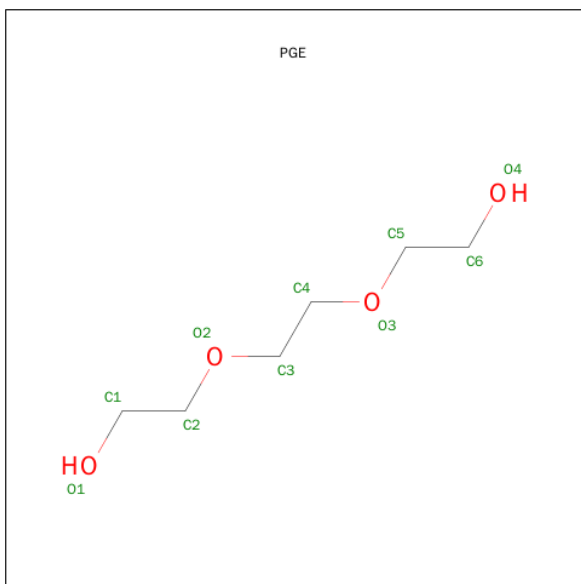
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			2	1	1		

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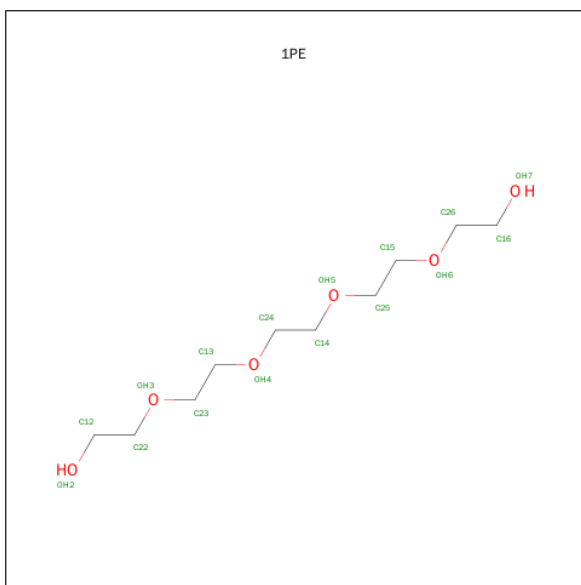
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



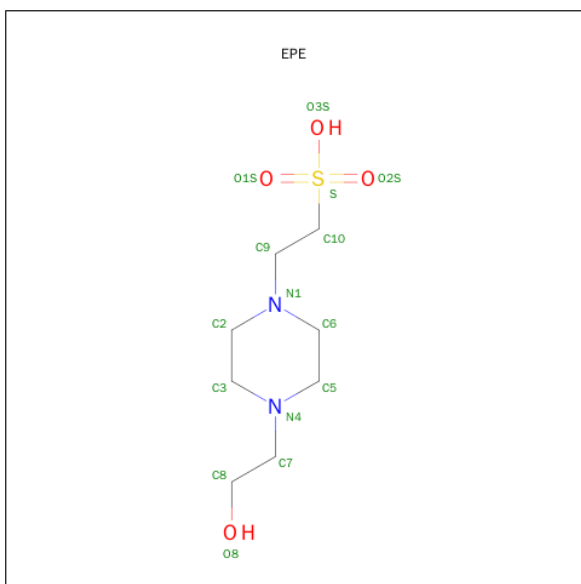
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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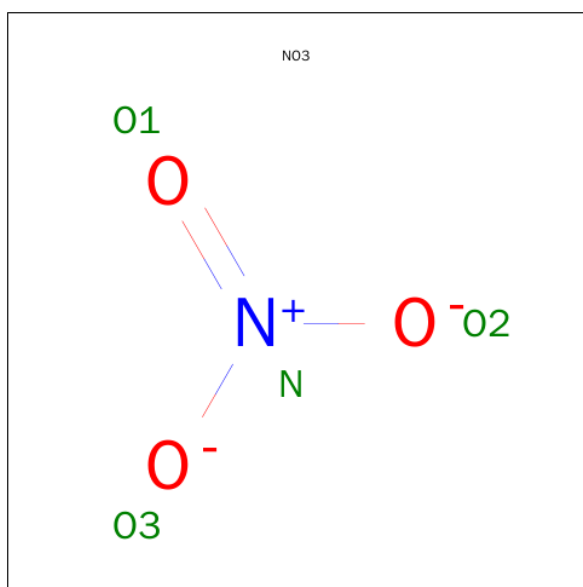
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	N	O	0	0
			4	1	3		
7	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 8 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
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

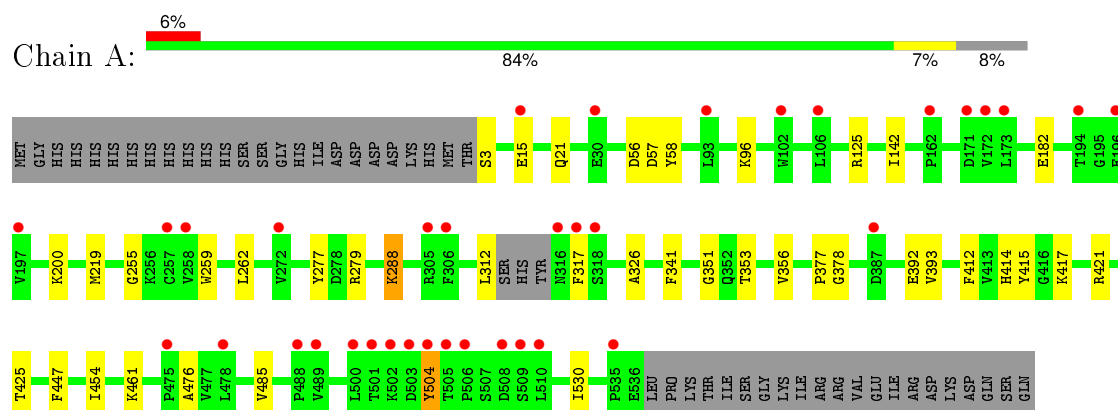
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	204	Total	O	0	0
			204	204		
9	B	225	Total	O	0	0
			225	225		

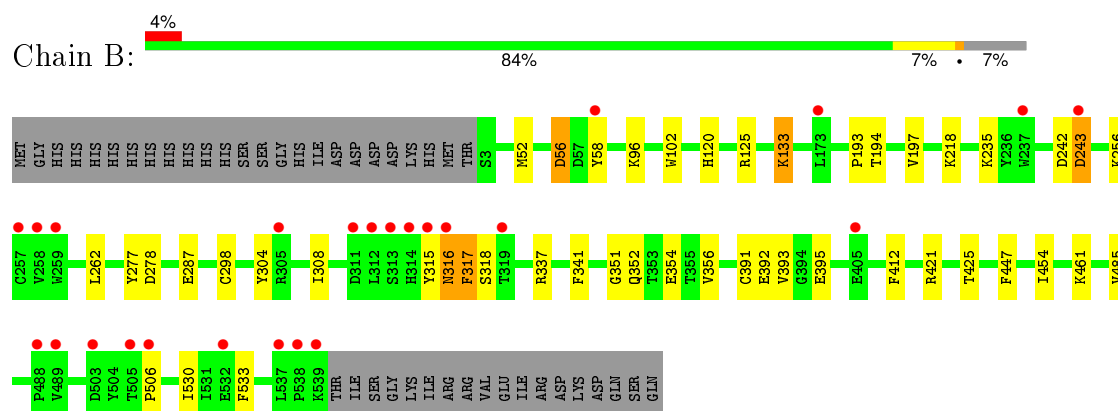
### 3 Residue-property plots [i](#)

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: AMP-binding protein



- Molecule 1: AMP-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.70Å 96.37Å 141.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.10 29.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.88-2.10) 99.9 (29.88-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.175 , 0.207 0.176 , 0.206	Depositor DCC
$R_{free}$ test set	3704 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 61.8	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 85208 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, PGE, FOR, 1PE, EPE, NO3

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	0.49	1/4317 (0.0%)	0.56	0/5869
1	B	0.49	0/4360	0.57	0/5933
All	All	0.49	1/8677 (0.0%)	0.57	0/11802

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	504	TYR	C-O	5.00	1.32	1.23

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	4191	0	3993	32	0
1	B	4233	0	4033	38	0
2	A	2	0	0	0	0
2	B	2	0	0	4	0
3	A	10	0	14	5	0
3	B	20	0	28	2	0
4	A	32	0	44	2	0
5	A	30	0	34	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	17	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	0	0	0
7	B	4	0	0	0	0
8	A	24	0	32	9	0
8	B	18	0	24	1	0
9	A	204	0	0	4	0
9	B	225	0	0	3	0
All	All	9016	0	8219	71	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 4.

All (71) 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:256:LYS:NZ	2:B:999:FOR:C	1.76	1.39
1:B:256:LYS:HZ3	2:B:999:FOR:C	1.32	1.23
1:B:242:ASP:O	1:B:243:ASP:CB	1.91	1.14
1:B:242:ASP:O	1:B:243:ASP:HB2	1.23	1.00
1:B:256:LYS:HZ1	2:B:999:FOR:C	1.59	0.95
1:B:315:TYR:O	1:B:317:PHE:N	2.18	0.76
1:B:56:ASP:HB3	1:B:58:TYR:H	1.50	0.74
9:A:1093:HOH:O	1:B:218:LYS:HE3	1.89	0.73
1:A:454:ILE:HD13	1:A:461:LYS:HE2	1.72	0.71
1:A:56:ASP:HB3	1:A:58:TYR:H	1.53	0.70
8:A:1005:GOL:H31	9:A:1169:HOH:O	1.94	0.67
1:B:391:CYS:HB3	1:B:395:GLU:HG3	1.77	0.66
1:B:485:VAL:HG21	1:B:530:ILE:HD12	1.77	0.66
1:A:485:VAL:HG21	1:A:530:ILE:HD12	1.79	0.64
1:A:353:THR:HG23	8:A:1005:GOL:H12	1.80	0.64
1:B:277:TYR:CZ	5:B:998:EPE:H61	2.34	0.62
8:A:1005:GOL:C3	9:A:1169:HOH:O	2.47	0.62
1:B:447:PHE:CD2	8:B:1003:GOL:H12	2.36	0.61
1:A:415:TYR:CE1	8:A:1004:GOL:H31	2.36	0.61
1:B:352:GLN:HG2	1:B:354:GLU:OE1	2.03	0.59
1:B:256:LYS:NZ	1:B:298:CYS:SG	2.77	0.57
1:A:277:TYR:CZ	5:A:996:EPE:H61	2.40	0.57
1:A:417:LYS:O	1:B:133:LYS:HE3	2.05	0.56
1:B:392:GLU:O	1:B:395:GLU:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ARG:O	1:B:425:THR:HG23	2.06	0.55
1:B:304:TYR:O	1:B:308:ILE:HG12	2.08	0.54
1:A:353:THR:CG2	8:A:1005:GOL:H12	2.38	0.54
1:B:256:LYS:CE	2:B:999:FOR:C	2.73	0.53
1:A:421:ARG:O	1:A:425:THR:HG23	2.10	0.52
1:A:312:LEU:HD12	1:A:341:PHE:HB3	1.92	0.51
1:B:351:GLY:H	3:B:993:PGE:H52	1.75	0.51
1:B:278:ASP:OD2	9:B:1270:HOH:O	2.19	0.51
1:A:378:GLY:HA3	8:A:1002:GOL:H2	1.93	0.51
1:A:392:GLU:HG3	1:A:393:VAL:N	2.26	0.51
1:A:461:LYS:H	4:A:994:1PE:H261	1.77	0.50
1:A:326:ALA:HB1	4:A:994:1PE:H221	1.93	0.49
1:B:454:ILE:HD13	1:B:461:LYS:HE3	1.94	0.49
1:B:287:GLU:HG3	1:B:315:TYR:CE1	2.47	0.49
1:A:96:LYS:HG3	1:A:142:ILE:HD13	1.93	0.48
1:A:447:PHE:CD2	8:A:1003:GOL:H31	2.49	0.48
1:B:242:ASP:O	1:B:243:ASP:HB3	2.03	0.48
1:B:506:PRO:HB3	1:B:533:PHE:CD2	2.48	0.48
1:B:287:GLU:HG3	1:B:315:TYR:CD1	2.50	0.47
1:B:392:GLU:HG3	1:B:393:VAL:N	2.30	0.47
1:B:235:LYS:HE2	9:B:1115:HOH:O	2.14	0.46
1:B:96:LYS:HD3	1:B:120:HIS:CG	2.50	0.46
1:A:288:LYS:HE2	3:A:991:PGE:H32	1.98	0.46
1:B:193:PRO:HB3	1:B:197:VAL:HG13	1.96	0.46
1:B:425:THR:HG21	9:B:1320:HOH:O	2.16	0.46
1:A:425:THR:HG21	9:A:1189:HOH:O	2.15	0.45
1:A:288:LYS:HZ3	3:A:991:PGE:H62	1.81	0.45
1:A:255:GLY:H	8:A:1005:GOL:H11	1.80	0.45
1:A:277:TYR:CE2	5:A:996:EPE:H61	2.52	0.44
1:B:194:THR:O	1:B:197:VAL:HG12	2.18	0.44
1:B:242:ASP:OD2	1:B:242:ASP:O	2.36	0.43
1:A:288:LYS:NZ	3:A:991:PGE:H62	2.33	0.43
1:B:315:TYR:O	1:B:316:ASN:C	2.56	0.43
1:A:392:GLU:CG	1:A:393:VAL:N	2.82	0.43
1:A:288:LYS:NZ	3:A:991:PGE:H22	2.34	0.43
1:A:259:TRP:HH2	1:A:351:GLY:HA3	1.84	0.42
1:A:21:GLN:HA	1:A:377:PRO:HG3	2.01	0.42
1:A:288:LYS:HZ3	3:A:991:PGE:H22	1.84	0.42
1:A:353:THR:HG23	8:A:1005:GOL:C1	2.48	0.42
1:A:312:LEU:HD12	1:A:341:PHE:CB	2.50	0.42
1:B:308:ILE:HD12	1:B:337:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MET:HB2	1:B:52:MET:HE2	1.71	0.41
1:A:476:ALA:HA	1:A:504:TYR:CD2	2.56	0.41
1:A:219:MET:O	1:A:415:TYR:HA	2.21	0.40
1:B:287:GLU:HB3	3:B:992:PGE:H2	2.03	0.40
1:A:392:GLU:CG	1:A:393:VAL:H	2.34	0.40
1:B:52:MET:HE1	1:B:102:TRP:CE2	2.56	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	530/580 (91%)	522 (98%)	6 (1%)	2 (0%)	39	37
1	B	537/580 (93%)	524 (98%)	9 (2%)	4 (1%)	26	21
All	All	1067/1160 (92%)	1046 (98%)	15 (1%)	6 (1%)	30	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	ASP
1	B	316	ASN
1	A	262	LEU
1	B	262	LEU
1	A	356	VAL
1	B	356	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/503 (87%)	427 (98%)	11 (2%)	55	59
1	B	444/503 (88%)	437 (98%)	7 (2%)	70	76
All	All	882/1006 (88%)	864 (98%)	18 (2%)	61	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	15	GLU
1	A	57	ASP
1	A	125	ARG
1	A	182	GLU
1	A	200	LYS
1	A	279	ARG
1	A	288	LYS
1	A	317	PHE
1	A	412	PHE
1	A	414	HIS
1	B	56	ASP
1	B	125	ARG
1	B	133	LYS
1	B	317	PHE
1	B	318	SER
1	B	341	PHE
1	B	412	PHE

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

Mol	Chain	Res	Type
1	A	7	GLN
1	A	336	ASN
1	B	336	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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
7	NO3	A	1001	-	3,3,3	3.15	3 (100%)	3,3,3	0.09	0
8	GOL	A	1002	-	5,5,5	0.34	0	5,5,5	0.73	0
8	GOL	A	1003	-	5,5,5	0.34	0	5,5,5	0.25	0
8	GOL	A	1004	-	5,5,5	0.24	0	5,5,5	0.76	0
8	GOL	A	1005	-	5,5,5	0.55	0	5,5,5	0.53	0
3	PGE	A	991	-	9,9,9	0.56	0	8,8,8	0.22	0
4	1PE	A	994	-	15,15,15	0.52	0	14,14,14	0.36	0
4	1PE	A	995	-	15,15,15	0.54	0	14,14,14	0.20	0
5	EPE	A	996	-	14,15,15	0.46	0	18,20,20	2.21	4 (22%)
5	EPE	A	997	-	14,15,15	0.39	0	18,20,20	1.57	2 (11%)
2	FOR	A	999	-	0,1,1	0.00	-	0,0,0	0.00	-
7	NO3	B	1001	-	3,3,3	3.27	3 (100%)	3,3,3	0.23	0
8	GOL	B	1002	-	5,5,5	0.28	0	5,5,5	0.36	0
8	GOL	B	1003	-	5,5,5	0.30	0	5,5,5	0.43	0
8	GOL	B	1004	-	5,5,5	0.41	0	5,5,5	0.31	0
3	PGE	B	992	-	9,9,9	0.46	0	8,8,8	0.21	0
3	PGE	B	993	-	9,9,9	0.58	0	8,8,8	0.34	0
5	EPE	B	998	-	14,15,15	0.42	0	18,20,20	2.09	5 (27%)
2	FOR	B	999	-	0,1,1	0.00	-	0,0,0	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
7	NO3	A	1001	-	-	0/0/0/0	0/0/0/0
8	GOL	A	1002	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
8	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
3	PGE	A	991	-	-	0/7/7/7	0/0/0/0
4	1PE	A	994	-	-	0/13/13/13	0/0/0/0
4	1PE	A	995	-	-	0/13/13/13	0/0/0/0
5	EPE	A	996	-	-	0/9/19/19	0/1/1/1
5	EPE	A	997	-	-	0/9/19/19	0/1/1/1
2	FOR	A	999	-	-	0/0/0/0	0/0/0/0
7	NO3	B	1001	-	-	0/0/0/0	0/0/0/0
8	GOL	B	1002	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1003	-	-	0/4/4/4	0/0/0/0
8	GOL	B	1004	-	-	0/4/4/4	0/0/0/0
3	PGE	B	992	-	-	0/7/7/7	0/0/0/0
3	PGE	B	993	-	-	0/7/7/7	0/0/0/0
5	EPE	B	998	-	-	0/9/19/19	0/1/1/1
2	FOR	B	999	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1001	NO3	O2-N	2.79	1.39	1.25
7	A	1001	NO3	O3-N	2.86	1.40	1.25
7	B	1001	NO3	O3-N	2.96	1.40	1.25
7	B	1001	NO3	O2-N	3.00	1.40	1.25
7	A	1001	NO3	O1-N	3.71	1.39	1.24
7	B	1001	NO3	O1-N	3.79	1.39	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	998	EPE	C7-N4-C5	2.22	116.95	111.27
5	B	998	EPE	C2-C3-N4	2.30	114.74	110.63
5	B	998	EPE	C7-N4-C3	2.32	117.21	111.27
5	A	996	EPE	C7-N4-C3	2.48	117.62	111.27
5	A	996	EPE	C7-N4-C5	2.67	118.11	111.27
5	A	997	EPE	C7-N4-C5	3.17	119.40	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	997	EPE	C5-N4-C3	4.09	117.75	108.90
5	A	996	EPE	C5-N4-C3	4.58	118.82	108.90
5	B	998	EPE	O1S-S-C10	4.79	110.99	106.91
5	B	998	EPE	C5-N4-C3	5.03	119.78	108.90
5	A	996	EPE	O1S-S-C10	6.44	112.40	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1002	GOL	1	0
8	A	1003	GOL	1	0
8	A	1004	GOL	1	0
8	A	1005	GOL	6	0
3	A	991	PGE	5	0
4	A	994	1PE	2	0
5	A	996	EPE	2	0
8	B	1003	GOL	1	0
3	B	992	PGE	1	0
3	B	993	PGE	1	0
5	B	998	EPE	1	0
2	B	999	FOR	4	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	531/580 (91%)	0.29	36 (6%)	20 28	18, 27, 38, 44	0
1	B	537/580 (92%)	0.23	25 (4%)	35 44	17, 25, 38, 49	0
All	All	1068/1160 (92%)	0.26	61 (5%)	27 35	17, 26, 38, 49	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	TYR	6.4
1	A	318	SER	6.2
1	A	172	VAL	6.1
1	B	314	HIS	5.6
1	A	503	ASP	5.2
1	A	171	ASP	4.5
1	A	504	TYR	4.1
1	B	538	PRO	4.1
1	A	196	GLU	3.9
1	B	313	SER	3.8
1	A	501	THR	3.7
1	B	243	ASP	3.5
1	A	506	PRO	3.5
1	A	489	VAL	3.5
1	B	505	THR	3.3
1	B	506	PRO	3.3
1	B	488	PRO	3.2
1	B	312	LEU	3.2
1	A	488	PRO	3.1
1	A	510	LEU	3.0
1	A	197	VAL	2.9
1	A	500	LEU	2.9
1	A	316	ASN	2.9
1	B	537	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	539	LYS	2.7
1	B	58	TYR	2.7
1	B	311	ASP	2.7
1	B	316	ASN	2.6
1	A	194	THR	2.6
1	B	405	GLU	2.6
1	A	162	PRO	2.5
1	A	387	ASP	2.5
1	A	173	LEU	2.5
1	A	508	ASP	2.5
1	A	305	ARG	2.5
1	B	258	VAL	2.4
1	A	93	LEU	2.4
1	A	15	GLU	2.4
1	A	475	PRO	2.3
1	A	257	CYS	2.3
1	A	258	VAL	2.3
1	A	106	LEU	2.3
1	A	102	TRP	2.3
1	A	306	PHE	2.3
1	A	535	PRO	2.2
1	A	30[A]	GLU	2.2
1	B	237	TRP	2.2
1	A	502	LYS	2.2
1	B	259	TRP	2.2
1	B	319	THR	2.2
1	A	317	PHE	2.2
1	A	509	SER	2.2
1	B	257	CYS	2.1
1	A	505	THR	2.1
1	B	489	VAL	2.1
1	B	305	ARG	2.1
1	A	272	VAL	2.1
1	B	503	ASP	2.0
1	A	478	LEU	2.0
1	B	173	LEU	2.0
1	B	532	GLU	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
7	NO3	B	1001	4/4	0.96	0.17	4.41	37,37,37,38	0
8	GOL	A	1005	6/6	0.86	0.26	2.97	42,44,46,46	0
4	1PE	A	994	16/16	0.85	0.24	2.80	45,48,55,55	0
8	GOL	A	1002	6/6	0.81	0.22	2.76	39,41,41,41	0
8	GOL	B	1004	6/6	0.86	0.22	2.73	41,43,44,45	0
5	EPE	A	997	15/15	0.92	0.15	2.40	42,44,49,52	0
3	PGE	B	993	10/10	0.81	0.26	2.37	40,43,45,46	0
5	EPE	B	998	15/15	0.95	0.17	1.72	34,43,47,47	0
8	GOL	B	1002	6/6	0.98	0.15	1.67	24,26,27,29	0
3	PGE	A	991	10/10	0.69	0.22	1.40	51,55,58,58	0
6	MG	A	1000	1/1	0.87	0.13	0.99	47,47,47,47	0
5	EPE	A	996	15/15	0.94	0.17	0.73	31,40,44,44	0
4	1PE	A	995	16/16	0.77	0.17	0.59	56,57,59,59	0
3	PGE	B	992	10/10	0.92	0.19	0.45	49,50,51,51	0
8	GOL	A	1004	6/6	0.95	0.13	0.38	25,27,27,28	0
7	NO3	A	1001	4/4	0.95	0.13	0.15	37,37,38,38	0
8	GOL	A	1003	6/6	0.93	0.12	0.10	46,47,48,49	0
8	GOL	B	1003	6/6	0.90	0.13	-0.61	33,37,38,40	0
2	FOR	A	999	2/2	0.97	0.10	-2.01	19,19,19,20	0
2	FOR	B	999	2/2	0.97	0.08	-2.98	20,20,20,21	0
6	MG	B	1000	1/1	0.71	0.12	-	58,58,58,58	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.