Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:39 AM GMT

PDB ID	:	3BMA
Title	:	Crystal structure of D-alanyl-lipoteichoic acid synthetase from Streptococcus pneumoniae R6
Authors	:	Patskovsky, Y.; Sridhar, V.; Bonanno, J.B.; Smith, D.; Rutter, M.; Iizuka, M.; Koss, J.; Bain, K.; Gheyi, T.; Wasserman, S.R.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-12-12
Resolution	:	2.24 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

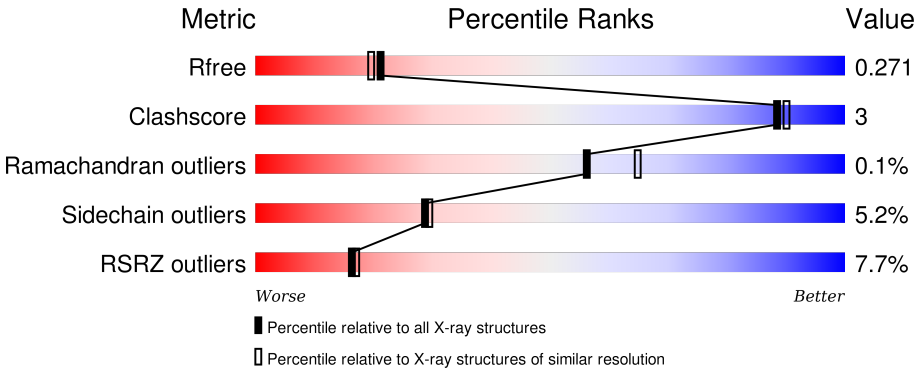
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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 >=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 <=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	407	5% 86% 10% •
1	B	407	4% 86% 9% • •
1	C	407	6% 87% 10% •
1	D	407	% 88% 8% •
1	E	407	6% 85% 11% •

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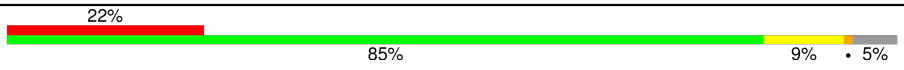
Mol	Chain	Length	Quality of chain
1	F	407	

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	SO4	A	1	-	-	-	X
2	SO4	A	15	-	-	-	X
2	SO4	A	3	-	-	-	X
2	SO4	B	5	-	-	-	X
2	SO4	D	7	-	-	-	X
2	SO4	D	8	-	-	-	X
2	SO4	F	14	-	-	-	X
3	GOL	A	439	-	-	-	X
3	GOL	C	1	-	-	-	X
3	GOL	C	436	-	-	-	X
3	GOL	C	437	-	-	-	X
3	GOL	E	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20324 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 D-alanyl-lipoteichoic acid synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	6	0
			3237	2080	543	604	10			
1	B	393	Total	C	N	O	S	0	6	0
			3255	2092	549	604	10			
1	C	394	Total	C	N	O	S	0	13	0
			3293	2118	552	613	10			
1	D	389	Total	C	N	O	S	0	9	0
			3233	2082	540	600	11			
1	E	390	Total	C	N	O	S	0	3	0
			3208	2058	541	599	10			
1	F	387	Total	C	N	O	S	0	2	0
			3173	2037	533	593	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	EXPRESSION TAG	UNP Q8DN13
A	30	SER	-	EXPRESSION TAG	UNP Q8DN13
A	31	LEU	-	EXPRESSION TAG	UNP Q8DN13
A	217	ARG	CYS	ENGINEERED	UNP Q8DN13
A	428	GLU	-	EXPRESSION TAG	UNP Q8DN13
A	429	GLY	-	EXPRESSION TAG	UNP Q8DN13
A	430	HIS	-	EXPRESSION TAG	UNP Q8DN13
A	431	HIS	-	EXPRESSION TAG	UNP Q8DN13
A	432	HIS	-	EXPRESSION TAG	UNP Q8DN13
A	433	HIS	-	EXPRESSION TAG	UNP Q8DN13
A	434	HIS	-	EXPRESSION TAG	UNP Q8DN13
A	435	HIS	-	EXPRESSION TAG	UNP Q8DN13
B	29	MET	-	EXPRESSION TAG	UNP Q8DN13
B	30	SER	-	EXPRESSION TAG	UNP Q8DN13
B	31	LEU	-	EXPRESSION TAG	UNP Q8DN13
B	217	ARG	CYS	ENGINEERED	UNP Q8DN13
B	428	GLU	-	EXPRESSION TAG	UNP Q8DN13

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	GLY	-	EXPRESSION TAG	UNP Q8DN13
B	430	HIS	-	EXPRESSION TAG	UNP Q8DN13
B	431	HIS	-	EXPRESSION TAG	UNP Q8DN13
B	432	HIS	-	EXPRESSION TAG	UNP Q8DN13
B	433	HIS	-	EXPRESSION TAG	UNP Q8DN13
B	434	HIS	-	EXPRESSION TAG	UNP Q8DN13
B	435	HIS	-	EXPRESSION TAG	UNP Q8DN13
C	29	MET	-	EXPRESSION TAG	UNP Q8DN13
C	30	SER	-	EXPRESSION TAG	UNP Q8DN13
C	31	LEU	-	EXPRESSION TAG	UNP Q8DN13
C	217	ARG	CYS	ENGINEERED	UNP Q8DN13
C	428	GLU	-	EXPRESSION TAG	UNP Q8DN13
C	429	GLY	-	EXPRESSION TAG	UNP Q8DN13
C	430	HIS	-	EXPRESSION TAG	UNP Q8DN13
C	431	HIS	-	EXPRESSION TAG	UNP Q8DN13
C	432	HIS	-	EXPRESSION TAG	UNP Q8DN13
C	433	HIS	-	EXPRESSION TAG	UNP Q8DN13
C	434	HIS	-	EXPRESSION TAG	UNP Q8DN13
C	435	HIS	-	EXPRESSION TAG	UNP Q8DN13
D	29	MET	-	EXPRESSION TAG	UNP Q8DN13
D	30	SER	-	EXPRESSION TAG	UNP Q8DN13
D	31	LEU	-	EXPRESSION TAG	UNP Q8DN13
D	217	ARG	CYS	ENGINEERED	UNP Q8DN13
D	428	GLU	-	EXPRESSION TAG	UNP Q8DN13
D	429	GLY	-	EXPRESSION TAG	UNP Q8DN13
D	430	HIS	-	EXPRESSION TAG	UNP Q8DN13
D	431	HIS	-	EXPRESSION TAG	UNP Q8DN13
D	432	HIS	-	EXPRESSION TAG	UNP Q8DN13
D	433	HIS	-	EXPRESSION TAG	UNP Q8DN13
D	434	HIS	-	EXPRESSION TAG	UNP Q8DN13
D	435	HIS	-	EXPRESSION TAG	UNP Q8DN13
E	29	MET	-	EXPRESSION TAG	UNP Q8DN13
E	30	SER	-	EXPRESSION TAG	UNP Q8DN13
E	31	LEU	-	EXPRESSION TAG	UNP Q8DN13
E	217	ARG	CYS	ENGINEERED	UNP Q8DN13
E	428	GLU	-	EXPRESSION TAG	UNP Q8DN13
E	429	GLY	-	EXPRESSION TAG	UNP Q8DN13
E	430	HIS	-	EXPRESSION TAG	UNP Q8DN13
E	431	HIS	-	EXPRESSION TAG	UNP Q8DN13
E	432	HIS	-	EXPRESSION TAG	UNP Q8DN13
E	433	HIS	-	EXPRESSION TAG	UNP Q8DN13
E	434	HIS	-	EXPRESSION TAG	UNP Q8DN13

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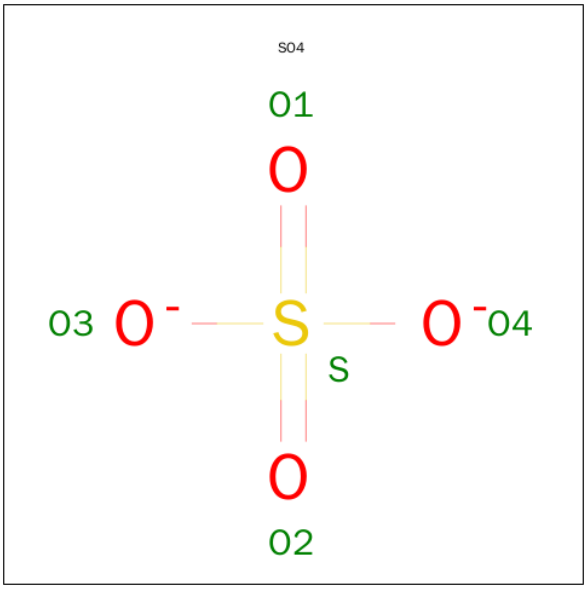
Chain	Residue	Modelled	Actual	Comment	Reference
E	435	HIS	-	EXPRESSION TAG	UNP Q8DN13
F	29	MET	-	EXPRESSION TAG	UNP Q8DN13
F	30	SER	-	EXPRESSION TAG	UNP Q8DN13
F	31	LEU	-	EXPRESSION TAG	UNP Q8DN13
F	217	ARG	CYS	ENGINEERED	UNP Q8DN13
F	428	GLU	-	EXPRESSION TAG	UNP Q8DN13
F	429	GLY	-	EXPRESSION TAG	UNP Q8DN13
F	430	HIS	-	EXPRESSION TAG	UNP Q8DN13
F	431	HIS	-	EXPRESSION TAG	UNP Q8DN13
F	432	HIS	-	EXPRESSION TAG	UNP Q8DN13
F	433	HIS	-	EXPRESSION TAG	UNP Q8DN13
F	434	HIS	-	EXPRESSION TAG	UNP Q8DN13
F	435	HIS	-	EXPRESSION TAG	UNP Q8DN13

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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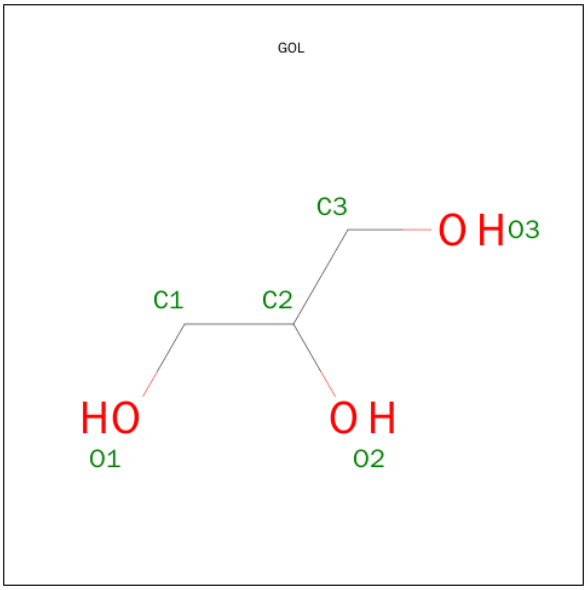
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

- 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 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

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

- Molecule 4 is water.

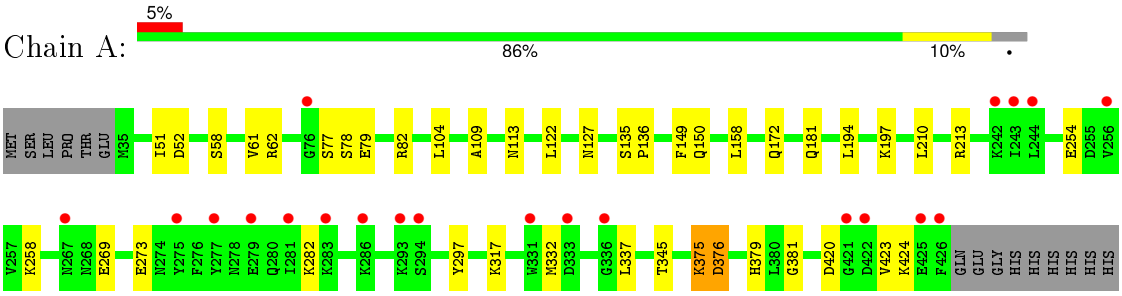
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	159	Total O 159 159	0	0
4	B	176	Total O 176 176	0	0
4	C	141	Total O 141 141	0	0
4	D	175	Total O 175 175	0	0
4	E	102	Total O 102 102	0	0
4	F	42	Total O 42 42	0	0

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.

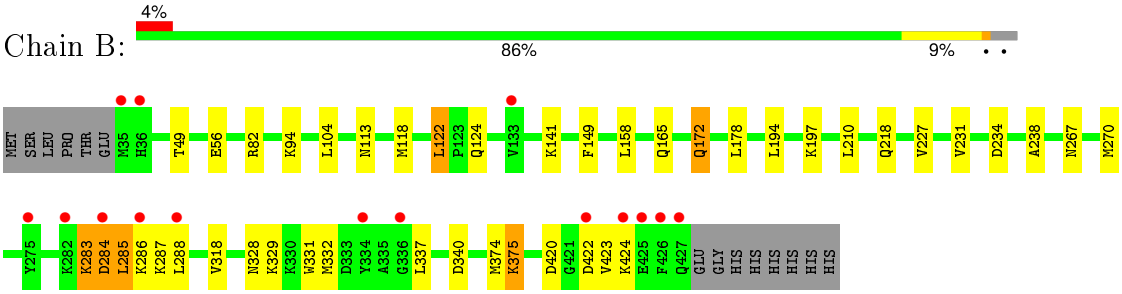
- Molecule 1: D-alanyl-lipoteichoic acid synthetase

Chain A:



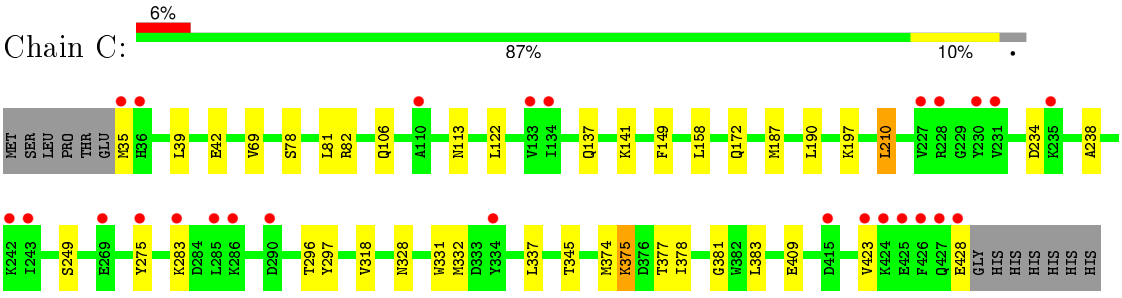
- Molecule 1: D-alanyl-lipoteichoic acid synthetase

Chain B:



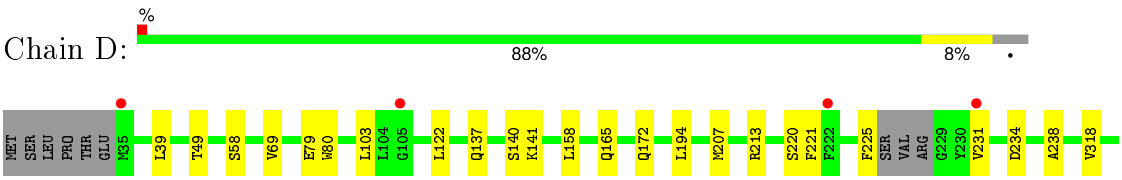
- Molecule 1: D-alanyl-lipoteichoic acid synthetase

Chain C:



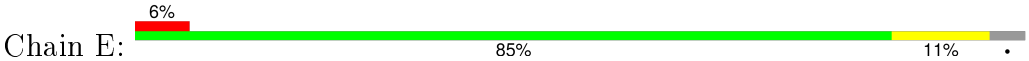
- Molecule 1: D-alanyl-lipoteichoic acid synthetase

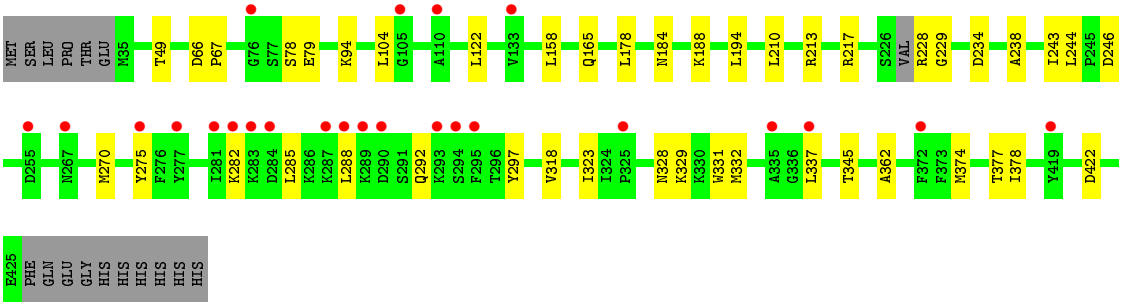
Chain D:



• Molecule 1: D-alanyl-lipoteichoic acid synthetase

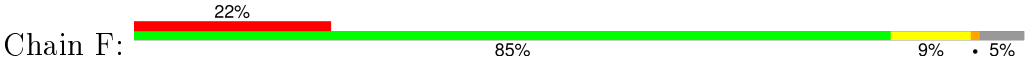
Chain E:

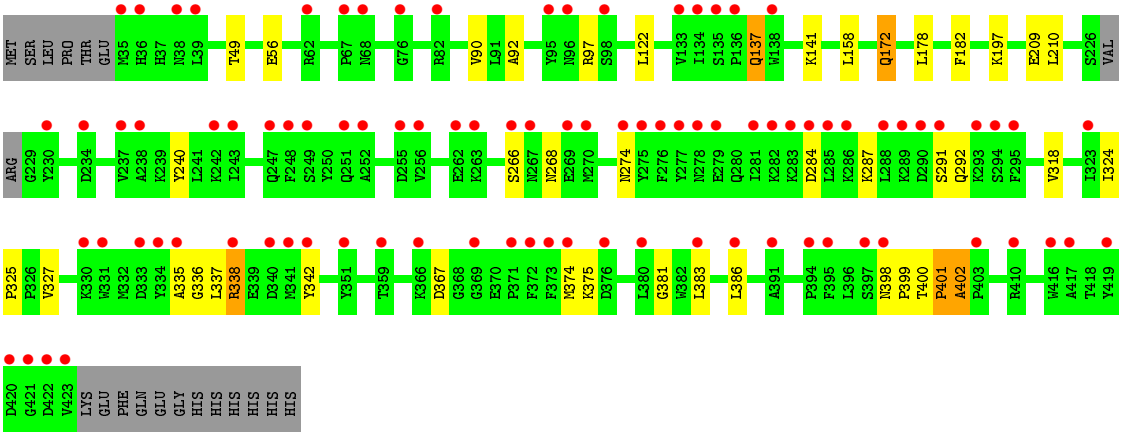




• Molecule 1: D-alanyl-lipoteichoic acid synthetase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.96Å 148.06Å 208.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.24 34.24 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.24) 99.3 (34.24-2.24)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.214 , 0.271 0.214 , 0.271	Depositor DCC
R_{free} test set	4142 reflections (3.12%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 137151 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20324	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.37	0/3341	0.55	0/4511
1	B	0.38	0/3362	0.55	0/4537
1	C	0.36	0/3418	0.53	0/4612
1	D	0.37	0/3345	0.56	0/4512
1	E	0.36	0/3301	0.55	1/4456 (0.0%)
1	F	0.37	0/3263	0.51	0/4407
All	All	0.37	0/20030	0.54	1/27035 (0.0%)

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	F	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	210	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	335	ALA	Peptide
1	F	336	GLY	Peptide
1	F	400	THR	Peptide

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Mol	Chain	Res	Type	Group
1	F	401	PRO	Peptide

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	3237	0	3145	17	0
1	B	3255	0	3175	23	0
1	C	3293	0	3226	20	0
1	D	3233	0	3154	7	0
1	E	3208	0	3107	16	0
1	F	3173	0	3067	18	0
2	A	15	0	0	0	0
2	B	25	0	0	1	0
2	D	20	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
3	A	30	0	40	2	0
3	C	24	0	32	2	0
3	E	6	0	8	1	0
4	A	159	0	0	0	0
4	B	176	0	0	1	0
4	C	141	0	0	3	0
4	D	175	0	0	0	0
4	E	102	0	0	1	0
4	F	42	0	0	1	0
All	All	20324	0	18954	97	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 3.

All (97) 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:284:ASP:OD2	1:B:287:LYS:HE3	1.68	0.93
1:B:285:LEU:N	1:B:285:LEU:HD12	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137[A]:GLN:NE2	2:F:14:SO4:O1	2.21	0.73
1:F:337:LEU:O	1:F:338:ARG:HB2	1.96	0.66
1:D:221:PHE:HZ	1:F:182:PHE:HB3	1.63	0.63
1:A:297:TYR:HB2	1:A:345:THR:HG21	1.81	0.62
1:B:113:ASN:HD21	1:B:149:PHE:HA	1.64	0.61
1:B:284:ASP:OD2	1:B:287:LYS:CE	2.45	0.61
1:B:172:GLN:HG3	1:B:197:LYS:HG2	1.82	0.61
1:C:113:ASN:HD21	1:C:149:PHE:HA	1.67	0.59
1:C:172:GLN:HG3	1:C:197:LYS:HG2	1.86	0.58
1:C:332:MET:HB2	1:C:337:LEU:HB3	1.86	0.57
1:B:332:MET:HB2	1:B:337:LEU:HB3	1.85	0.57
1:F:375:LYS:HB2	1:F:381:GLY:HA3	1.87	0.56
1:B:285:LEU:N	1:B:285:LEU:CD1	2.68	0.56
1:B:285:LEU:O	1:B:286:LYS:C	2.44	0.55
1:F:337:LEU:O	1:F:338:ARG:CB	2.53	0.55
1:A:51:ILE:H	3:A:436:GOL:H2	1.71	0.55
1:B:284:ASP:HB3	1:B:287:LYS:HG3	1.89	0.55
1:C:296:THR:H	3:C:437:GOL:H2	1.71	0.55
1:A:113:ASN:HD21	1:A:149:PHE:HA	1.72	0.55
3:A:438:GOL:H12	1:B:218:GLN:HG2	1.89	0.54
1:F:266:SER:H	1:F:274:ASN:HD21	1.55	0.54
1:A:210:LEU:HD21	1:B:210:LEU:HD21	1.88	0.54
1:B:285:LEU:O	1:B:288:LEU:N	2.41	0.54
1:F:90:VAL:HG21	1:F:240:TYR:HB2	1.90	0.54
1:C:297:TYR:HB2	1:C:345[A]:THR:HG21	1.89	0.54
1:D:221:PHE:CZ	1:F:182:PHE:HB3	2.43	0.54
1:C:210[A]:LEU:CD2	4:C:480:HOH:O	2.56	0.53
1:D:58:SER:HB3	1:D:220:SER:HA	1.90	0.53
1:B:285:LEU:H	1:B:285:LEU:HD12	1.72	0.52
1:E:165:GLN:HG2	1:E:194:LEU:HD21	1.90	0.52
1:A:376:ASP:HB3	1:A:379:HIS:H	1.75	0.52
1:A:332:MET:HB2	1:A:337:LEU:HB3	1.93	0.51
1:B:124:GLN:NE2	2:B:4:SO4:O4	2.41	0.51
1:B:165:GLN:HG2	1:B:194:LEU:HD21	1.92	0.51
1:B:234:ASP:HA	1:B:238:ALA:HB3	1.93	0.50
1:F:401:PRO:O	1:F:402:ALA:HB3	2.11	0.49
1:E:217:ARG:NH1	4:E:473:HOH:O	2.45	0.49
1:A:375:LYS:HB2	1:A:381:GLY:HA3	1.95	0.49
1:B:285:LEU:CD1	1:B:285:LEU:H	2.24	0.48
1:C:377:THR:HG23	1:C:378:ILE:HG12	1.95	0.48
1:F:284:ASP:HB3	1:F:287:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:SER:O	1:A:62:ARG:HB2	2.14	0.47
1:B:328:ASN:HB3	1:B:331:TRP:HB3	1.97	0.47
1:E:234:ASP:HA	1:E:238:ALA:HB3	1.95	0.47
1:E:292:GLN:HB3	1:E:337:LEU:HD23	1.96	0.47
1:A:254:GLU:O	1:A:258:LYS:HB2	2.15	0.47
1:F:172:GLN:HG3	1:F:197:LYS:HG2	1.96	0.47
1:C:375:LYS:HB2	1:C:381:GLY:HA3	1.97	0.47
1:D:39:LEU:HD13	1:D:69:VAL:HG21	1.97	0.46
1:C:81:LEU:HD21	1:C:106:GLN:HE22	1.80	0.46
1:A:213:ARG:HH22	1:E:213:ARG:HH22	1.63	0.46
1:F:398:ASN:HA	1:F:399:PRO:HD3	1.87	0.45
1:F:292:GLN:CD	1:F:337:LEU:HD12	2.37	0.45
1:A:77[B]:SER:OG	1:A:109:ALA:O	2.33	0.45
1:D:234:ASP:HA	1:D:238:ALA:HB3	1.99	0.45
1:E:329:LYS:HA	1:E:332:MET:HG2	1.99	0.45
1:E:285:LEU:HA	1:E:288:LEU:HD12	1.99	0.44
1:E:184:ASN:HA	1:E:188:LYS:HD2	2.00	0.44
1:C:39:LEU:HD13	1:C:69:VAL:HG21	2.00	0.44
1:F:383:LEU:HA	1:F:386:LEU:HD12	1.99	0.44
1:C:328:ASN:HB3	1:C:331:TRP:HB3	2.00	0.43
1:E:229:GLY:HA2	3:E:1:GOL:H11	2.00	0.43
1:E:297:TYR:HB2	1:E:345:THR:HG21	1.99	0.43
1:C:210[A]:LEU:HD23	4:C:480:HOH:O	2.19	0.43
1:C:383:LEU:HB3	3:C:1:GOL:H32	2.01	0.43
1:C:234:ASP:HA	1:C:238:ALA:HB3	2.00	0.43
1:F:92:ALA:HA	1:F:97:ARG:HD2	2.01	0.43
1:E:323:ILE:HG13	1:E:362:ALA:HB3	2.00	0.43
1:C:42:GLU:HA	4:C:533:HOH:O	2.17	0.43
1:E:377:THR:HG23	1:E:378:ILE:HG12	2.01	0.42
1:F:56:GLU:HG3	4:F:436:HOH:O	2.19	0.42
1:B:329:LYS:HA	1:B:332:MET:HG2	2.02	0.42
1:C:297:TYR:HB2	1:C:345[B]:THR:HG21	2.02	0.42
1:D:80:TRP:HB3	1:D:103:LEU:HD13	2.02	0.41
1:B:113:ASN:ND2	4:B:478:HOH:O	2.54	0.41
1:E:66:ASP:HA	1:E:67:PRO:HD3	1.81	0.41
1:A:150:GLN:HG3	1:A:181:GLN:HE21	1.86	0.41
1:E:328:ASN:HB3	1:E:331:TRP:HB3	2.02	0.41
1:F:325:PRO:O	1:F:342:TYR:OH	2.38	0.41
1:A:127:ASN:HD21	1:A:317:LYS:HD2	1.86	0.41
1:B:283:LYS:H	1:B:283:LYS:HG2	1.72	0.41
1:E:282:LYS:HA	1:E:285:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ARG:HB3	1:B:375:LYS:HE2	2.03	0.41
1:F:324:ILE:HA	1:F:325:PRO:HD3	1.90	0.41
1:D:165:GLN:HG2	1:D:194:LEU:HD21	2.03	0.40
1:A:82:ARG:HB3	1:A:375:LYS:HE2	2.03	0.40
1:A:172:GLN:HG3	1:A:197[B]:LYS:HG2	2.03	0.40
1:A:79:GLU:HG2	1:A:79:GLU:H	1.68	0.40
1:B:118:MET:O	1:B:122:LEU:HD13	2.22	0.40
1:A:135:SER:HA	1:A:136:PRO:HD3	1.93	0.40
1:E:332:MET:HB2	1:E:337:LEU:HB3	2.03	0.40
1:C:187:MET:HB3	1:C:190:LEU:HD12	2.03	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	396/407 (97%)	381 (96%)	15 (4%)	0	100	100
1	B	398/407 (98%)	385 (97%)	12 (3%)	1 (0%)	46	51
1	C	405/407 (100%)	393 (97%)	12 (3%)	0	100	100
1	D	393/407 (97%)	380 (97%)	13 (3%)	0	100	100
1	E	389/407 (96%)	371 (95%)	18 (5%)	0	100	100
1	F	385/407 (95%)	362 (94%)	21 (6%)	2 (0%)	34	34
All	All	2366/2442 (97%)	2272 (96%)	91 (4%)	3 (0%)	56	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	402	ALA
1	B	284	ASP
1	F	338	ARG

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	349/357 (98%)	333 (95%)	16 (5%)	33	36
1	B	351/357 (98%)	328 (93%)	23 (7%)	21	19
1	C	358/357 (100%)	338 (94%)	20 (6%)	26	25
1	D	349/357 (98%)	328 (94%)	21 (6%)	24	22
1	E	344/357 (96%)	327 (95%)	17 (5%)	31	33
1	F	340/357 (95%)	324 (95%)	16 (5%)	32	35
All	All	2091/2142 (98%)	1978 (95%)	113 (5%)	29	27

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	61	VAL
1	A	78	SER
1	A	104	LEU
1	A	122	LEU
1	A	158	LEU
1	A	194	LEU
1	A	269[A]	GLU
1	A	269[B]	GLU
1	A	273	GLU
1	A	282	LYS
1	A	375	LYS
1	A	376	ASP
1	A	420	ASP
1	A	423	VAL
1	A	424	LYS
1	B	49	THR
1	B	56	GLU
1	B	94	LYS
1	B	104	LEU
1	B	122	LEU
1	B	141	LYS

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	172	GLN
1	B	178	LEU
1	B	227	VAL
1	B	231	VAL
1	B	267	ASN
1	B	270	MET
1	B	283	LYS
1	B	285	LEU
1	B	318	VAL
1	B	340	ASP
1	B	374	MET
1	B	375	LYS
1	B	420	ASP
1	B	422	ASP
1	B	423	VAL
1	B	424	LYS
1	C	35	MET
1	C	78	SER
1	C	82[A]	ARG
1	C	82[B]	ARG
1	C	122	LEU
1	C	137	GLN
1	C	141	LYS
1	C	158	LEU
1	C	210[A]	LEU
1	C	210[B]	LEU
1	C	249	SER
1	C	275	TYR
1	C	283	LYS
1	C	318	VAL
1	C	374	MET
1	C	375	LYS
1	C	409[A]	GLU
1	C	409[B]	GLU
1	C	423	VAL
1	C	428	GLU
1	D	49	THR
1	D	79	GLU
1	D	122	LEU
1	D	137[A]	GLN
1	D	137[B]	GLN

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Mol	Chain	Res	Type
1	D	140	SER
1	D	141	LYS
1	D	158	LEU
1	D	172	GLN
1	D	207	MET
1	D	213	ARG
1	D	225	PHE
1	D	231	VAL
1	D	318	VAL
1	D	329	LYS
1	D	337	LEU
1	D	375	LYS
1	D	380	LEU
1	D	383	LEU
1	D	385	TRP
1	D	422	ASP
1	E	49	THR
1	E	78	SER
1	E	79	GLU
1	E	94	LYS
1	E	104	LEU
1	E	122	LEU
1	E	158	LEU
1	E	178	LEU
1	E	228	ARG
1	E	243	ILE
1	E	244	LEU
1	E	246	ASP
1	E	270	MET
1	E	275	TYR
1	E	318	VAL
1	E	374	MET
1	E	422	ASP
1	F	49	THR
1	F	122	LEU
1	F	137[A]	GLN
1	F	137[B]	GLN
1	F	141	LYS
1	F	158	LEU
1	F	172	GLN
1	F	178	LEU
1	F	209	GLU

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Mol	Chain	Res	Type
1	F	210	LEU
1	F	268	ASN
1	F	291	SER
1	F	318	VAL
1	F	327	VAL
1	F	367	ASP
1	F	374	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	124	GLN
1	A	127	ASN
1	A	150	GLN
1	A	164	HIS
1	B	38	ASN
1	B	113	ASN
1	B	127	ASN
1	B	150	GLN
1	B	184	ASN
1	B	267	ASN
1	B	319	ASN
1	B	344	GLN
1	B	360	ASN
1	C	106	GLN
1	C	113	ASN
1	C	124	GLN
1	C	150	GLN
1	C	343	GLN
1	C	344	GLN
1	C	360	ASN
1	C	408	ASN
1	D	106	GLN
1	D	150	GLN
1	D	280	GLN
1	D	398	ASN
1	E	124	GLN
1	E	127	ASN
1	E	150	GLN
1	E	192	GLN
1	E	344	GLN

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Mol	Chain	Res	Type
1	E	360	ASN
1	E	408	ASN
1	F	38	ASN
1	F	106	GLN
1	F	124	GLN
1	F	172	GLN
1	F	274	ASN
1	F	319	ASN
1	F	344	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.07	0
2	SO4	A	15	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	A	3	-	4,4,4	0.25	0	6,6,6	0.09	0
3	GOL	A	436	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	A	437	-	5,5,5	0.32	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	A	438	-	5,5,5	0.35	0	5,5,5	0.14	0
3	GOL	A	439	-	5,5,5	0.33	0	5,5,5	0.17	0
3	GOL	A	440	-	5,5,5	0.35	0	5,5,5	0.20	0
2	SO4	B	10	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	2	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	B	4	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	B	5	-	4,4,4	0.28	0	6,6,6	0.07	0
2	SO4	B	6	-	4,4,4	0.22	0	6,6,6	0.13	0
3	GOL	C	1	-	5,5,5	0.31	0	5,5,5	0.22	0
3	GOL	C	436	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GOL	C	437	-	5,5,5	0.45	0	5,5,5	0.30	0
3	GOL	C	438	-	5,5,5	0.33	0	5,5,5	0.30	0
2	SO4	D	11	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	D	7	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	D	8	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	D	9	-	4,4,4	0.19	0	6,6,6	0.13	0
3	GOL	E	1	-	5,5,5	0.36	0	5,5,5	0.27	0
2	SO4	E	13	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	F	14	-	4,4,4	0.26	0	6,6,6	0.13	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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	A	15	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
3	GOL	A	436	-	-	0/4/4/4	0/0/0/0
3	GOL	A	437	-	-	0/4/4/4	0/0/0/0
3	GOL	A	438	-	-	0/4/4/4	0/0/0/0
3	GOL	A	439	-	-	0/4/4/4	0/0/0/0
3	GOL	A	440	-	-	0/4/4/4	0/0/0/0
2	SO4	B	10	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4	-	-	0/0/0/0	0/0/0/0
2	SO4	B	5	-	-	0/0/0/0	0/0/0/0
2	SO4	B	6	-	-	0/0/0/0	0/0/0/0
3	GOL	C	1	-	-	0/4/4/4	0/0/0/0
3	GOL	C	436	-	-	0/4/4/4	0/0/0/0
3	GOL	C	437	-	-	0/4/4/4	0/0/0/0
3	GOL	C	438	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	11	-	-	0/0/0/0	0/0/0/0
2	SO4	D	7	-	-	0/0/0/0	0/0/0/0
2	SO4	D	8	-	-	0/0/0/0	0/0/0/0
2	SO4	D	9	-	-	0/0/0/0	0/0/0/0
3	GOL	E	1	-	-	0/4/4/4	0/0/0/0
2	SO4	E	13	-	-	0/0/0/0	0/0/0/0
2	SO4	F	14	-	-	0/0/0/0	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.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	436	GOL	1	0
3	A	438	GOL	1	0
2	B	4	SO4	1	0
3	C	1	GOL	1	0
3	C	437	GOL	1	0
3	E	1	GOL	1	0
2	F	14	SO4	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	392/407 (96%)	0.14	21 (5%) 29 31	15, 38, 80, 110	0
1	B	393/407 (96%)	0.05	15 (3%) 44 46	13, 39, 79, 108	0
1	C	394/407 (96%)	0.19	26 (6%) 22 23	19, 43, 83, 122	0
1	D	389/407 (95%)	-0.16	4 (1%) 84 85	17, 34, 63, 103	0
1	E	390/407 (95%)	0.22	24 (6%) 24 25	18, 46, 95, 111	0
1	F	387/407 (95%)	1.10	91 (23%) 1 1	22, 73, 114, 126	0
All	All	2345/2442 (96%)	0.26	181 (7%) 16 17	13, 43, 96, 126	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	421	GLY	8.6
1	F	372	PHE	8.2
1	F	36	HIS	7.6
1	F	35	MET	7.4
1	E	283	LYS	6.5
1	F	286	LYS	6.2
1	F	275	TYR	6.2
1	A	426	PHE	5.8
1	F	371	PRO	5.8
1	F	269	GLU	5.8
1	B	36	HIS	5.7
1	B	275	TYR	5.7
1	E	275	TYR	5.6
1	F	283	LYS	5.5
1	C	35	MET	5.4
1	F	335	ALA	5.3
1	F	67	PRO	5.1
1	F	331	TRP	5.0
1	A	281	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	231	VAL	4.8
1	F	284	ASP	4.7
1	E	284	ASP	4.6
1	F	419	TYR	4.5
1	F	95	TYR	4.5
1	C	228	ARG	4.5
1	F	248	PHE	4.4
1	B	425	GLU	4.3
1	F	278	ASN	4.3
1	F	334	TYR	4.2
1	C	275	TYR	4.2
1	F	333	ASP	4.1
1	C	231	VAL	4.0
1	B	35	MET	3.9
1	A	277	TYR	3.9
1	A	275	TYR	3.9
1	F	267	ASN	3.9
1	F	420	ASP	3.8
1	F	289	LYS	3.8
1	B	424	LYS	3.8
1	F	351	TYR	3.7
1	C	283	LYS	3.7
1	F	279	GLU	3.7
1	F	68	ASN	3.7
1	F	281	ILE	3.6
1	A	242	LYS	3.6
1	F	293	LYS	3.6
1	F	422	ASP	3.6
1	F	39	LEU	3.6
1	F	98	SER	3.5
1	F	417	ALA	3.5
1	A	283	LYS	3.5
1	F	242	LYS	3.4
1	F	291	SER	3.4
1	B	334	TYR	3.4
1	C	424	LYS	3.4
1	C	425	GLU	3.4
1	A	243	ILE	3.4
1	A	425	GLU	3.3
1	E	290	ASP	3.3
1	E	294	SER	3.3
1	B	427	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	35[A]	MET	3.3
1	F	340	ASP	3.3
1	C	285	LEU	3.2
1	E	337	LEU	3.2
1	C	428	GLU	3.2
1	F	323	ILE	3.1
1	F	290	ASP	3.1
1	F	416	TRP	3.1
1	A	422	ASP	3.1
1	F	294	SER	3.1
1	E	295	PHE	3.1
1	C	36	HIS	3.0
1	F	274	ASN	3.0
1	B	133	VAL	3.0
1	F	262	GLU	2.9
1	E	288	LEU	2.9
1	F	270	MET	2.9
1	F	282	LYS	2.9
1	E	372	PHE	2.9
1	F	82[A]	ARG	2.8
1	F	373	PHE	2.8
1	F	251	GLN	2.8
1	E	335	ALA	2.8
1	F	391	ALA	2.8
1	C	227	VAL	2.8
1	E	133	VAL	2.8
1	F	249	SER	2.8
1	E	293	LYS	2.8
1	F	423	VAL	2.8
1	C	427	GLN	2.8
1	D	222	PHE	2.8
1	F	369	GLY	2.8
1	C	423	VAL	2.7
1	F	410	ARG	2.7
1	C	286	LYS	2.7
1	F	342	TYR	2.7
1	A	244	LEU	2.7
1	F	134	ILE	2.7
1	C	426	PHE	2.7
1	F	243	ILE	2.7
1	C	269	GLU	2.7
1	E	255	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	242	LYS	2.7
1	F	255	ASP	2.6
1	A	256	VAL	2.6
1	F	256	VAL	2.6
1	F	138	TRP	2.6
1	A	279	GLU	2.6
1	A	267	ASN	2.6
1	F	238	ALA	2.6
1	F	285	LEU	2.6
1	F	380	LEU	2.6
1	C	243	ILE	2.6
1	F	359	THR	2.6
1	E	277	TYR	2.6
1	F	252	ALA	2.6
1	F	277	TYR	2.5
1	A	294	SER	2.5
1	F	398	ASN	2.5
1	F	383	LEU	2.5
1	F	263	LYS	2.5
1	D	105	GLY	2.5
1	F	266	SER	2.5
1	C	334	TYR	2.5
1	F	386	LEU	2.5
1	C	133	VAL	2.5
1	A	336	GLY	2.4
1	B	336	GLY	2.4
1	B	284	ASP	2.4
1	F	76	GLY	2.4
1	F	96	ASN	2.4
1	B	426	PHE	2.4
1	F	395	PHE	2.4
1	E	419	TYR	2.4
1	B	282	LYS	2.4
1	F	397	SER	2.4
1	F	403	PRO	2.4
1	F	295	PHE	2.4
1	F	330	LYS	2.4
1	A	421	GLY	2.3
1	F	341	MET	2.3
1	B	422	ASP	2.3
1	F	234	ASP	2.3
1	E	281	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	288	LEU	2.3
1	F	374	MET	2.3
1	F	338	ARG	2.2
1	F	247	GLN	2.2
1	E	325	PRO	2.2
1	E	282	LYS	2.2
1	E	267	ASN	2.2
1	F	38	ASN	2.2
1	F	133	VAL	2.2
1	F	366	LYS	2.2
1	F	394	PRO	2.2
1	A	331	TRP	2.2
1	B	286	LYS	2.2
1	C	110	ALA	2.2
1	F	135	SER	2.1
1	A	333	ASP	2.1
1	C	290	ASP	2.1
1	E	110	ALA	2.1
1	E	289	LYS	2.1
1	F	237	VAL	2.1
1	F	136	PRO	2.1
1	A	286	LYS	2.1
1	C	415	ASP	2.1
1	A	76	GLY	2.1
1	F	288	LEU	2.1
1	E	105	GLY	2.1
1	C	235	LYS	2.1
1	F	376	ASP	2.1
1	F	276	PHE	2.1
1	C	230	TYR	2.1
1	F	230	TYR	2.1
1	C	134	ILE	2.1
1	E	76	GLY	2.0
1	A	293	LYS	2.0
1	E	287	LYS	2.0
1	F	62	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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^{th} 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^2)	Q<0.9
3	GOL	C	436	6/6	0.73	0.40	10.76	49,65,72,74	0
3	GOL	A	439	6/6	0.87	0.24	6.88	68,70,72,74	0
3	GOL	C	437	6/6	0.88	0.29	6.62	51,55,60,63	0
2	SO4	B	5	5/5	0.95	0.28	5.62	26,30,38,40	5
2	SO4	A	1	5/5	0.81	0.23	5.56	44,46,54,56	5
3	GOL	C	1	6/6	0.68	0.32	4.54	69,72,77,77	0
2	SO4	D	8	5/5	0.88	0.28	4.03	26,39,41,50	5
2	SO4	D	7	5/5	0.97	0.34	3.66	38,40,45,50	5
2	SO4	F	14	5/5	0.93	0.36	3.02	59,60,62,62	5
2	SO4	A	3	5/5	0.96	0.33	2.82	40,47,52,54	5
2	SO4	A	15	5/5	0.92	0.19	2.38	39,39,49,49	5
3	GOL	E	1	6/6	0.82	0.24	2.30	51,67,73,79	0
3	GOL	A	437	6/6	0.90	0.17	0.92	28,51,60,66	0
3	GOL	A	436	6/6	0.92	0.15	0.52	37,42,56,62	0
3	GOL	A	438	6/6	0.96	0.13	0.33	27,43,49,61	0
2	SO4	B	2	5/5	0.97	0.10	-0.86	72,77,79,82	0
2	SO4	B	10	5/5	0.91	0.16	-0.90	46,47,50,56	5
2	SO4	E	13	5/5	0.93	0.14	-1.31	103,106,108,108	0
2	SO4	B	6	5/5	0.95	0.14	-	34,41,49,50	5
2	SO4	B	4	5/5	0.94	0.16	-	34,38,41,43	5
2	SO4	D	9	5/5	0.93	0.15	-	21,25,35,40	5
3	GOL	A	440	6/6	0.88	0.22	-	72,79,82,83	0
2	SO4	D	11	5/5	0.92	0.12	-	35,40,46,48	5
3	GOL	C	438	6/6	0.76	0.32	-	81,85,88,89	0

6.5 Other polymers (i)

There are no such residues in this entry.