



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:01 PM UTC

PDB ID : 3BMA / pdb_00003bma
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

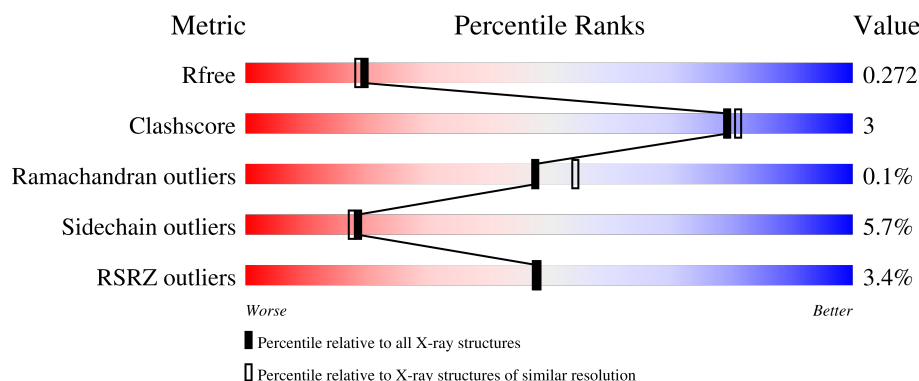
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	% 84% 11% ..
1	B	407	% 85% 10% ..
1	C	407	% 86% 10% ..
1	D	407	% 87% 8% .

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	407	% 86% 10% • •
1	F	407	13% 84% 10% • 5%

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 mutation	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 mutation	UNP Q8DN13
B	428	GLU	-	expression tag	UNP Q8DN13

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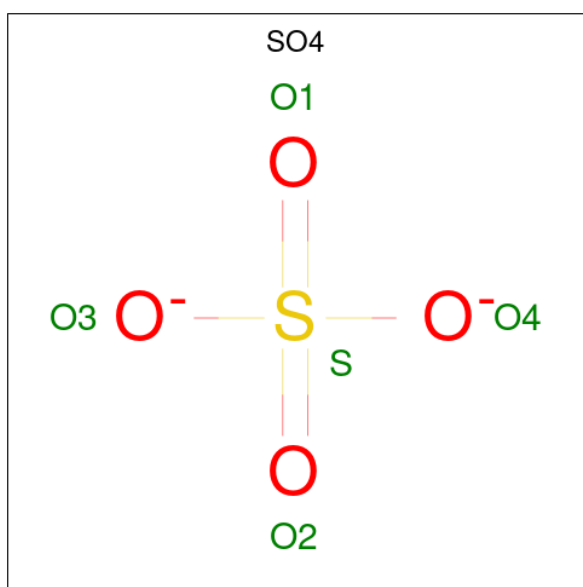
Chain	Residue	Modelled	Actual	Comment	Reference
B	429	GLY	-	expression tag	UNP Q8DN13
B	430	HIS	-	expression tag	UNP Q8DN13
B	431	HIS	-	expression tag	UNP Q8DN13
B	432	HIS	-	expression tag	UNP Q8DN13
B	433	HIS	-	expression tag	UNP Q8DN13
B	434	HIS	-	expression tag	UNP Q8DN13
B	435	HIS	-	expression tag	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 mutation	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 mutation	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 mutation	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 mutation	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 (CCD ID: SO4) (formula: O₄S).



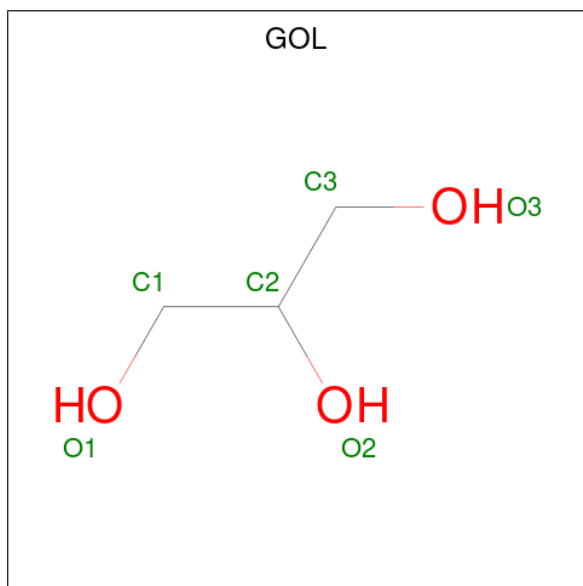
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

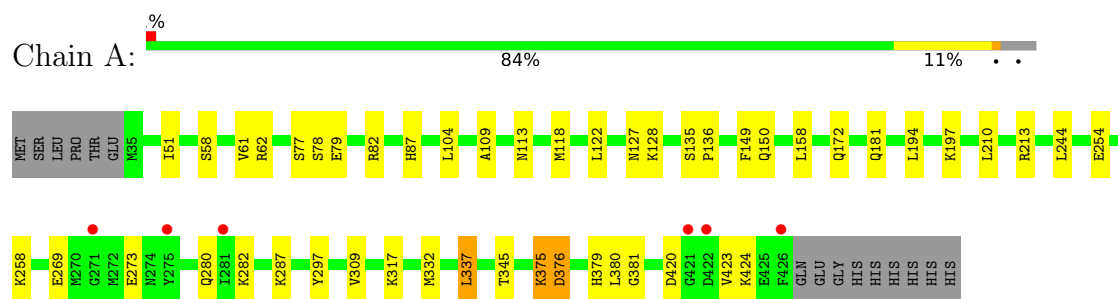
- Molecule 4 is water.

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

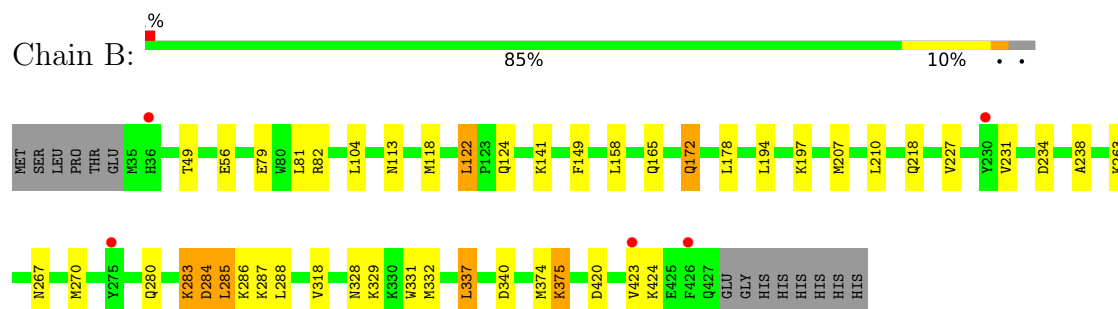
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

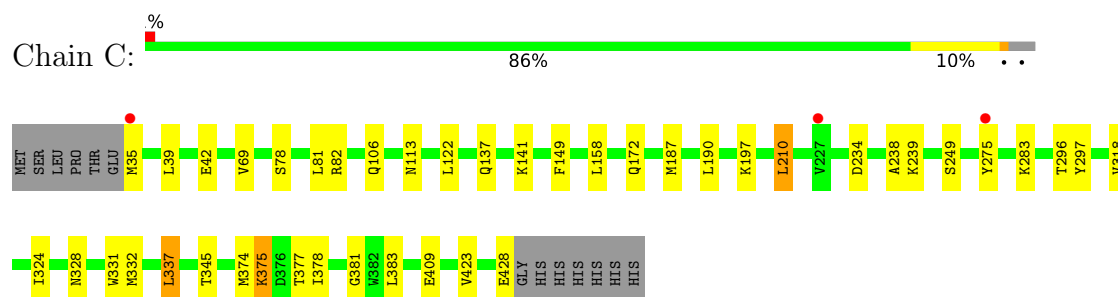
- Molecule 1: D-alanyl-lipoteichoic acid synthetase



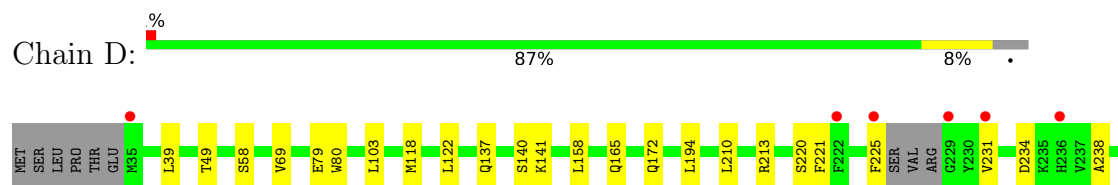
- Molecule 1: D-alanyl-lipoteichoic acid synthetase



- Molecule 1: D-alanyl-lipoteichoic acid synthetase

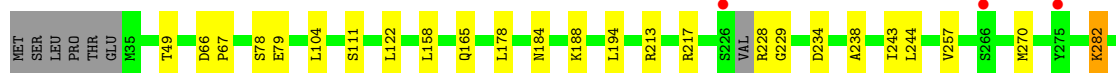
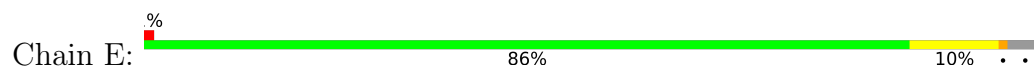


- Molecule 1: D-alanyl-lipoteichoic acid synthetase

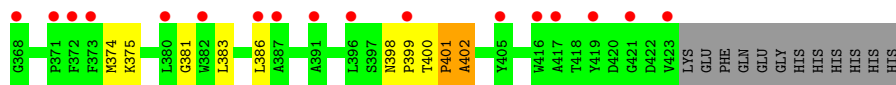
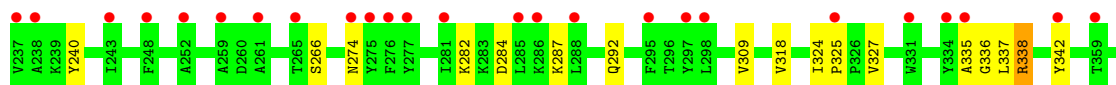
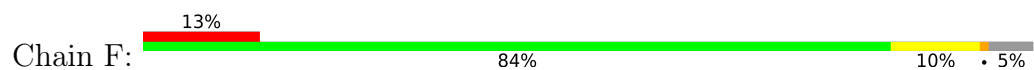




• Molecule 1: D-alanyl-lipoteichoic acid synthetase



• Molecule 1: D-alanyl-lipoteichoic acid synthetase



4 Data and refinement statistics

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 20.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.24) 99.1 (20.00-2.24)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.214 , 0.271 0.215 , 0.272	Depositor DCC
R_{free} test set	4146 reflections (3.00%)	wwPDB-VP
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 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.47	0/3341	0.89	2/4511 (0.0%)
1	B	0.48	0/3362	0.88	0/4537
1	C	0.46	0/3418	0.87	2/4612 (0.0%)
1	D	0.46	0/3345	0.88	0/4512
1	E	0.46	0/3301	0.87	1/4456 (0.0%)
1	F	0.47	0/3263	0.84	0/4407
All	All	0.47	0/20030	0.87	5/27035 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	324	ILE	CA-C-N	5.58	123.67	119.66
1	C	324	ILE	C-N-CA	5.58	123.67	119.66
1	A	87	HIS	CA-C-N	5.35	125.42	119.32
1	A	87	HIS	C-N-CA	5.35	125.42	119.32
1	E	111	SER	N-CA-C	5.02	117.48	111.71

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
1	F	401	PRO	Peptide

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	3237	0	3145	19	0
1	B	3255	0	3175	25	0
1	C	3293	0	3226	20	0
1	D	3233	0	3154	9	0
1	E	3208	0	3107	16	0
1	F	3173	0	3067	19	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	0	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	102	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 (102) 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:HD12	1:B:285:LEU:N	2.03	0.74
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:D:210:LEU:HD11	1:F:207:MET:HE1	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:B:285:LEU:O	1:B:286:LYS:C	2.44	0.60
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: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:A:113:ASN:HD21	1:A:149:PHE:HA	1.72	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
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:C:297:TYR:HB2	1:C:345[A]:THR:HG21	1.89	0.54
1:F:90:VAL:HG21	1:F:240:TYR:HB2	1.90	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:HD12	1:B:285:LEU:H	1.72	0.52
1:D:118:MET:HE1	1:D:309:VAL:HG13	1.91	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:292:GLN:CD	1:F:337:LEU:HD12	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:58:SER:O	1:A:62:ARG:HB2	2.14	0.47
1:F:284:ASP:HB3	1:F:287:LYS:HG2	1.97	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: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:B:284:ASP:CG	1:B:287:LYS:HE3	2.41	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:234:ASP:HA	1:C:238:ALA:HB3	2.00	0.43
1:C:383:LEU:HB3	3:C:1:GOL:H32	2.01	0.43
1:F:92:ALA:HA	1:F:97:ARG:HD2	2.01	0.43
1:F:118:MET:HE1	1:F:309:VAL:HG13	2.01	0.43
1:C:42:GLU:HA	4:C:533:HOH:O	2.17	0.43
1:E:323:ILE:HG13	1:E:362:ALA:HB3	2.00	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:A:150:GLN:HG3	1:A:181:GLN:HE21	1.86	0.41
1:E:66:ASP:HA	1:E:67:PRO:HD3	1.81	0.41
1:E:328:ASN:HB3	1:E:331:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:PRO:O	1:F:342:TYR:OH	2.38	0.41
1:A:118:MET:HE1	1:A:309:VAL:HG13	2.03	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:B:82:ARG:HB3	1:B:375:LYS:HE2	2.03	0.41
1:E:282:LYS:HA	1:E:285:LEU:HD23	2.02	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:79:GLU:H	1:A:79:GLU:HG2	1.68	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:210:LEU:HD11	1:B:207:MET:HE1	2.03	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:C:187:MET:HB3	1:C:190:LEU:HD12	2.03	0.40
1:E:332:MET:HB2	1:E:337:LEU:HB3	2.03	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	396/407 (97%)	381 (96%)	15 (4%)	0	100	100
1	B	398/407 (98%)	385 (97%)	12 (3%)	1 (0%)	36	38
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%)	24	23
All	All	2366/2442 (97%)	2272 (96%)	91 (4%)	3 (0%)	48	54

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%)	328 (94%)	21 (6%)	17	16
1	B	351/357 (98%)	325 (93%)	26 (7%)	13	10
1	C	358/357 (100%)	336 (94%)	22 (6%)	17	15
1	D	349/357 (98%)	328 (94%)	21 (6%)	17	16
1	E	344/357 (96%)	326 (95%)	18 (5%)	21	20
1	F	340/357 (95%)	327 (96%)	13 (4%)	29	34
All	All	2091/2142 (98%)	1970 (94%)	121 (6%)	18	17

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	78	SER
1	A	104	LEU
1	A	122	LEU
1	A	128	LYS
1	A	158	LEU
1	A	194	LEU
1	A	244	LEU
1	A	269[A]	GLU
1	A	269[B]	GLU
1	A	273	GLU
1	A	280	GLN
1	A	282	LYS
1	A	287	LYS

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Mol	Chain	Res	Type
1	A	337	LEU
1	A	375	LYS
1	A	376	ASP
1	A	380	LEU
1	A	420	ASP
1	A	423	VAL
1	A	424	LYS
1	B	49	THR
1	B	56	GLU
1	B	79	GLU
1	B	81	LEU
1	B	104	LEU
1	B	122	LEU
1	B	141	LYS
1	B	158	LEU
1	B	172	GLN
1	B	178	LEU
1	B	227	VAL
1	B	231	VAL
1	B	263	LYS
1	B	267	ASN
1	B	270	MET
1	B	280	GLN
1	B	283	LYS
1	B	285	LEU
1	B	318	VAL
1	B	337	LEU
1	B	340	ASP
1	B	374	MET
1	B	375	LYS
1	B	420	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

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Mol	Chain	Res	Type
1	C	210[B]	LEU
1	C	239	LYS
1	C	249	SER
1	C	275	TYR
1	C	283	LYS
1	C	318	VAL
1	C	337	LEU
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
1	D	140	SER
1	D	141	LYS
1	D	158	LEU
1	D	172	GLN
1	D	213	ARG
1	D	225	PHE
1	D	231	VAL
1	D	258	LYS
1	D	270	MET
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	422	ASP
1	E	49	THR
1	E	78	SER
1	E	79	GLU
1	E	104	LEU
1	E	122	LEU
1	E	158	LEU
1	E	178	LEU
1	E	228	ARG

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Mol	Chain	Res	Type
1	E	243	ILE
1	E	244	LEU
1	E	257	VAL
1	E	270	MET
1	E	282	LYS
1	E	318	VAL
1	E	323	ILE
1	E	337	LEU
1	E	374	MET
1	E	422	ASP
1	F	49	THR
1	F	104	LEU
1	F	122	LEU
1	F	141	LYS
1	F	158	LEU
1	F	172	GLN
1	F	178	LEU
1	F	209	GLU
1	F	210	LEU
1	F	282	LYS
1	F	318	VAL
1	F	327	VAL
1	F	374	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	113	ASN
1	A	150	GLN
1	A	164	HIS
1	A	172	GLN
1	A	180	GLN
1	A	184	ASN
1	A	192	GLN
1	A	280	GLN
1	B	38	ASN
1	B	113	ASN
1	B	127	ASN
1	B	151	GLN
1	B	184	ASN
1	B	267	ASN

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Mol	Chain	Res	Type
1	B	312	GLN
1	B	344	GLN
1	B	408	ASN
1	C	106	GLN
1	C	113	ASN
1	C	137	GLN
1	C	150	GLN
1	C	218	GLN
1	C	247	GLN
1	C	251	GLN
1	C	280	GLN
1	C	312	GLN
1	C	344	GLN
1	C	360	ASN
1	C	408	ASN
1	D	37	HIS
1	D	119	GLN
1	D	124	GLN
1	D	142	ASN
1	D	150	GLN
1	D	151	GLN
1	D	280	GLN
1	D	312	GLN
1	D	398	ASN
1	E	120	GLN
1	E	124	GLN
1	E	127	ASN
1	E	150	GLN
1	E	172	GLN
1	E	192	GLN
1	E	205	ASN
1	E	267	ASN
1	E	344	GLN
1	E	408	ASN
1	F	38	ASN
1	F	106	GLN
1	F	267	ASN
1	F	274	ASN
1	F	319	ASN
1	F	328	ASN
1	F	344	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	8	-	4,4,4	0.18	0	6,6,6	0.14	0
3	GOL	E	1	-	5,5,5	0.40	0	5,5,5	0.36	0
2	SO4	B	4	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	A	15	-	4,4,4	0.23	0	6,6,6	0.14	0
3	GOL	C	1	-	5,5,5	0.34	0	5,5,5	0.26	0
2	SO4	B	10	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	E	13	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	A	3	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	D	7	-	4,4,4	0.23	0	6,6,6	0.08	0
3	GOL	C	438	-	5,5,5	0.37	0	5,5,5	0.30	0
2	SO4	B	6	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	F	14	-	4,4,4	0.23	0	6,6,6	0.13	0
3	GOL	A	439	-	5,5,5	0.37	0	5,5,5	0.22	0
3	GOL	A	440	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	A	436	-	5,5,5	0.39	0	5,5,5	0.34	0
2	SO4	D	11	-	4,4,4	0.23	0	6,6,6	0.12	0
3	GOL	A	438	-	5,5,5	0.38	0	5,5,5	0.24	0
2	SO4	B	5	-	4,4,4	0.25	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	437	-	5,5,5	0.34	0	5,5,5	0.47	0
2	SO4	A	1	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	D	9	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	B	2	-	4,4,4	0.24	0	6,6,6	0.14	0
3	GOL	C	437	-	5,5,5	0.46	0	5,5,5	0.37	0
3	GOL	C	436	-	5,5,5	0.38	0	5,5,5	0.31	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
3	GOL	A	440	-	-	2/4/4/4	-
3	GOL	E	1	-	-	2/4/4/4	-
3	GOL	A	436	-	-	4/4/4/4	-
3	GOL	A	438	-	-	3/4/4/4	-
3	GOL	C	438	-	-	2/4/4/4	-
3	GOL	A	437	-	-	4/4/4/4	-
3	GOL	A	439	-	-	2/4/4/4	-
3	GOL	C	437	-	-	4/4/4/4	-
3	GOL	C	1	-	-	4/4/4/4	-
3	GOL	C	436	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	436	GOL	O1-C1-C2-C3
3	A	436	GOL	C1-C2-C3-O3
3	A	437	GOL	O1-C1-C2-O2
3	A	437	GOL	O1-C1-C2-C3
3	A	438	GOL	C1-C2-C3-O3
3	A	438	GOL	O2-C2-C3-O3
3	A	439	GOL	O1-C1-C2-C3
3	A	440	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	440	GOL	O2-C2-C3-O3
3	C	1	GOL	C1-C2-C3-O3
3	C	436	GOL	O1-C1-C2-C3
3	A	437	GOL	C1-C2-C3-O3
3	C	1	GOL	O1-C1-C2-C3
3	C	437	GOL	O1-C1-C2-C3
3	C	437	GOL	C1-C2-C3-O3
3	C	438	GOL	C1-C2-C3-O3
3	E	1	GOL	O1-C1-C2-C3
3	A	436	GOL	O1-C1-C2-O2
3	A	436	GOL	O2-C2-C3-O3
3	A	439	GOL	O1-C1-C2-O2
3	C	1	GOL	O2-C2-C3-O3
3	C	437	GOL	O1-C1-C2-O2
3	E	1	GOL	O1-C1-C2-O2
3	C	436	GOL	O1-C1-C2-O2
3	C	438	GOL	O2-C2-C3-O3
3	A	437	GOL	O2-C2-C3-O3
3	C	1	GOL	O1-C1-C2-O2
3	A	438	GOL	O1-C1-C2-C3
3	C	437	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	GOL	1	0
2	B	4	SO4	1	0
3	C	1	GOL	1	0
3	A	436	GOL	1	0
3	A	438	GOL	1	0
3	C	437	GOL	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, 95th 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%)	-0.12	6 (1%) 72 73	15, 38, 80, 110	6 (1%)
1	B	393/407 (96%)	-0.24	5 (1%) 75 77	13, 39, 79, 108	6 (1%)
1	C	394/407 (96%)	-0.04	3 (0%) 82 84	16, 43, 83, 122	13 (3%)
1	D	389/407 (95%)	-0.35	6 (1%) 72 73	17, 34, 62, 103	9 (2%)
1	E	390/407 (95%)	0.01	6 (1%) 72 73	18, 46, 95, 111	3 (0%)
1	F	387/407 (95%)	0.84	54 (13%) 6 5	22, 73, 114, 126	2 (0%)
All	All	2345/2442 (96%)	0.02	80 (3%) 48 48	13, 43, 96, 126	39 (1%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	372	PHE	5.8
1	F	229	GLY	4.0
1	D	35[A]	MET	3.9
1	F	371	PRO	3.9
1	F	423	VAL	3.7
1	F	231	VAL	3.6
1	D	225	PHE	3.5
1	F	373	PHE	3.5
1	F	421	GLY	3.4
1	E	423	VAL	3.3
1	C	227	VAL	3.2
1	F	281	ILE	3.1
1	F	416	TRP	3.1
1	F	275	TYR	3.1
1	A	271	GLY	3.1
1	E	275	TYR	3.0
1	D	229	GLY	3.0
1	F	35	MET	3.0
1	D	222	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	95	TYR	2.9
1	F	237	VAL	2.9
1	F	243	ILE	2.8
1	F	368	GLY	2.8
1	F	342	TYR	2.7
1	B	426	PHE	2.7
1	F	261	ALA	2.6
1	A	426	PHE	2.6
1	B	423	VAL	2.6
1	F	288	LEU	2.6
1	B	275	TYR	2.6
1	F	39	LEU	2.6
1	F	36	HIS	2.6
1	F	331	TRP	2.5
1	E	226	SER	2.5
1	F	419	TYR	2.5
1	C	35	MET	2.5
1	F	259	ALA	2.5
1	F	248	PHE	2.4
1	F	236	HIS	2.4
1	F	386	LEU	2.4
1	A	275	TYR	2.4
1	F	387	ALA	2.4
1	F	226	SER	2.4
1	F	297	TYR	2.4
1	F	325	PRO	2.4
1	F	391	ALA	2.4
1	A	422	ASP	2.3
1	F	399	PRO	2.3
1	A	281	ILE	2.3
1	E	337	LEU	2.3
1	D	231	VAL	2.3
1	F	274	ASN	2.3
1	F	359	THR	2.3
1	F	286	LYS	2.3
1	F	295	PHE	2.2
1	F	285	LEU	2.2
1	F	265	THR	2.2
1	C	275	TYR	2.2
1	F	405	TYR	2.2
1	F	233	TYR	2.1
1	F	277	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	421	GLY	2.1
1	F	238	ALA	2.1
1	F	335	ALA	2.1
1	F	334	TYR	2.1
1	B	36	HIS	2.1
1	F	82[A]	ARG	2.1
1	F	417	ALA	2.1
1	B	230	TYR	2.1
1	E	369	GLY	2.1
1	E	266	SER	2.1
1	D	236	HIS	2.1
1	F	380	LEU	2.1
1	F	67	PRO	2.1
1	F	90	VAL	2.1
1	F	252	ALA	2.0
1	F	298	LEU	2.0
1	F	396	LEU	2.0
1	F	276	PHE	2.0
1	F	382	TRP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	1	6/6	0.74	0.17	69,72,77,77	0
2	SO4	A	1	5/5	0.75	0.12	44,46,54,56	5
3	GOL	C	438	6/6	0.75	0.15	81,85,88,89	0
2	SO4	D	11	5/5	0.78	0.13	35,40,46,48	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	E	13	5/5	0.79	0.11	103,106,108,108	0
3	GOL	C	436	6/6	0.81	0.14	49,65,72,74	0
2	SO4	D	8	5/5	0.81	0.15	26,39,41,50	5
3	GOL	E	1	6/6	0.82	0.19	51,67,73,79	0
2	SO4	F	14	5/5	0.83	0.13	59,60,62,62	5
2	SO4	B	4	5/5	0.84	0.14	34,38,41,43	5
3	GOL	A	437	6/6	0.85	0.13	28,51,60,66	0
3	GOL	A	440	6/6	0.85	0.13	72,79,82,83	0
2	SO4	B	10	5/5	0.85	0.10	46,47,50,56	5
3	GOL	A	439	6/6	0.86	0.17	68,70,72,74	0
3	GOL	C	437	6/6	0.87	0.17	51,55,60,63	0
2	SO4	B	6	5/5	0.88	0.13	34,41,49,50	5
2	SO4	A	15	5/5	0.88	0.14	39,39,49,49	5
3	GOL	A	436	6/6	0.89	0.12	37,42,56,62	0
2	SO4	D	7	5/5	0.90	0.14	38,40,45,50	5
2	SO4	B	2	5/5	0.90	0.12	72,77,79,82	0
2	SO4	A	3	5/5	0.91	0.17	40,47,52,54	5
2	SO4	B	5	5/5	0.91	0.12	26,30,38,40	5
3	GOL	A	438	6/6	0.93	0.09	27,43,49,61	0
2	SO4	D	9	5/5	0.93	0.09	21,25,35,40	5

6.5 Other polymers

There are no such residues in this entry.