Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 02:18 PM EST

PDB ID	:	3C48
Title	:	Structure of the retaining glycosyltransferase MshA: The first step in mycothiol biosynthesis. Organism: Corynebacterium glutamicum- APO (OPEN) structure.
Authors	:	Vetting, M.W.; Frantom, P.A.; Blanchard, J.S.
Deposited on	:	2008-01-29
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

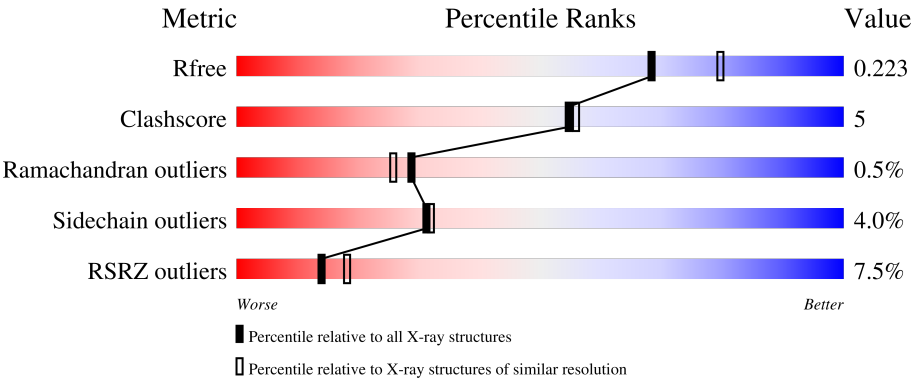
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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 <=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	438	9% 78% 11% • 9%
1	B	438	4% 77% 12% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6593 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 Predicted glycosyltransferases.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3087	1933	551	591	12			
1	B	396	Total	C	N	O	S	0	0	0
			3061	1917	549	583	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8NTA6
A	-18	GLY	-	expression tag	UNP Q8NTA6
A	-17	SER	-	expression tag	UNP Q8NTA6
A	-16	SER	-	expression tag	UNP Q8NTA6
A	-15	HIS	-	expression tag	UNP Q8NTA6
A	-14	HIS	-	expression tag	UNP Q8NTA6
A	-13	HIS	-	expression tag	UNP Q8NTA6
A	-12	HIS	-	expression tag	UNP Q8NTA6
A	-11	HIS	-	expression tag	UNP Q8NTA6
A	-10	HIS	-	expression tag	UNP Q8NTA6
A	-9	SER	-	expression tag	UNP Q8NTA6
A	-8	SER	-	expression tag	UNP Q8NTA6
A	-7	GLY	-	expression tag	UNP Q8NTA6
A	-6	LEU	-	expression tag	UNP Q8NTA6
A	-5	VAL	-	expression tag	UNP Q8NTA6
A	-4	PRO	-	expression tag	UNP Q8NTA6
A	-3	ARG	-	expression tag	UNP Q8NTA6
A	-2	GLY	-	expression tag	UNP Q8NTA6
A	-1	SER	-	expression tag	UNP Q8NTA6
A	0	HIS	-	expression tag	UNP Q8NTA6
B	-19	MET	-	expression tag	UNP Q8NTA6
B	-18	GLY	-	expression tag	UNP Q8NTA6
B	-17	SER	-	expression tag	UNP Q8NTA6
B	-16	SER	-	expression tag	UNP Q8NTA6
B	-15	HIS	-	expression tag	UNP Q8NTA6

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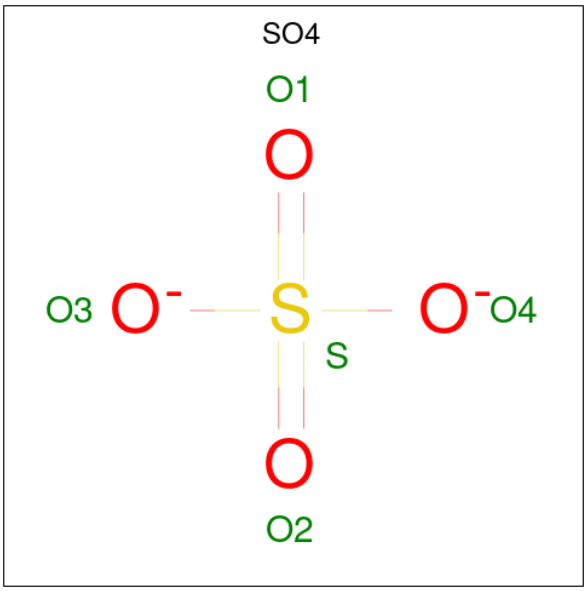
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8NTA6
B	-13	HIS	-	expression tag	UNP Q8NTA6
B	-12	HIS	-	expression tag	UNP Q8NTA6
B	-11	HIS	-	expression tag	UNP Q8NTA6
B	-10	HIS	-	expression tag	UNP Q8NTA6
B	-9	SER	-	expression tag	UNP Q8NTA6
B	-8	SER	-	expression tag	UNP Q8NTA6
B	-7	GLY	-	expression tag	UNP Q8NTA6
B	-6	LEU	-	expression tag	UNP Q8NTA6
B	-5	VAL	-	expression tag	UNP Q8NTA6
B	-4	PRO	-	expression tag	UNP Q8NTA6
B	-3	ARG	-	expression tag	UNP Q8NTA6
B	-2	GLY	-	expression tag	UNP Q8NTA6
B	-1	SER	-	expression tag	UNP Q8NTA6
B	0	HIS	-	expression tag	UNP Q8NTA6

- 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

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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	B	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

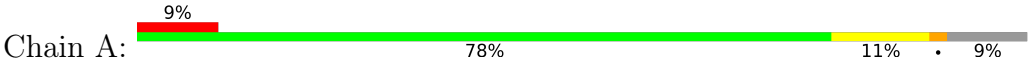
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	170	Total O 170 170	0	0
3	B	235	Total O 235 235	0	0

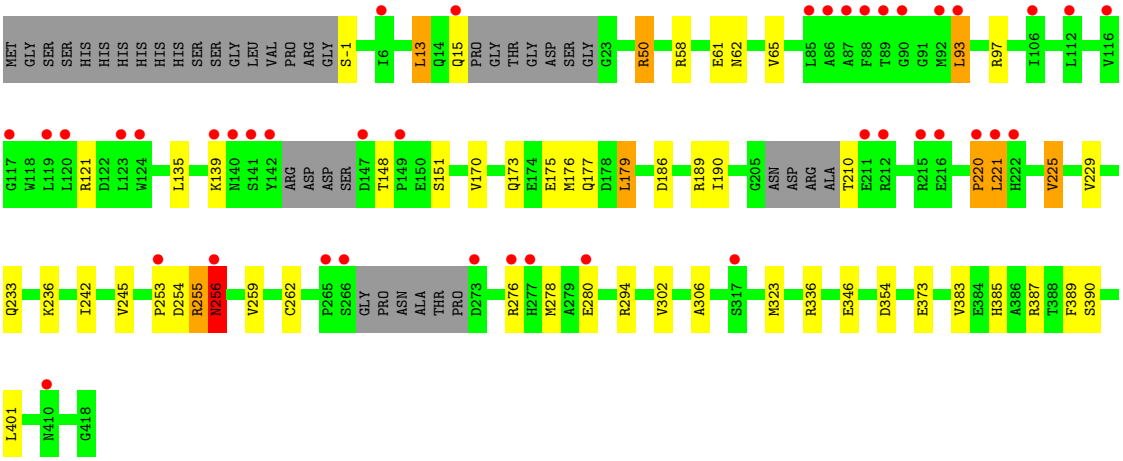
3 Residue-property plots (i)

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

• Molecule 1: Predicted glycosyltransferases

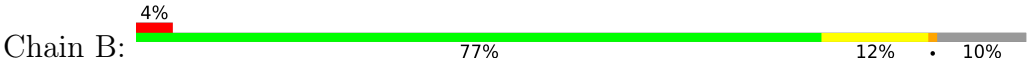
Chain A:

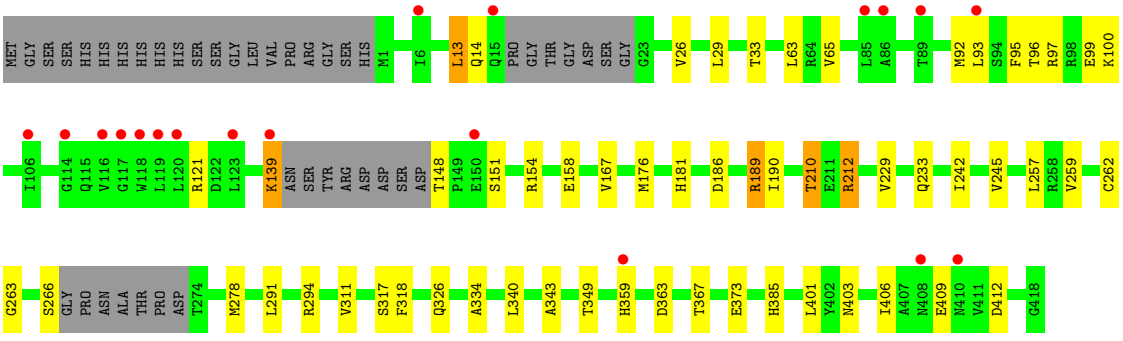




• Molecule 1: Predicted glycosyltransferases

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	79.74Å 79.74Å 148.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.53 – 2.10 34.53 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.53-2.10) 98.7 (34.53-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.222 0.179 , 0.223	Depositor DCC
R_{free} test set	3075 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.035 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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, 0.333 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: 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	0.77	5/3148 (0.2%)	0.78	4/4278 (0.1%)
1	B	0.74	0/3121	0.75	1/4242 (0.0%)
All	All	0.76	5/6269 (0.1%)	0.77	5/8520 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ASP	CG-OD1	-13.96	0.93	1.25
1	A	253	PRO	CA-C	7.06	1.67	1.52
1	A	255	ARG	NE-CZ	5.58	1.40	1.33
1	A	255	ARG	CD-NE	-5.45	1.37	1.46
1	A	253	PRO	C-O	-5.23	1.12	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254	ASP	CB-CG-OD1	-9.09	110.12	118.30
1	A	254	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	A	254	ASP	OD1-CG-OD2	7.84	138.19	123.30
1	B	318	PHE	N-CA-CB	7.50	124.10	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	ASN	N-CA-C	5.81	126.68	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	ASN	Peptide
1	B	317	SER	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	3087	0	3033	33	0
1	B	3061	0	3022	30	0
2	A	15	0	0	1	0
2	B	25	0	0	2	0
3	A	170	0	0	2	0
3	B	235	0	0	4	0
All	All	6593	0	6055	63	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 5.

All (63) 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:A:50:ARG:HH21	1:A:50:ARG:HG2	1.30	0.95
1:B:210:THR:HG21	3:B:537:HOH:O	1.70	0.92
1:B:412:ASP:OD1	3:B:542:HOH:O	1.96	0.82
1:A:186:ASP:OD2	1:A:189:ARG:NH2	2.22	0.73
1:A:220:PRO:HA	1:A:221:LEU:HB2	1.73	0.70
1:A:323:MET:HG2	1:A:390:SER:CB	2.24	0.68
1:B:242:ILE:HB	1:B:278:MET:HE1	1.74	0.68
1:A:58:ARG:HH21	1:A:62:ASN:H	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:HD2	2:A:420:SO4:O1	1.95	0.66
1:A:229:VAL:HA	1:A:262:CYS:O	1.96	0.66
1:A:135:LEU:HD11	1:A:179:LEU:HD13	1.77	0.66
1:A:13:LEU:HD13	1:A:65:VAL:HG21	1.79	0.65
1:A:50:ARG:HG2	1:A:50:ARG:NH2	2.05	0.65
1:B:13:LEU:HD13	1:B:65:VAL:HG21	1.77	0.65
1:A:225:VAL:HG22	1:A:306:ALA:HA	1.78	0.64
1:B:406:ILE:O	1:B:409:GLU:HG2	1.98	0.63
1:A:323:MET:HG2	1:A:390:SER:OG	2.01	0.61
1:B:139:LYS:HD3	2:B:423:SO4:O3	2.01	0.60
1:B:212:ARG:HD3	2:B:421:SO4:O2	2.02	0.59
1:A:276:ARG:O	1:A:280:GLU:HG3	2.02	0.59
1:A:242:ILE:HB	1:A:278:MET:HE2	1.88	0.56
1:B:363:ASP:O	1:B:367:THR:HG23	2.05	0.56
1:A:173:GLN:O	1:A:177:GLN:HG3	2.09	0.53
1:A:176:MET:HG3	1:A:190:ILE:HG21	1.91	0.53
1:B:176:MET:HG3	1:B:190:ILE:HG21	1.91	0.53
1:B:409:GLU:HG3	1:B:409:GLU:O	2.09	0.52
1:B:373:GLU:H	1:B:373:GLU:CD	2.13	0.52
1:B:186:ASP:HB3	1:B:189:ARG:HG2	1.92	0.51
1:A:336:ARG:NH2	1:A:346:GLU:OE1	2.43	0.51
1:A:323:MET:HG2	1:A:390:SER:HB2	1.93	0.50
1:A:245:VAL:HG21	1:A:259:VAL:HG21	1.93	0.50
1:B:334:ALA:HB1	1:B:340:LEU:HD13	1.94	0.50
1:B:167:VAL:HG11	1:B:401:LEU:HD11	1.93	0.49
1:A:58:ARG:NH2	1:A:62:ASN:H	2.07	0.49
1:B:148:THR:N	1:B:151:SER:HG	2.10	0.49
1:A:383:VAL:O	1:A:387:ARG:HG3	2.12	0.49
1:A:170:VAL:HB	1:A:175:GLU:HB3	1.95	0.48
1:B:343:ALA:O	1:B:385:HIS:HE1	1.97	0.48
1:B:93:LEU:O	1:B:97:ARG:HG3	2.15	0.47
1:A:336:ARG:HD2	1:A:354:ASP:OD1	2.15	0.46
1:B:181:HIS:HD2	3:B:595:HOH:O	1.99	0.46
1:B:326:GLN:NE2	1:B:349:THR:OG1	2.49	0.46
1:A:93:LEU:O	1:A:97:ARG:HG3	2.16	0.46
1:A:135:LEU:HD11	1:A:179:LEU:CD1	2.44	0.45
1:A:189:ARG:HD3	3:A:464:HOH:O	2.16	0.45
1:A:255:ARG:CG	1:A:256:ASN:N	2.79	0.44
1:B:403:ASN:ND2	3:B:631:HOH:O	2.49	0.44
1:B:233:GLN:HB3	1:B:266:SER:HB3	1.99	0.44
1:A:236:LYS:HA	1:A:236:LYS:HD3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:HIS:O	1:A:389:PHE:HB2	2.18	0.43
1:B:33:THR:HA	1:B:63:LEU:HD22	2.00	0.43
1:A:148:THR:H	1:A:151:SER:HG	1.66	0.43
1:B:229:VAL:HA	1:B:262:CYS:O	2.19	0.43
1:A:13:LEU:CD1	1:A:65:VAL:HG21	2.47	0.42
1:B:95:PHE:CE1	1:B:99:GLU:HG3	2.55	0.42
1:B:92:MET:O	1:B:96:THR:HG23	2.20	0.41
1:B:291:LEU:HB3	1:B:294:ARG:NH2	2.35	0.41
1:A:61:GLU:O	1:A:62:ASN:HB2	2.20	0.41
1:B:13:LEU:CD1	1:B:65:VAL:HG21	2.47	0.41
1:B:186:ASP:HB3	1:B:189:ARG:CG	2.49	0.41
1:B:154:ARG:O	1:B:158:GLU:HG3	2.21	0.40
1:B:245:VAL:HG21	1:B:259:VAL:HG21	2.04	0.40
1:A:401:LEU:HD12	3:A:483:HOH:O	2.21	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	389/438 (89%)	376 (97%)	10 (3%)	3 (1%)	19	15
1	B	388/438 (89%)	376 (97%)	11 (3%)	1 (0%)	41	41
All	All	777/876 (89%)	752 (97%)	21 (3%)	4 (0%)	29	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	A	256	ASN
1	A	220	PRO
1	B	263	GLY

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	327/357 (92%)	314 (96%)	13 (4%)	31 32
1	B	323/357 (90%)	310 (96%)	13 (4%)	31 32
All	All	650/714 (91%)	624 (96%)	26 (4%)	31 32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	13	LEU
1	A	15	GLN
1	A	50	ARG
1	A	93	LEU
1	A	121	ARG
1	A	179	LEU
1	A	210	THR
1	A	225	VAL
1	A	233	GLN
1	A	294	ARG
1	A	302	VAL
1	A	373	GLU
1	B	13	LEU
1	B	14	GLN
1	B	26	VAL
1	B	29	LEU
1	B	100	LYS
1	B	121	ARG
1	B	139	LYS
1	B	189	ARG
1	B	210	THR
1	B	212	ARG
1	B	257	LEU
1	B	311	VAL
1	B	359	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	25	ASN
1	A	38	GLN
1	A	233	GLN
1	B	14	GLN
1	B	25	ASN
1	B	38	GLN
1	B	67	ASN
1	B	256	ASN
1	B	326	GLN
1	B	385	HIS
1	B	403	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	B	419	-	4,4,4	0.15	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	423	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	A	420	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	B	422	-	4,4,4	0.17	0	6,6,6	0.28	0
2	SO4	A	421	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	B	421	-	4,4,4	0.10	0	6,6,6	0.25	0
2	SO4	A	419	-	4,4,4	0.40	0	6,6,6	0.30	0
2	SO4	B	420	-	4,4,4	0.17	0	6,6,6	0.26	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	423	SO4	1	0
2	A	420	SO4	1	0
2	B	421	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	399/438 (91%)	0.38	41 (10%) 6 8	25, 38, 51, 58	0
1	B	396/438 (90%)	0.09	19 (4%) 30 36	27, 33, 44, 59	0
All	All	795/876 (90%)	0.24	60 (7%) 14 18	25, 34, 50, 59	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	TYR	6.8
1	A	116	VAL	5.4
1	A	220	PRO	5.1
1	A	85	LEU	5.0
1	B	119	LEU	4.8
1	A	215	ARG	4.8
1	A	119	LEU	4.6
1	B	410	ASN	4.5
1	A	221	LEU	4.4
1	A	277	HIS	4.4
1	A	120	LEU	4.3
1	A	212	ARG	4.2
1	B	89	THR	4.2
1	B	116	VAL	4.1
1	B	85	LEU	4.0
1	B	86	ALA	3.9
1	A	216	GLU	3.9
1	A	89	THR	3.9
1	A	86	ALA	3.8
1	A	123	LEU	3.7
1	A	211	GLU	3.6
1	B	120	LEU	3.5
1	A	265	PRO	3.5
1	A	139	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLN	3.3
1	B	150	GLU	3.2
1	A	87	ALA	3.2
1	B	118	TRP	3.2
1	A	141	SER	3.0
1	B	139	LYS	3.0
1	A	117	GLY	3.0
1	B	6	ILE	2.9
1	B	15	GLN	2.9
1	A	106	ILE	2.9
1	A	88	PHE	2.8
1	A	140	ASN	2.8
1	A	266	SER	2.8
1	B	117	GLY	2.7
1	A	253	PRO	2.7
1	A	93	LEU	2.6
1	B	123	LEU	2.6
1	A	90	GLY	2.6
1	A	273	ASP	2.5
1	A	124	TRP	2.4
1	A	6	ILE	2.4
1	B	359	HIS	2.3
1	A	222	HIS	2.3
1	A	256	ASN	2.3
1	A	149	PRO	2.3
1	A	92	MET	2.2
1	A	112	LEU	2.2
1	B	93	LEU	2.2
1	A	410	ASN	2.2
1	A	317	SER	2.1
1	B	106	ILE	2.1
1	A	276	ARG	2.1
1	B	408	ASN	2.0
1	A	280	GLU	2.0
1	A	147	ASP	2.0
1	B	114	GLY	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 monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
2	SO4	B	423	5/5	0.92	0.27	72,73,74,75	0
2	SO4	B	422	5/5	0.95	0.39	70,71,72,73	0
2	SO4	B	421	5/5	0.96	0.31	68,69,69,70	0
2	SO4	A	420	5/5	0.97	0.18	62,62,63,63	0
2	SO4	A	421	5/5	0.97	0.28	65,65,66,66	0
2	SO4	B	419	5/5	0.97	0.17	50,51,52,53	0
2	SO4	A	419	5/5	0.98	0.21	31,32,33,37	0
2	SO4	B	420	5/5	1.00	0.03	26,26,26,31	0

6.5 Other polymers (i)

There are no such residues in this entry.