



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:10 PM GMT

PDB ID : 3G05
Title : Crystal structure of N-terminal domain (2-550) of E.coli MnmG
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2009-01-27
Resolution : 3.49 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

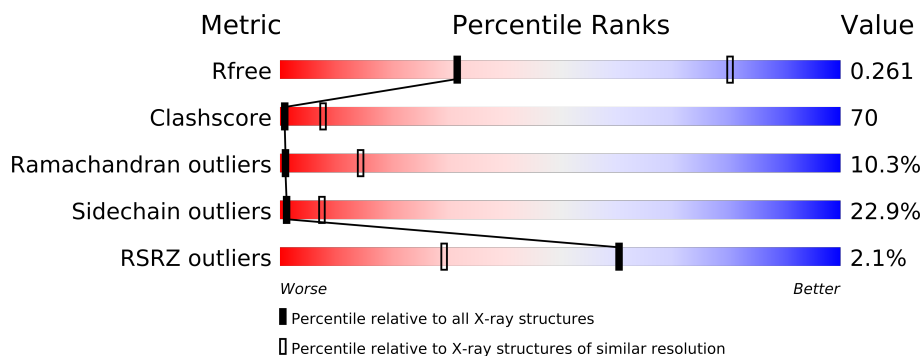
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

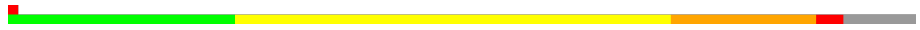
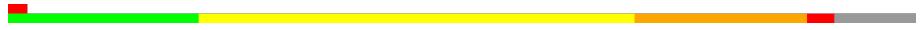
The reported resolution of this entry is 3.49 Å.

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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8156 atoms, of which 0 are hydrogen and 0 are deuterium.

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 tRNA uridine 5-carboxymethylaminomethylmodification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4073	2551	728	776	18			
1	B	524	Total	C	N	O	S	0	0	0
			4063	2540	730	775	18			

There are 54 discrepancies between the modelled and reference sequences:

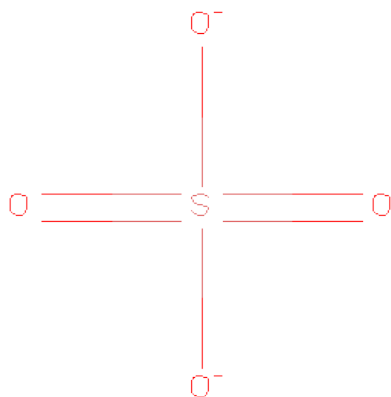
Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	EXPRESSION TAG	UNP Q8XAY0
A	-26	GLY	-	EXPRESSION TAG	UNP Q8XAY0
A	-25	SER	-	EXPRESSION TAG	UNP Q8XAY0
A	-24	SER	-	EXPRESSION TAG	UNP Q8XAY0
A	-23	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-22	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-21	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-20	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-19	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-18	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-17	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-16	HIS	-	EXPRESSION TAG	UNP Q8XAY0
A	-15	ASP	-	EXPRESSION TAG	UNP Q8XAY0
A	-14	TYR	-	EXPRESSION TAG	UNP Q8XAY0
A	-13	ASP	-	EXPRESSION TAG	UNP Q8XAY0
A	-12	ILE	-	EXPRESSION TAG	UNP Q8XAY0
A	-11	PRO	-	EXPRESSION TAG	UNP Q8XAY0
A	-10	THR	-	EXPRESSION TAG	UNP Q8XAY0
A	-9	THR	-	EXPRESSION TAG	UNP Q8XAY0
A	-8	GLU	-	EXPRESSION TAG	UNP Q8XAY0
A	-7	ASN	-	EXPRESSION TAG	UNP Q8XAY0
A	-6	LEU	-	EXPRESSION TAG	UNP Q8XAY0
A	-5	TYR	-	EXPRESSION TAG	UNP Q8XAY0
A	-4	PHE	-	EXPRESSION TAG	UNP Q8XAY0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	EXPRESSION TAG	UNP Q8XAY0
A	-2	GLY	-	EXPRESSION TAG	UNP Q8XAY0
A	-1	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-27	MET	-	EXPRESSION TAG	UNP Q8XAY0
B	-26	GLY	-	EXPRESSION TAG	UNP Q8XAY0
B	-25	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-24	SER	-	EXPRESSION TAG	UNP Q8XAY0
B	-23	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-22	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-21	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-20	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-19	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-18	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-17	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-16	HIS	-	EXPRESSION TAG	UNP Q8XAY0
B	-15	ASP	-	EXPRESSION TAG	UNP Q8XAY0
B	-14	TYR	-	EXPRESSION TAG	UNP Q8XAY0
B	-13	ASP	-	EXPRESSION TAG	UNP Q8XAY0
B	-12	ILE	-	EXPRESSION TAG	UNP Q8XAY0
B	-11	PRO	-	EXPRESSION TAG	UNP Q8XAY0
B	-10	THR	-	EXPRESSION TAG	UNP Q8XAY0
B	-9	THR	-	EXPRESSION TAG	UNP Q8XAY0
B	-8	GLU	-	EXPRESSION TAG	UNP Q8XAY0
B	-7	ASN	-	EXPRESSION TAG	UNP Q8XAY0
B	-6	LEU	-	EXPRESSION TAG	UNP Q8XAY0
B	-5	TYR	-	EXPRESSION TAG	UNP Q8XAY0
B	-4	PHE	-	EXPRESSION TAG	UNP Q8XAY0
B	-3	GLN	-	EXPRESSION TAG	UNP Q8XAY0
B	-2	GLY	-	EXPRESSION TAG	UNP Q8XAY0
B	-1	SER	-	EXPRESSION TAG	UNP Q8XAY0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



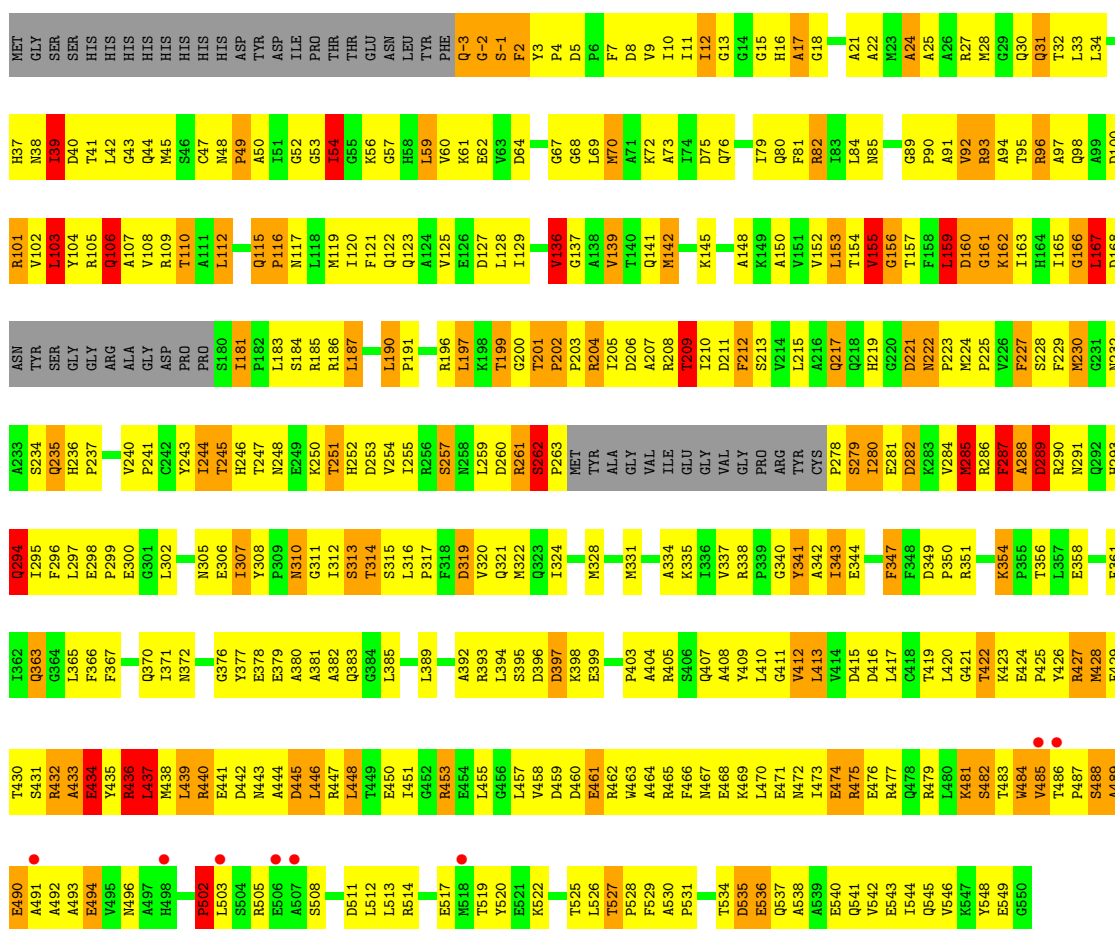
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

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.

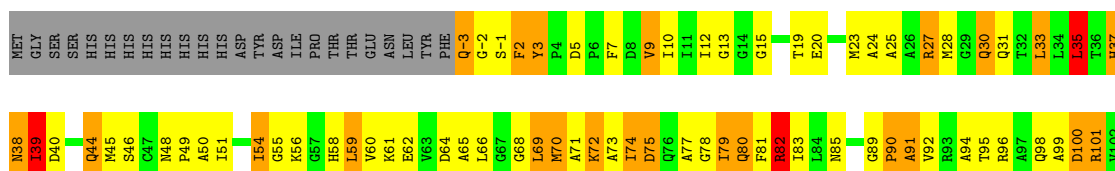
- Molecule 1: tRNA uridine 5-carboxymethylaminomethylmodification enzyme mnmG

Chain A: 



- Molecule 1: tRNA uridine 5-carboxymethylaminomethylmodification enzyme mnmG

Chain B: 



E536	Q537	A538	A539	E540	Q541	V542	E543	I544	Q545	V546	K547	Y548	E549	G550	L103	Y104	R105	Q106	A107	V108	R109	T110	A111	L112	E113	N114	Q115	P116	N117	L118	M119	I120	F121	Q122	Q123	A124	V125	E126	L127	L128	I129	V130	E131	N132	D133	R134	V135	V136	G137	A138	V139	T140	Q141	L144	K145	F146	R147	A148	K149	A150	V151	V152	L153	T154	V155	G156	T157	F158	L159	D160	G161	K162	I163		
															H164	I165	G166	LEU	ASP	ASN	TYR	SER	GLY	GLY	ARG	ALA	GLY	ASP	PRO	S180	I181	P182	L183	S184	R185	R186	L187	R188	E189	L190	P191	L192	R193	V194	G195	R196	L197	K198	T199	G200	V139	T140	Q141	R204	L205	D206	A207	R208	T209	I210	D211	F212	V151	S213	V214	L215	A216	Q217	I280	Q218	H219	N222	P223	M224	P225
															V226	F227	S228	F229	M230	G231	N232	A233	S234	Q235	H236	P237	Q238	Q239	V240	P241	C242	Y243	I244	T245	H246	T247	N248	E249	K250	R251	H252	D253	V254	I255	R256	L259	D260	R261	S262	PRO	MET	TTR	ALA	GLY	VAL	ILE	GLU	GLY	VAL	GLY	PRO	ARG	TYR	CYS	P278	S279	I280	E281	K283	V284	M285	R286			
															F287	A288	D289	R290	N291	Q292	H293	Q294	I295	F296	L297	E298	P299	E300	G301	L302	T303	S304	N305	E306	I307	Y308	P309	N310	G311	R312	S313	T314	S315	L316	P317	F318	D319	Q320	Q321	N322	Q323	T324	V325	R326	S327	N390	A391	Q392	Q393	N331	E332	N333	A334	K335	I336	V337	R338	P339	G340	Y341	A342	T343	E344	Y345	D346
															F347	F348	D349	P350	R351	P355	T356	L357	E358	S359	K360	F361	I362	Q363	G364	L365	F366	F367	A368	Q370	I371	N372	G373	G376	Y377	E378	E379	A380	A381	A382	Q383	G384	L385	L386	A387	G388	L389	N390	A391	Q392	R393	L394	S395	D396	D397	K398	E399	G400	W401	A402	P403	A404	R405	S406	Q407	A408	Y409				
															L410	G411	V412	L413	V414	D415	D416	L417	L420	G421	T422	K423	E424	P425	Y426	R427	M428	F429	T430	S431	R432	A433	N434	Y435	R436	L437	M438	L439	R440	E441	D442	M443	A444	D445	L446	R447	L448	T449	E450	I451	G452	R453	E454	L455	G456	L457	V458	D459	D460	E461	R462	W463	F466	N467	E468	K469	L470	E471			
															M472	I473	E474	R475	E476	R479	L480	K481	S482	T483	W484	V485	T486	P487	S488	A489	E490	A491	A492	A493	E494	V495	N496	L499	T500	A501	P502	L503	S504	R505	E506	A507	S508	D511	L512	L513	R514	R515	P516	E517	M518	T519	Y520	E521	K522	L523	T524	T525	L526	P527	P528	F529	A532	L533	T534	D535					

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.59Å 144.59Å 271.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.49 49.74 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.49) 99.7 (49.74-3.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.227 , 0.265 0.226 , 0.261	Depositor DCC
R_{free} test set	2137 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 83.5	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 42342 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8156	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.84	1/4146 (0.0%)	1.15	20/5615 (0.4%)
1	B	0.75	0/4134	1.11	15/5596 (0.3%)
All	All	0.80	1/8280 (0.0%)	1.13	35/11211 (0.3%)

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	1	7
1	B	0	4
All	All	1	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	505	ARG	CZ-NH2	24.30	1.64	1.33

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	B	290	ARG	N-CA-C	-10.74	82.01	111.00
1	A	505	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	B	100	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	505	ARG	NH1-CZ-NH2	-7.68	110.95	119.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	291	ASN	CA

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-1	SER	Mainchain,Peptide
1	A	159	LEU	Peptide
1	A	261	ARG	Peptide
1	A	287	PHE	Peptide
1	A	288	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4073	0	4026	563	0
1	B	4063	0	4029	581	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
All	All	8156	0	8055	1141	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 70.

The worst 5 of 1141 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:ASP:CA	1:A:291:ASN:HA	1.56	1.32
1:B:180:SER:O	1:B:181:ILE:HG22	1.24	1.31
1:B:154:THR:O	1:B:155:VAL:CG1	1.79	1.29
1:A:285:MET:CE	1:A:285:MET:HA	1.59	1.26
1:A:289:ASP:C	1:A:291:ASN:HA	1.56	1.26

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	521/576 (90%)	383 (74%)	88 (17%)	50 (10%)	1	17
1	B	518/576 (90%)	363 (70%)	98 (19%)	57 (11%)	1	13
All	All	1039/1152 (90%)	746 (72%)	186 (18%)	107 (10%)	1	14

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLY
1	A	142	MET
1	A	160	ASP
1	A	167	LEU
1	A	212	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/474 (90%)	338 (79%)	88 (21%)	2	10
1	B	427/474 (90%)	320 (75%)	107 (25%)	1	6
All	All	853/948 (90%)	658 (77%)	195 (23%)	1	7

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	-3	GLN
1	B	114	ASN
1	B	471	GLU
1	B	9	VAL

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Mol	Chain	Res	Type
1	B	46	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	B	44	GLN
1	B	383	GLN
1	B	30	GLN
1	B	31	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	551	-	4,4,4	0.27	0	6,6,6	0.33	0
2	SO4	A	552	-	4,4,4	0.23	0	6,6,6	0.42	0
2	SO4	B	1	-	4,4,4	0.19	0	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	551	-	4,4,4	0.13	0	6,6,6	0.25	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	551	-	-	0/0/0/0	0/0/0/0
2	SO4	A	552	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	551	-	-	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	527/576 (91%)	0.16	8 (1%) 70 36	53, 73, 123, 136	0
1	B	524/576 (90%)	0.29	14 (2%) 52 24	55, 79, 130, 137	0
All	All	1051/1152 (91%)	0.23	22 (2%) 60 29	53, 75, 128, 137	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	HIS	3.3
1	A	503	LEU	3.2
1	B	507	ALA	3.2
1	B	506	GLU	3.2
1	B	289	ASP	3.0

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	1	5/5	0.33	1.61	77,78,78,78	0
2	SO4	A	551	5/5	0.23	0.21	71,72,72,72	0
2	SO4	B	551	5/5	0.25	0.09	85,85,85,86	0
2	SO4	A	552	5/5	0.23	-0.60	79,79,79,80	0

6.5 Other polymers

There are no such residues in this entry.