



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 12:43 PM EDT

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 : unknown
Resolution : 3.49 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

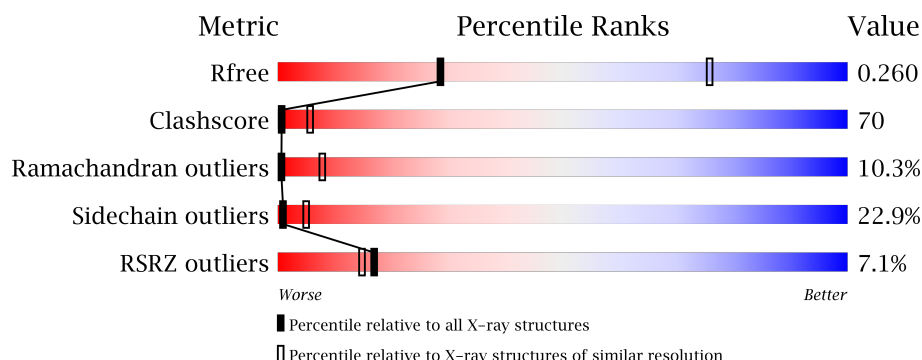
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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 $\leq 5\%$. 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	576	<div> <div>5%</div> <div>25%</div> <div>48%</div> <div>16%</div> <div>9%</div> </div>
1	B	576	<div> <div>9%</div> <div>21%</div> <div>48%</div> <div>19%</div> <div>9%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8156 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 tRNA uridine 5-carboxymethylaminomethyl modification 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).

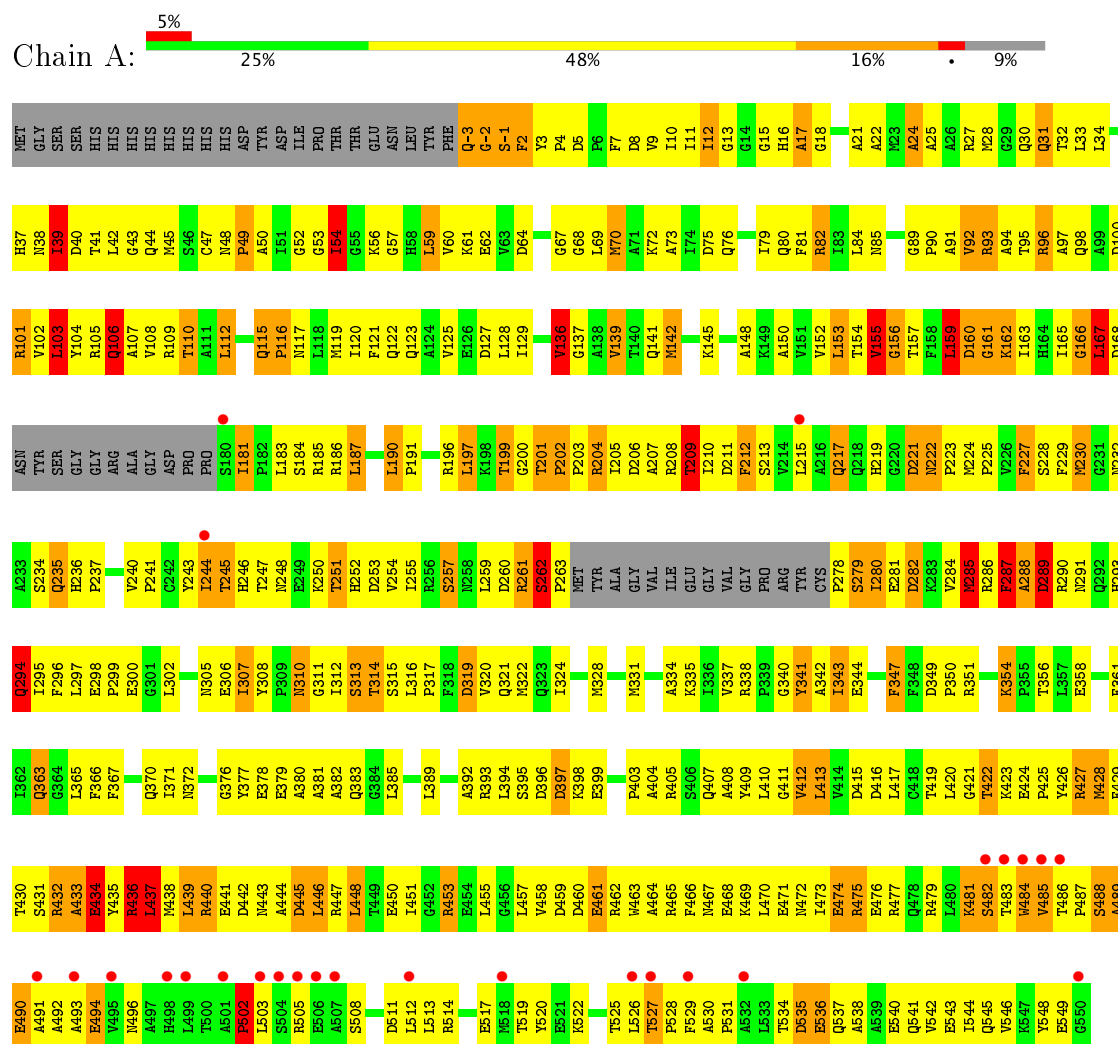


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

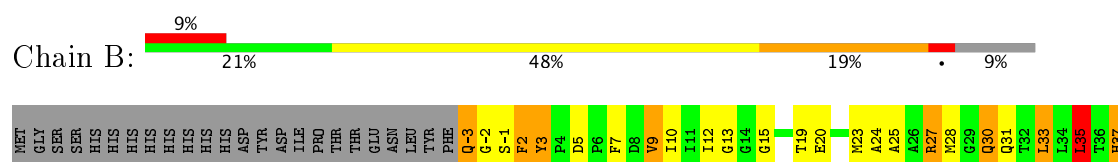
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG



T534	I472	L410	F347	F287	V226	H164	I103	I338
D535	I473	G411	F348	A288	F227	I165	Y104	I339
E536	E474	V412	D949	D289	S228	G166	Q106	D40
Q537	R475	L413	P350	R290	F229	LEU	R105	
A538	E476	V414	R351	N291	N230	ASP	A107	Q44
A539		D415	P355	Q292	G231	ASN	V108	K45
E540	R479	D416	T356	H293	H232	TYR	R109	S46
Q541	L480	L417	L357	Q294	A233	SER	T110	C47
Y542	K481		S234	L295	S234	GLY	A111	N48
E543	S482	L420	S358	F295	Q235	GLY	L112	P49
T544	T483	G421	S359	L297	H236	ARG	E113	A50
Q545	W484	T422	K360	E298	P237	ALA	N114	
Y546	V485	K423	F361	P299	Q238	GLY	Q115	
K547	T486	E424	L362	E300	Q239	ASP	P116	
Y548	P487	P425	Q363	G301	V240	PRO	N117	
E549	S488	Y426	G364	L302	P241	PRO	L118	
G550	A489	R427	L365	T303	C242	S180	M119	
	E490	M428	F366	S304	Y243	I181	I120	
	A491	F429	F367	N305	T244	P182	I121	
	A492	T430	A366	E306	T245	L183	Q122	
	A493	S431	G369	L307	H246	S184	Q123	
	E494	R432	Q370	Y308	T247	R185	A124	
	V495	A433	I371	P309	N248	R186	V125	
	N496	E434	N372	N310	E249	L187	E126	
	A497	Y435	G373	G311	K250	R188	D127	
	H498	R436		I312	T251	E189	L128	
	E499	L437	G376	S313	H252	L190	I129	
	T500	M438	Y377	T314	D253	P191	V130	
	A501	L439	E378	S315	V254	L192	E131	
	P502	R440	E379	L316	T255	R193	N132	
	L503	P441	A380	P317	R256	V194	D133	
	S504	D442	A381	F318		G195	R134	
	R505	M443	A382	D319	L259	R196	V135	
	E506	A444	Q383	V320	D260	L197	V136	
	A507	D445	G384	Q321	R261	K198	D75	
	S508	L446	L385	M322	S262	T199	A138	
	G509	R447	L386	Q323	PRO	G200	V139	
	E510	L448	A387	I324	MET	G200	A77	
	D511	T449	G388	V325	TYR	T201	T140	
	L512	E450	L389	R326	ALA	R204	Q141	
	L513	I451	N390	S327	GLY	I205	L144	
	R514	G452	A391	M328	VAL	D206	K145	
	R515	R453	A392	Q329	ILE	A207	F146	
	P516	E454	R393	G330	GLU	R208	R147	
	E517	L455	L394	M331	GLY	T209	A148	
	M518	G456	S395	E332	VAL	I210	K149	
	T519	L457	D396	N333	GLY	D211	A150	
	Y520	V458	D397	A334	PRO	F212	V151	
	E521	D459	K398	K335	ARG	S213	V152	
	K522	D460	E399	I336	TYR	V214	I153	
	L523	E461	G400	V337	CYS	L215	T154	
	T524	R462	W401	R338	P278	A216	V155	
	T525	W463	A402	P339	S279	G156	A94	
	L526		P403	G340	I280	Q217	T95	
	T527	F466	A404	Y341	E281	Q218	T157	
	P528	M467	R405	A342	D282	E219	F158	
	F529	E468	S406	I343	K283	L159	A97	
		R469	Q407	E344	V284	I160	Q98	
		L470	A408	Y345	M285	D160	A99	
		E471	Y409	D346	R286	K162	D100	
						R101	I102	
						I163		

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	Depositor
R, R_{free}	0.227 , 0.265 0.224 , 0.260	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 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	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.

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 [i](#)

5.1 Standard geometry [i](#)

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 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	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

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 70.

The worst 5 of 1141 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: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 [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	521/576 (90%)	383 (74%)	88 (17%)	50 (10%)	1	9
1	B	518/576 (90%)	363 (70%)	98 (19%)	57 (11%)	0	7
All	All	1039/1152 (90%)	746 (72%)	186 (18%)	107 (10%)	0	8

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 [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	426/474 (90%)	338 (79%)	88 (21%)	1	7
1	B	427/474 (90%)	320 (75%)	107 (25%)	0	4
All	All	853/948 (90%)	658 (77%)	195 (23%)	1	5

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

Mol	Chain	Res	Type
1	B	-3	GLN

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Mol	Chain	Res	Type
1	B	114	ASN
1	B	471	GLU
1	B	9	VAL
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 molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.17	0	6,6,6	0.50	0
2	SO4	A	552	-	4,4,4	0.19	0	6,6,6	0.56	0
2	SO4	B	1	-	4,4,4	0.25	0	6,6,6	0.52	0
2	SO4	B	551	-	4,4,4	0.24	0	6,6,6	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
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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	551	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.36	26 (4%)	30 24	53, 73, 123, 136	0
1	B	524/576 (90%)	0.60	49 (9%)	9 9	55, 79, 130, 137	0
All	All	1051/1152 (91%)	0.48	75 (7%)	17 15	53, 75, 128, 137	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LEU	5.6
1	A	485	VAL	5.5
1	B	507	ALA	5.4
1	B	289	ASP	5.3
1	B	164	HIS	5.1

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	B	1	5/5	0.96	0.33	1.36	77,78,78,78	0
2	SO4	A	551	5/5	0.97	0.23	-0.02	71,72,72,72	0
2	SO4	A	552	5/5	0.93	0.26	-	79,79,79,80	0
2	SO4	B	551	5/5	0.91	0.25	-	85,85,85,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.