wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2024 – 06:26 PM EST

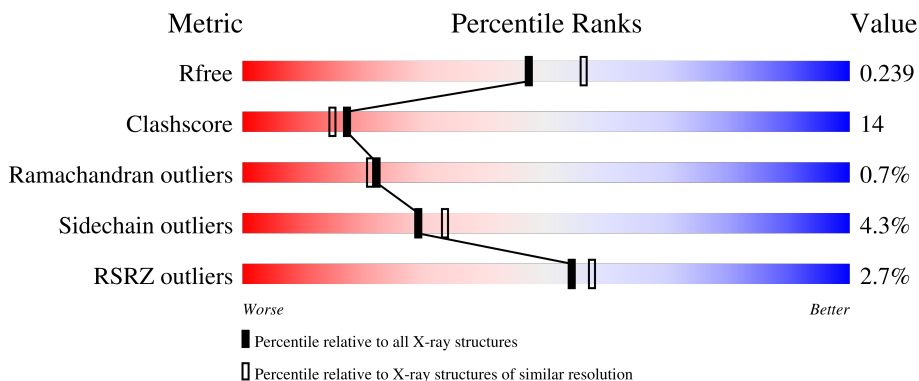|		
PDB ID	:	3GXA
Title	:	Crystal structure of GNA1946
Authors	:	Yang, X.; Shen, Y.
Deposited on	:	2009-04-02
Resolution	:	2.25 Å(reported)

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 2.25 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.
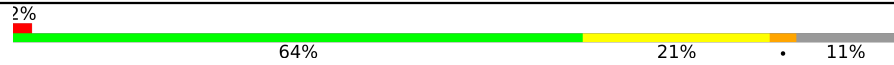
Metric	Percentile Ranks	Value
Rfree		0.239
Clashscore		14
Ramachandran outliers		0.7%
Sidechain outliers		4.3%
RSRZ outliers		2.7%

Worse　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	275	64%　　　20%　•　13%
1	B	275	2% 66%　　　19%　•　13%
1	C	275	7% 59%　　　27%　•　11%
1	D	275	2% 67%　　　18%　•　13%
1	E	275	% 63%　　　21%　•　13%

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Mol	Chain	Length	Quality of chain
1	F	275	

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12179 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 Outer membrane lipoprotein GNA1946.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	B	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	C	244	Total	C	N	O	S	0	0	0
			1915	1228	311	373	3			
1	D	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	E	239	Total	C	N	O	S	0	0	0
			1884	1211	305	365	3			
1	F	244	Total	C	N	O	S	0	0	0
			1915	1228	311	373	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP Q7BMQ8
A	288	LEU	-	expression tag	UNP Q7BMQ8
A	289	GLU	-	expression tag	UNP Q7BMQ8
A	290	HIS	-	expression tag	UNP Q7BMQ8
A	291	HIS	-	expression tag	UNP Q7BMQ8
A	292	HIS	-	expression tag	UNP Q7BMQ8
A	293	HIS	-	expression tag	UNP Q7BMQ8
A	294	HIS	-	expression tag	UNP Q7BMQ8
A	295	HIS	-	expression tag	UNP Q7BMQ8
B	21	MET	-	expression tag	UNP Q7BMQ8
B	288	LEU	-	expression tag	UNP Q7BMQ8
B	289	GLU	-	expression tag	UNP Q7BMQ8
B	290	HIS	-	expression tag	UNP Q7BMQ8
B	291	HIS	-	expression tag	UNP Q7BMQ8
B	292	HIS	-	expression tag	UNP Q7BMQ8
B	293	HIS	-	expression tag	UNP Q7BMQ8
B	294	HIS	-	expression tag	UNP Q7BMQ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	295	HIS	-	expression tag	UNP Q7BMQ8
C	21	MET	-	expression tag	UNP Q7BMQ8
C	288	LEU	-	expression tag	UNP Q7BMQ8
C	289	GLU	-	expression tag	UNP Q7BMQ8
C	290	HIS	-	expression tag	UNP Q7BMQ8
C	291	HIS	-	expression tag	UNP Q7BMQ8
C	292	HIS	-	expression tag	UNP Q7BMQ8
C	293	HIS	-	expression tag	UNP Q7BMQ8
C	294	HIS	-	expression tag	UNP Q7BMQ8
C	295	HIS	-	expression tag	UNP Q7BMQ8
D	21	MET	-	expression tag	UNP Q7BMQ8
D	288	LEU	-	expression tag	UNP Q7BMQ8
D	289	GLU	-	expression tag	UNP Q7BMQ8
D	290	HIS	-	expression tag	UNP Q7BMQ8
D	291	HIS	-	expression tag	UNP Q7BMQ8
D	292	HIS	-	expression tag	UNP Q7BMQ8
D	293	HIS	-	expression tag	UNP Q7BMQ8
D	294	HIS	-	expression tag	UNP Q7BMQ8
D	295	HIS	-	expression tag	UNP Q7BMQ8
E	21	MET	-	expression tag	UNP Q7BMQ8
E	288	LEU	-	expression tag	UNP Q7BMQ8
E	289	GLU	-	expression tag	UNP Q7BMQ8
E	290	HIS	-	expression tag	UNP Q7BMQ8
E	291	HIS	-	expression tag	UNP Q7BMQ8
E	292	HIS	-	expression tag	UNP Q7BMQ8
E	293	HIS	-	expression tag	UNP Q7BMQ8
E	294	HIS	-	expression tag	UNP Q7BMQ8
E	295	HIS	-	expression tag	UNP Q7BMQ8
F	21	MET	-	expression tag	UNP Q7BMQ8
F	288	LEU	-	expression tag	UNP Q7BMQ8
F	289	GLU	-	expression tag	UNP Q7BMQ8
F	290	HIS	-	expression tag	UNP Q7BMQ8
F	291	HIS	-	expression tag	UNP Q7BMQ8
F	292	HIS	-	expression tag	UNP Q7BMQ8
F	293	HIS	-	expression tag	UNP Q7BMQ8
F	294	HIS	-	expression tag	UNP Q7BMQ8
F	295	HIS	-	expression tag	UNP Q7BMQ8

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

SO4

O1

O

O3 O⁻ — S — O⁻ O4

S

O

O2

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		
2	B	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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).
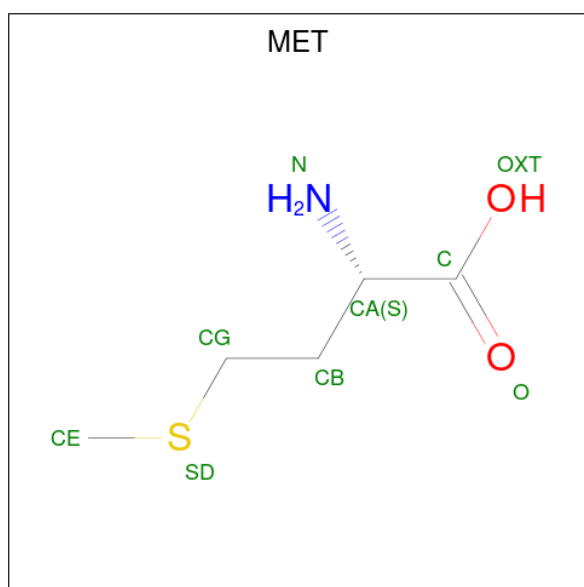
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 9	C 5	N 1	O 2	S 1	0	0
3	B	1	Total 9	C 5	N 1	O 2	S 1	0	0
3	C	1	Total 9	C 5	N 1	O 2	S 1	0	0
3	D	1	Total 9	C 5	N 1	O 2	S 1	0	0
3	E	1	Total 9	C 5	N 1	O 2	S 1	0	0
3	F	1	Total 9	C 5	N 1	O 2	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total 128	O 128	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	111	Total 111	O 111	0	0
4	C	100	Total 100	O 100	0	0
4	D	136	Total 136	O 136	0	0
4	E	105	Total 105	O 105	0	0
4	F	99	Total 99	O 99	0	0

3 Residue-property plots ⓘ

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 den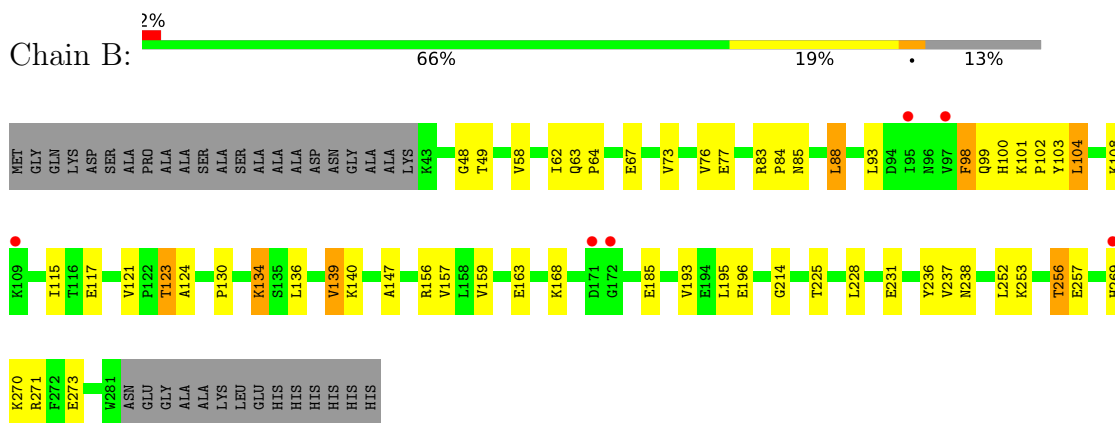sity. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
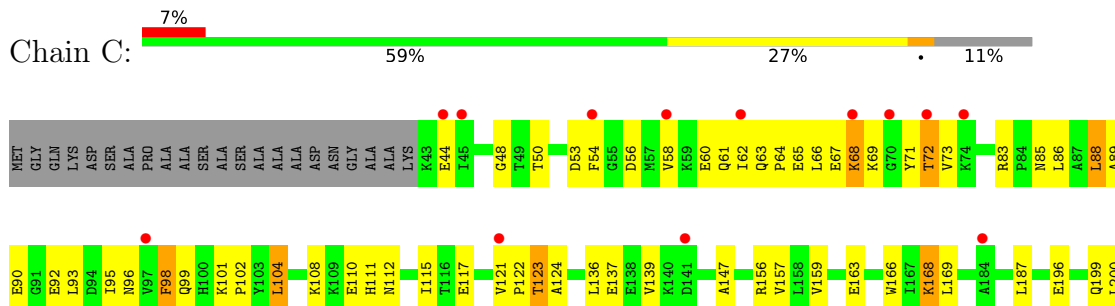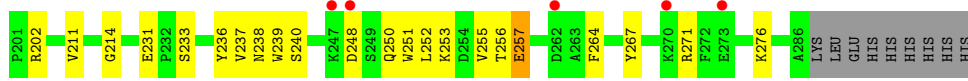
• Molecule 1: Outer membrane lipoprotein GNA1946

Chain A:
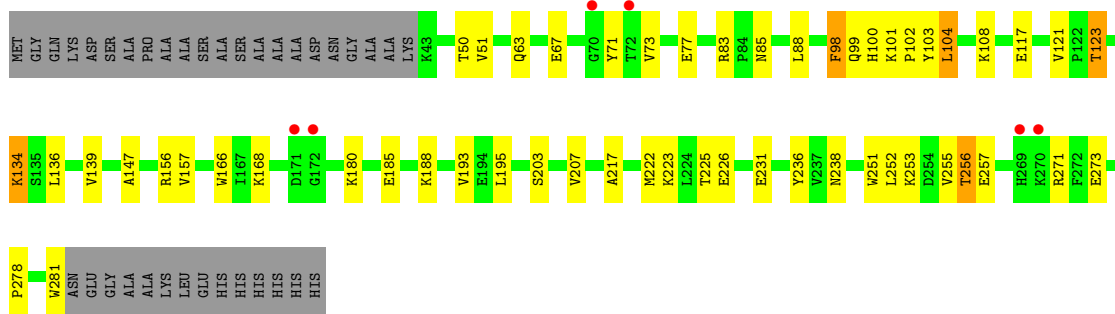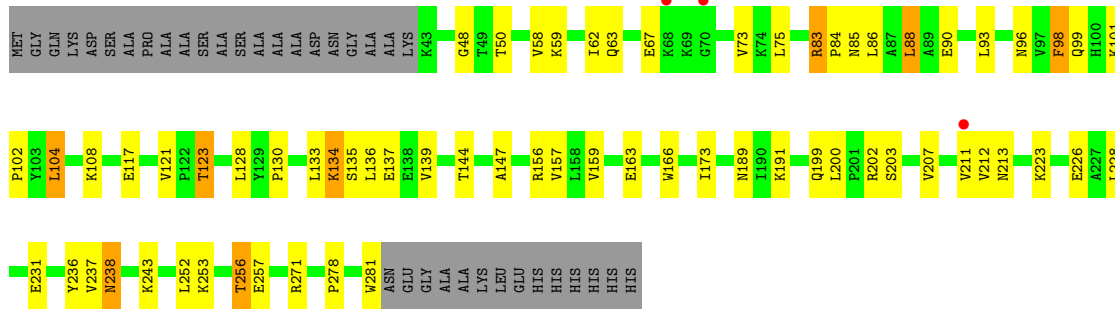

• Molecule 1: Outer membrane lipoprotein GNA1946

Chain B:

• Molecule 1: Outer membrane lipoprotein GNA1946

Chain C:

P201 R202 V211 G214 E231 P232 S233 Y236 V237 N238 W239 S240 K247 D248 S249 Q250 W251 L252 K253 D254 V255 T256 E257 D262 A263 F264 Y267 K270 R271 F272 E273 K276 A286 LYS LEU GLU HIS HIS HIS HIS HIS

- Molecule 1: Outer membrane lipoprotein GNA1946

Chain D:

2%

67% 18% 13%

MET GLY GLN LYS ASP SER ALA PRO ALA ALA SER ALA ALA SER ALA ALA ASP ASN GLY ALA ALA LYS K43 T50 V51 Q63 E67 G70 Y71 T72 V73 E77 R83 P84 N85 L88 F98 Q99 H100 K101 P102 Y103 L104 K108 E117 V121 P122 T123

K134 S135 L136 V139 A147 R156 V157 W166 I167 K168 D171 G172 K180 E185 K188 V193 E194 L195 S203 V207 A217 M222 K223 L224 T225 E226 E231 Y236 V237 N238 W251 L252 K253 D254 V255 T256 E257 H269 K270 R271 F272 E273

P278 W281 ASN GLU GLY ALA ALA LYS GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Outer membrane lipoprotein GNA1946

Chain E:

%

63% 21% 13%

MET GLY GLN LYS ASP SER ALA PRO ALA ALA SER ALA ALA SER ALA ALA ASP ASN GLY ALA ALA LYS K43 G48 T49 T50 V58 K59 I62 Q63 E67 K68 K69 G70 V73 K74 L75 R83 P84 N85 L86 A87 L88 A89 E90 L93 N96 V97 F98 Q99 H100 K101

P102 Y103 L104 K108 E117 V121 P122 T123 L128 Y129 P130 L133 K134 S135 L136 E137 E138 V139 T144 A147 R156 V157 L158 V159 E163 W166 I173 N189 I190 K191 Q199 L200 P201 R202 S203 V207 V211 V212 N213 K223 E226 A227 L228

E231 Y236 V237 N238 K243 L252 K253 T256 E257 R271 P278 W281 ASN GLU GLY ALA ALA LYS LEU GLU HIS HIS HIS HIS HIS

- Molecule 1: Outer membrane lipoprotein GNA1946

Chain F:

2%

64% 21% 11%

MET GLY GLN LYS ASP SER ALA PRO ALA ALA SER ALA ALA SER ALA ALA ASP ASN GLY ALA ALA LYS K43 E44 G48 V51 V58 K59 E60 Q61 I62 Q63 P64 E65 L66 E67 K68 K69 T72 V73 F78 T79 N85 L88 A89 E90 I95 N96 V97 F98 Q99 H100

Y103 L104 D105 D106 F107 K108 K109 E110 H111 I115 T116 V121 P122 T123 L126 L136 V139 K140 T144 A147 R156 V157 M160 L164 G165 W166 I167 K168 K191 I192 V193 E194 L195 E196 R202 F209 A210 V211 S219 F229 Q230 E231 P232

Y236 V237 N238 W239 S240 K243 L252 K253 T256 E257 A258 Y259 D262 H269 K270 R271 A286 LYS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.39Å 122.81Å 160.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.55 – 2.25 21.55 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.4 (21.55-2.25) 94.5 (21.55-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.26Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.206 , 0.239 0.206 , 0.239	Depositor DCC
R_{free} test set	5130 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 41.1	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12179	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.41	0/1927	0.67	0/2615
1	B	0.38	0/1927	0.66	0/2615
1	C	0.36	0/1958	0.61	0/2657
1	D	0.37	0/1927	0.63	0/2615
1	E	0.37	0/1927	0.65	0/2615
1	F	0.37	0/1958	0.65	0/2657
All	All	0.38	0/11624	0.64	0/15774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1884	0	1855	49	0
1	B	1884	0	1855	54	0
1	C	1915	0	1880	67	0
1	D	1884	0	1855	49	0
1	E	1884	0	1855	53	0
1	F	1915	0	1880	60	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	30	0	0	1	0
2	C	5	0	0	1	0
2	D	20	0	0	1	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
3	A	9	0	8	1	0
3	B	9	0	8	1	0
3	C	9	0	8	1	0
3	D	9	0	8	1	0
3	E	9	0	8	1	0
3	F	9	0	8	1	0
4	A	128	0	0	2	0
4	B	111	0	0	3	0
4	C	100	0	0	8	0
4	D	136	0	0	0	0
4	E	105	0	0	0	0
4	F	99	0	0	2	0
All	All	12179	0	11228	316	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 14.

The worst 5 of 316 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:123:THR:HG21	1:B:238:ASN:H	1.12	1.12
1:E:123:THR:HG21	1:E:238:ASN:H	1.14	1.11
1:A:123:THR:HG21	1:A:238:ASN:H	1.16	1.05
1:C:123:THR:HG21	1:C:238:ASN:H	1.16	1.05
1:D:123:THR:HG21	1:D:238:ASN:H	1.17	1.04

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	237/275 (86%)	232 (98%)	4 (2%)	1 (0%)	34	37
1	B	237/275 (86%)	231 (98%)	5 (2%)	1 (0%)	34	37
1	C	242/275 (88%)	229 (95%)	9 (4%)	4 (2%)	9	4
1	D	237/275 (86%)	229 (97%)	7 (3%)	1 (0%)	34	37
1	E	237/275 (86%)	232 (98%)	4 (2%)	1 (0%)	34	37
1	F	242/275 (88%)	235 (97%)	5 (2%)	2 (1%)	19	17
All	All	1432/1650 (87%)	1388 (97%)	34 (2%)	10 (1%)	22	21

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PHE
1	C	98	PHE
1	E	98	PHE
1	B	98	PHE
1	C	68	LYS

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	202/225 (90%)	191 (95%)	11 (5%)	22	22
1	B	202/225 (90%)	195 (96%)	7 (4%)	36	43
1	C	204/225 (91%)	196 (96%)	8 (4%)	32	38
1	D	202/225 (90%)	197 (98%)	5 (2%)	47	56
1	E	202/225 (90%)	191 (95%)	11 (5%)	22	22
1	F	204/225 (91%)	193 (95%)	11 (5%)	22	22
All	All	1216/1350 (90%)	1163 (96%)	53 (4%)	29	32

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	123	THR
1	E	128	LEU
1	F	195	LEU
1	D	134	LYS
1	E	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	112	ASN
1	F	99	GLN
1	F	238	ASN
1	F	111	HIS
1	C	99	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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	F	11	-	4,4,4	0.24	0	6,6,6	0.04	0
2	SO4	B	8	-	4,4,4	0.22	0	6,6,6	0.06	0
3	MET	A	296	-	7,8,8	0.73	0	7,9,9	0.71	0
2	SO4	C	9	-	4,4,4	0.23	0	6,6,6	0.08	0
3	MET	F	600	-	7,8,8	0.73	0	7,9,9	0.78	0
3	MET	C	300	-	7,8,8	0.69	0	7,9,9	0.83	0
2	SO4	D	4	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	B	15	-	4,4,4	0.21	0	6,6,6	0.07	0
2	SO4	E	5	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	16	-	4,4,4	0.20	0	6,6,6	0.06	0
3	MET	E	500	-	7,8,8	0.76	0	7,9,9	0.68	0
2	SO4	F	6	-	4,4,4	0.21	0	6,6,6	0.10	0
2	SO4	D	12	-	4,4,4	0.25	0	6,6,6	0.05	0
3	MET	D	400	-	7,8,8	0.73	0	7,9,9	0.67	0
2	SO4	B	2	-	4,4,4	0.22	0	6,6,6	0.04	0
2	SO4	B	3	-	4,4,4	0.21	0	6,6,6	0.07	0
2	SO4	D	13	-	4,4,4	0.21	0	6,6,6	0.05	0
2	SO4	A	7	-	4,4,4	0.20	0	6,6,6	0.06	0
2	SO4	D	10	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	B	1	-	4,4,4	0.18	0	6,6,6	0.04	0
2	SO4	B	14	-	4,4,4	0.22	0	6,6,6	0.06	0
3	MET	B	296	-	7,8,8	0.83	0	7,9,9	0.71	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	MET	E	500	-	-	0/8/8/8	-
3	MET	C	300	-	-	2/8/8/8	-
3	MET	A	296	-	-	1/8/8/8	-
3	MET	D	400	-	-	0/8/8/8	-
3	MET	F	600	-	-	0/8/8/8	-
3	MET	B	296	-	-	0/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	300	MET	OXT-C-CA-N
3	C	300	MET	O-C-CA-N
3	A	296	MET	OXT-C-CA-N

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	296	MET	1	0
2	C	9	SO4	1	0
3	F	600	MET	1	0
3	C	300	MET	1	0
2	D	4	SO4	1	0
3	E	500	MET	1	0
3	D	400	MET	1	0
2	B	3	SO4	1	0
3	B	296	MET	1	0

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	239/275 (86%)	-0.31	1 (0%)	92	93	14, 22, 36, 42	0
1	B	239/275 (86%)	-0.14	6 (2%)	57	60	14, 25, 44, 50	0
1	C	244/275 (88%)	0.35	18 (7%)	14	15	18, 36, 55, 62	0
1	D	239/275 (86%)	-0.22	6 (2%)	57	60	14, 23, 43, 50	0
1	E	239/275 (86%)	-0.18	3 (1%)	77	79	16, 26, 41, 50	0
1	F	244/275 (88%)	-0.13	5 (2%)	65	68	16, 26, 47, 61	0
All	All	1444/1650 (87%)	-0.10	39 (2%)	54	57	14, 26, 46, 62	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	72	THR	4.8
1	D	269	HIS	4.3
1	F	68	LYS	4.0
1	B	172	GLY	3.7
1	F	269	HIS	3.6

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 monosaccharides in this entry.

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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. 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(Å^2)	Q<0.9
2	SO4	C	9	5/5	0.75	0.27	82,82,84,84	0
2	SO4	B	2	5/5	0.84	0.33	100,100,100,100	0
2	SO4	E	5	5/5	0.85	0.26	77,79,79,80	0
2	SO4	B	15	5/5	0.87	0.26	91,91,91,92	0
2	SO4	B	3	5/5	0.88	0.19	82,84,84,84	0
2	SO4	A	16	5/5	0.88	0.33	94,94,95,95	0
2	SO4	D	10	5/5	0.89	0.20	67,67,68,68	0
2	SO4	B	14	5/5	0.90	0.17	73,74,74,75	0
2	SO4	D	12	5/5	0.91	0.26	94,94,95,95	0
2	SO4	B	8	5/5	0.92	0.23	64,65,66,67	0
2	SO4	F	11	5/5	0.94	0.29	73,73,74,75	0
2	SO4	F	6	5/5	0.96	0.15	45,46,47,48	0
3	MET	A	296	9/9	0.97	0.14	17,17,18,19	0
3	MET	B	296	9/9	0.97	0.14	13,14,16,17	0
3	MET	E	500	9/9	0.97	0.17	15,17,20,20	0
2	SO4	A	7	5/5	0.98	0.13	33,35,35,37	0
2	SO4	B	1	5/5	0.98	0.09	36,38,39,40	0
3	MET	C	300	9/9	0.98	0.16	14,18,20,20	0
3	MET	D	400	9/9	0.98	0.15	13,14,17,17	0
2	SO4	D	13	5/5	0.98	0.15	69,69,69,69	0
2	SO4	D	4	5/5	0.99	0.09	27,28,30,30	0
3	MET	F	600	9/9	0.99	0.13	12,14,14,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.