



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 11:05 am BST

PDB ID : 2IWV
Title : Structure of the monomeric outer membrane porin OmpG in the open and closed conformation
Authors : Yildiz, O.; Vinothkumar, K.R.; Goswami, P.; Kuehlbrandt, W.
Deposited on : 2006-07-04
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

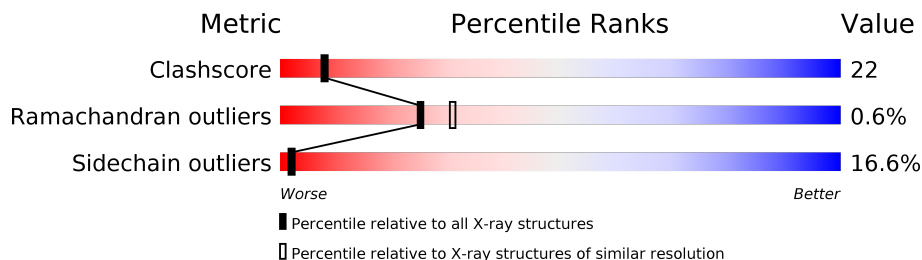
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	281	 57% 33% 7% ..
1	B	281	 59% 29% 9% ..
1	C	281	 59% 30% 7% ..
1	D	281	 59% 28% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LDA	A	1313	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LDA	A	1315	-	-	X	-
3	LDA	A	1318	-	-	X	-
3	LDA	A	1319	-	-	X	-
3	LDA	A	413	-	-	X	-
3	LDA	B	1292	-	-	X	-
3	LDA	C	1291	-	-	X	-
3	LDA	D	1301	-	-	X	-
3	LDA	D	1307	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12128 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.

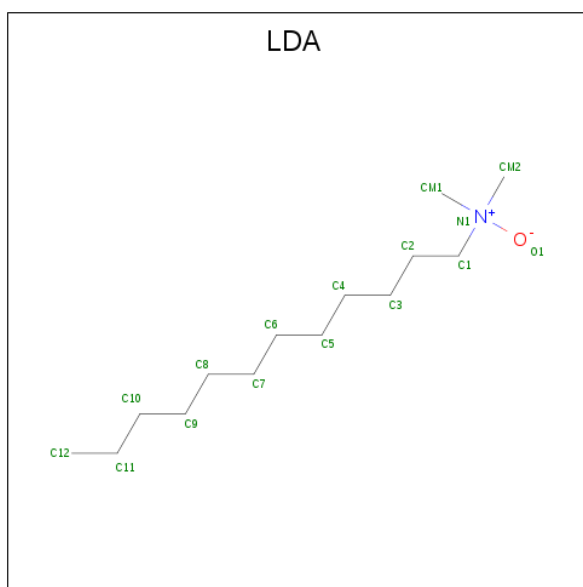
- Molecule 1 is a protein called OUTER MEMBRANE PROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	2298	1461	381	451	5	0	0	0
1	B	277	2298	1461	381	451	5	0	0	0
1	C	277	2298	1461	381	451	5	0	0	0
1	D	277	2298	1461	381	451	5	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	Ca	0	0
			9	9		
2	A	9	Total	Ca	0	0
			9	9		
2	D	7	Total	Ca	0	0
			7	7		
2	C	8	Total	Ca	0	0
			8	8		

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0

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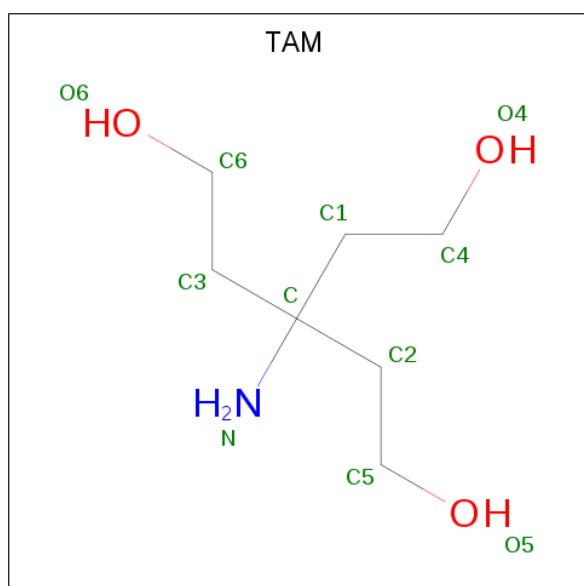
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0

- Molecule 4 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	124	Total	O	0	0
			124	124		
5	C	112	Total	O	0	0
			112	112		
5	D	114	Total	O	0	0
			114	114		

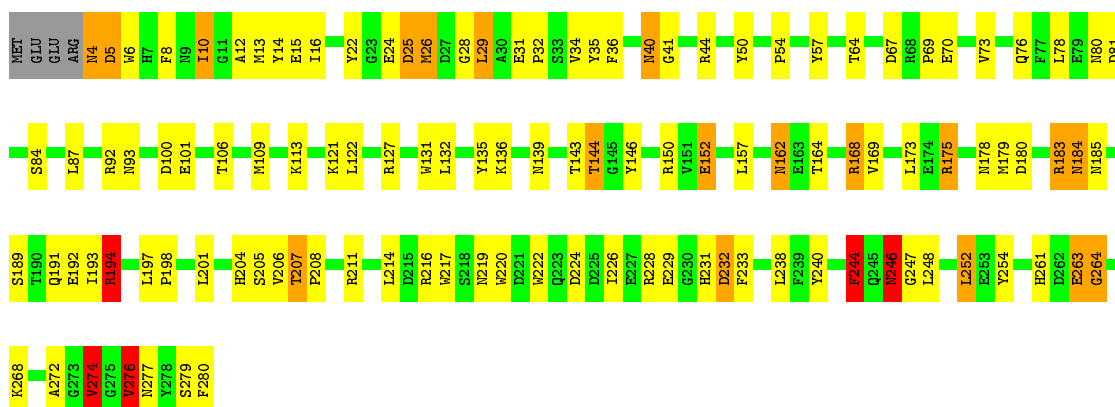
3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

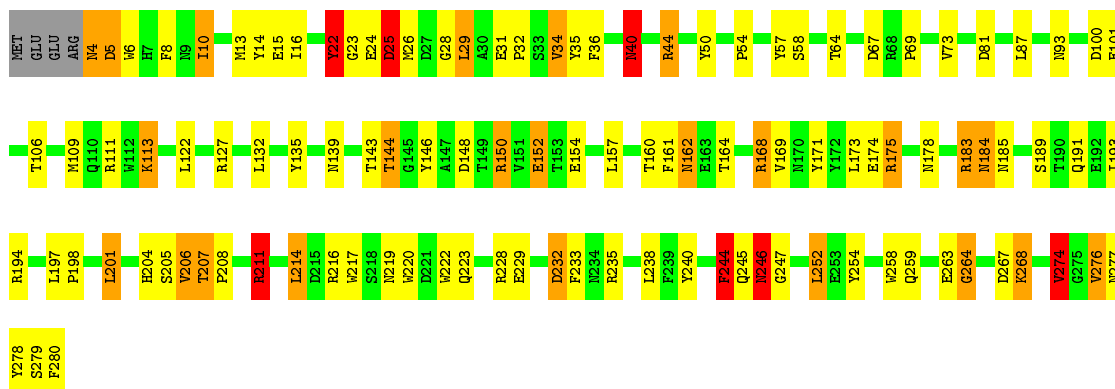
- Molecule 1: OUTER MEMBRANE PROTEIN G

Chain A:  57% 33% 7% ..



- Molecule 1: OUTER MEMBRANE PROTEIN G

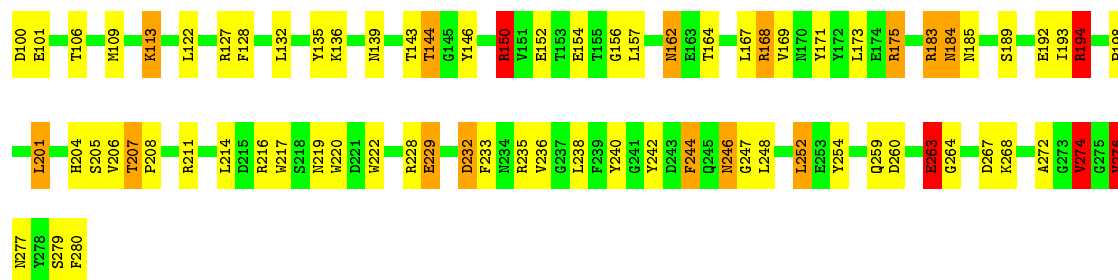
Chain B:  59% 29% 9% ..



- Molecule 1: OUTER MEMBRANE PROTEIN G

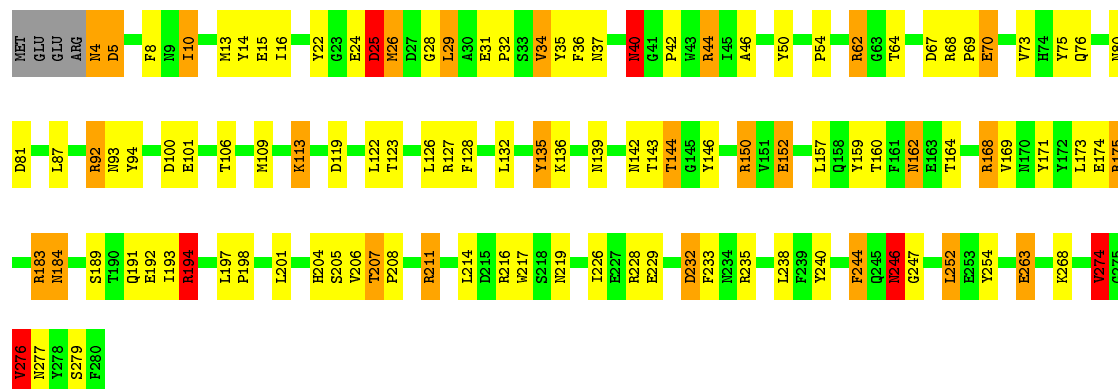
Chain C:  59% 30% 7% ..





- Molecule 1: OUTER MEMBRANE PROTEIN G

Chain D: 59% 28% 9% ..



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.60Å 77.00Å 103.90Å 79.30° 73.40° 74.30°	Depositor
Resolution (Å)	14.98 – 2.30	Depositor
% Data completeness (in resolution range)	100.0 (14.98-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12128	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

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: TAM, CA, LDA

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	0.97	1/2372 (0.0%)	1.05	10/3226 (0.3%)
1	B	1.03	3/2372 (0.1%)	1.14	16/3226 (0.5%)
1	C	1.04	2/2372 (0.1%)	1.08	10/3226 (0.3%)
1	D	1.03	7/2372 (0.3%)	1.10	15/3226 (0.5%)
All	All	1.01	13/9488 (0.1%)	1.09	51/12904 (0.4%)

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	8
1	B	0	7
1	C	0	7
1	D	0	6
All	All	0	28

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	GLU	CD-OE1	7.59	1.34	1.25
1	A	152	GLU	CD-OE1	6.70	1.33	1.25
1	D	46	ALA	CA-CB	6.59	1.66	1.52
1	D	152	GLU	CD-OE1	6.35	1.32	1.25
1	B	174	GLU	CD-OE2	6.11	1.32	1.25

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	ARG	NE-CZ-NH1	13.72	127.16	120.30
1	B	211	ARG	NE-CZ-NH1	-12.15	114.23	120.30
1	B	194	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	D	168	ARG	NE-CZ-NH2	-11.24	114.68	120.30
1	B	211	ARG	NE-CZ-NH2	10.76	125.68	120.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ARG	Peptide
1	A	244	PHE	Peptide
1	A	25	ASP	Peptide
1	A	4	ASN	Peptide
1	A	40	ASN	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	2298	0	2038	79	0
1	B	2298	0	2038	92	0
1	C	2298	0	2038	93	0
1	D	2298	0	2038	84	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	C	8	0	0	0	0
2	D	7	0	0	0	0
3	A	656	0	1271	95	0
3	B	688	0	1333	75	0
3	C	672	0	1302	78	0
3	D	416	0	806	54	0
4	B	11	0	17	1	0
5	A	110	0	0	8	0
5	B	124	0	0	12	0
5	C	112	0	0	11	0
5	D	114	0	0	7	0
All	All	12128	0	12881	527	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 22.

The worst 5 of 527 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:C:247:GLY:HA2	5:C:2095:HOH:O	1.38	1.22
3:C:1291:LDA:HM13	3:C:1323:LDA:H52	1.23	1.14
3:D:1301:LDA:H102	3:D:1308:LDA:H102	1.28	1.12
1:A:162:ASN:HD22	1:A:164:THR:H	1.02	1.01
1:D:162:ASN:HD22	1:D:164:THR:H	1.07	1.00

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	275/281 (98%)	259 (94%)	13 (5%)	3 (1%)	14 15
1	B	275/281 (98%)	260 (94%)	14 (5%)	1 (0%)	34 42
1	C	275/281 (98%)	262 (95%)	12 (4%)	1 (0%)	34 42
1	D	275/281 (98%)	259 (94%)	14 (5%)	2 (1%)	22 26
All	All	1100/1124 (98%)	1040 (94%)	53 (5%)	7 (1%)	25 31

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	41	GLY
1	A	184	ASN
1	B	184	ASN
1	C	184	ASN

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	235/239 (98%)	198 (84%)	37 (16%)	2	2
1	B	235/239 (98%)	195 (83%)	40 (17%)	2	2
1	C	235/239 (98%)	196 (83%)	39 (17%)	2	2
1	D	235/239 (98%)	195 (83%)	40 (17%)	2	2
All	All	940/956 (98%)	784 (83%)	156 (17%)	2	2

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	246	ASN
1	C	87	LEU
1	D	207	THR
1	B	263	GLU
1	C	13	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	246	ASN
1	C	110	GLN
1	D	185	ASN
1	C	93	ASN
1	C	139	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 33 are monoatomic - leaving 153 for Mogul analysis.

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
3	LDA	B	1316	-	12,15,15	2.08	1 (8%)	14,17,17	0.52	0
3	LDA	D	1297	-	12,15,15	2.02	1 (8%)	14,17,17	0.45	0
3	LDA	A	1303	-	12,15,15	2.61	1 (8%)	14,17,17	1.11	1 (7%)
3	LDA	D	1282	-	12,15,15	1.76	1 (8%)	14,17,17	0.82	1 (7%)
3	LDA	C	1318	-	12,15,15	1.90	1 (8%)	14,17,17	0.67	0
3	LDA	C	1300	-	12,15,15	2.11	1 (8%)	14,17,17	0.53	0
3	LDA	B	1294	-	12,15,15	2.07	1 (8%)	14,17,17	0.62	0
3	LDA	A	1299	-	12,15,15	1.89	1 (8%)	14,17,17	0.66	0
3	LDA	C	1320	-	12,15,15	2.01	1 (8%)	14,17,17	0.40	0
3	LDA	A	1324	-	12,15,15	2.03	1 (8%)	14,17,17	0.60	0
3	LDA	B	1325	-	12,15,15	2.05	1 (8%)	14,17,17	0.60	0
3	LDA	A	1305	-	12,15,15	1.91	1 (8%)	14,17,17	0.78	0
3	LDA	B	1307	-	12,15,15	2.02	1 (8%)	14,17,17	0.90	1 (7%)
3	LDA	C	1294	-	12,15,15	1.94	1 (8%)	14,17,17	0.74	0
3	LDA	B	1300	-	12,15,15	2.02	1 (8%)	14,17,17	0.55	0
3	LDA	B	1312	-	12,15,15	1.98	1 (8%)	14,17,17	0.61	0
3	LDA	C	1311	-	12,15,15	2.07	1 (8%)	14,17,17	0.55	0
3	LDA	D	1281	-	12,15,15	2.13	1 (8%)	14,17,17	1.03	0
3	LDA	B	1296	-	12,15,15	1.91	1 (8%)	14,17,17	0.71	0
3	LDA	B	1293	-	12,15,15	2.05	1 (8%)	14,17,17	0.54	0
3	LDA	A	1300	-	12,15,15	2.12	1 (8%)	14,17,17	0.55	0
3	LDA	B	1304	-	12,15,15	2.60	1 (8%)	14,17,17	1.72	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	B	1330	-	12,15,15	2.02	1 (8%)	14,17,17	0.78	0
3	LDA	A	1301	-	12,15,15	2.02	1 (8%)	14,17,17	0.42	0
3	LDA	A	1295	-	12,15,15	1.89	1 (8%)	14,17,17	0.77	0
3	LDA	A	1291	-	12,15,15	2.03	1 (8%)	14,17,17	0.68	0
3	LDA	B	1321	-	12,15,15	2.58	3 (25%)	14,17,17	1.26	2 (14%)
3	LDA	B	1292	-	12,15,15	1.96	1 (8%)	14,17,17	0.68	0
3	LDA	D	1310	-	12,15,15	1.94	1 (8%)	14,17,17	0.63	0
3	LDA	A	1304	-	12,15,15	2.65	1 (8%)	14,17,17	1.54	3 (21%)
3	LDA	C	1281	-	12,15,15	2.15	1 (8%)	14,17,17	0.53	0
3	LDA	B	413	-	12,15,15	1.99	1 (8%)	14,17,17	0.62	0
3	LDA	D	1294	-	12,15,15	2.07	1 (8%)	14,17,17	0.56	0
3	LDA	B	1327	-	12,15,15	2.28	2 (16%)	14,17,17	0.96	1 (7%)
3	LDA	C	1324	-	12,15,15	2.06	1 (8%)	14,17,17	0.50	0
3	LDA	B	1305	-	12,15,15	1.95	1 (8%)	14,17,17	0.79	0
3	LDA	A	1307	-	12,15,15	2.48	1 (8%)	14,17,17	1.41	1 (7%)
3	LDA	A	1319	-	12,15,15	1.89	1 (8%)	14,17,17	0.47	0
3	LDA	A	1313	-	12,15,15	1.98	1 (8%)	14,17,17	0.88	1 (7%)
3	LDA	B	1311	-	12,15,15	2.04	1 (8%)	14,17,17	0.72	0
3	LDA	B	1309	-	12,15,15	2.92	1 (8%)	14,17,17	1.91	3 (21%)
4	TAM	B	1289	-	7,10,10	0.88	0	9,12,12	0.75	0
3	LDA	A	1312	-	12,15,15	2.88	1 (8%)	14,17,17	1.95	2 (14%)
3	LDA	A	1316	-	12,15,15	2.03	1 (8%)	14,17,17	0.57	0
3	LDA	A	1309	-	12,15,15	2.01	1 (8%)	14,17,17	0.70	0
3	LDA	B	1317	-	12,15,15	2.05	1 (8%)	14,17,17	0.49	0
3	LDA	A	1296	-	12,15,15	2.02	1 (8%)	14,17,17	0.51	0
3	LDA	D	1296	-	12,15,15	1.93	1 (8%)	14,17,17	0.73	0
3	LDA	D	1303	-	12,15,15	2.06	1 (8%)	14,17,17	0.39	0
3	LDA	A	1317	-	12,15,15	2.00	1 (8%)	14,17,17	0.54	0
3	LDA	B	1315	-	12,15,15	2.16	1 (8%)	14,17,17	0.52	0
3	LDA	A	413	-	12,15,15	1.93	1 (8%)	14,17,17	0.59	0
3	LDA	C	1304	-	12,15,15	2.14	1 (8%)	14,17,17	0.47	0
3	LDA	B	1299	-	12,15,15	2.07	1 (8%)	14,17,17	0.94	1 (7%)
3	LDA	B	1318	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
3	LDA	B	1306	-	12,15,15	2.01	1 (8%)	14,17,17	0.73	0
3	LDA	A	1028	-	12,15,15	1.98	1 (8%)	14,17,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	B	1298	-	12,15,15	1.95	1 (8%)	14,17,17	0.57	0
3	LDA	A	1325	-	12,15,15	1.97	1 (8%)	14,17,17	0.57	0
3	LDA	A	1320	-	12,15,15	2.02	1 (8%)	14,17,17	0.73	0
3	LDA	B	1328	-	12,15,15	2.56	1 (8%)	14,17,17	1.24	2 (14%)
3	LDA	A	1326	-	12,15,15	2.12	1 (8%)	14,17,17	0.54	0
3	LDA	C	1307	-	12,15,15	2.16	1 (8%)	14,17,17	1.00	2 (14%)
3	LDA	B	1324	-	12,15,15	2.03	1 (8%)	14,17,17	0.50	0
3	LDA	A	1289	-	12,15,15	2.01	1 (8%)	14,17,17	0.63	0
3	LDA	A	1327	-	12,15,15	2.04	1 (8%)	14,17,17	0.72	0
3	LDA	D	1299	-	12,15,15	2.01	1 (8%)	14,17,17	0.88	1 (7%)
3	LDA	C	1315	-	12,15,15	2.00	1 (8%)	14,17,17	0.56	0
3	LDA	C	1308	-	12,15,15	1.86	1 (8%)	14,17,17	0.65	0
3	LDA	A	1292	-	12,15,15	2.01	1 (8%)	14,17,17	0.59	0
3	LDA	A	1321	-	12,15,15	2.04	1 (8%)	14,17,17	0.54	0
3	LDA	D	1307	-	12,15,15	1.98	1 (8%)	14,17,17	0.71	0
3	LDA	D	1308	-	12,15,15	2.48	1 (8%)	14,17,17	2.13	2 (14%)
3	LDA	A	1322	-	12,15,15	2.06	1 (8%)	14,17,17	0.42	0
3	LDA	B	1320	-	12,15,15	2.03	1 (8%)	14,17,17	0.52	0
3	LDA	A	1294	-	12,15,15	2.01	1 (8%)	14,17,17	0.85	0
3	LDA	C	1303	-	12,15,15	2.03	1 (8%)	14,17,17	0.69	0
3	LDA	C	1314	-	12,15,15	2.02	1 (8%)	14,17,17	0.59	0
3	LDA	C	1292	-	12,15,15	2.08	1 (8%)	14,17,17	0.52	0
3	LDA	D	1312	-	12,15,15	2.12	1 (8%)	14,17,17	0.43	0
3	LDA	C	1295	-	12,15,15	1.90	1 (8%)	14,17,17	0.75	0
3	LDA	D	1313	-	12,15,15	1.93	1 (8%)	14,17,17	0.57	0
3	LDA	B	1314	-	12,15,15	2.09	1 (8%)	14,17,17	0.54	0
3	LDA	C	1299	-	12,15,15	1.95	1 (8%)	14,17,17	0.66	0
3	LDA	A	1298	-	12,15,15	2.09	1 (8%)	14,17,17	0.93	1 (7%)
3	LDA	C	1290	-	12,15,15	1.96	1 (8%)	14,17,17	0.80	0
3	LDA	C	1309	-	12,15,15	2.06	1 (8%)	14,17,17	0.62	0
3	LDA	B	1323	-	12,15,15	2.06	1 (8%)	14,17,17	0.55	0
3	LDA	C	1291	-	12,15,15	2.04	1 (8%)	14,17,17	0.65	0
3	LDA	C	1310	-	12,15,15	2.00	1 (8%)	14,17,17	0.60	0
3	LDA	C	1321	-	12,15,15	2.03	1 (8%)	14,17,17	0.50	0
3	LDA	A	1297	-	12,15,15	1.92	1 (8%)	14,17,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	D	1305	-	12,15,15	2.03	1 (8%)	14,17,17	1.08	0
3	LDA	D	1301	-	12,15,15	2.10	1 (8%)	14,17,17	0.52	0
3	LDA	B	1290	-	12,15,15	2.08	1 (8%)	14,17,17	0.75	1 (7%)
3	LDA	D	1300	-	12,15,15	2.01	1 (8%)	14,17,17	0.59	0
3	LDA	C	1319	-	12,15,15	1.91	1 (8%)	14,17,17	0.82	0
3	LDA	D	1292	-	12,15,15	2.06	1 (8%)	14,17,17	0.65	0
3	LDA	D	1291	-	12,15,15	1.91	1 (8%)	14,17,17	0.81	0
3	LDA	A	1293	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
3	LDA	C	1301	-	12,15,15	2.04	1 (8%)	14,17,17	0.44	0
3	LDA	C	1326	-	12,15,15	2.02	1 (8%)	14,17,17	0.70	0
3	LDA	C	1328	-	12,15,15	2.06	1 (8%)	14,17,17	0.39	0
3	LDA	A	1310	-	12,15,15	2.02	1 (8%)	14,17,17	0.99	1 (7%)
3	LDA	A	1315	-	12,15,15	2.53	1 (8%)	14,17,17	2.04	1 (7%)
3	LDA	C	1325	-	12,15,15	1.89	1 (8%)	14,17,17	0.77	1 (7%)
3	LDA	D	1306	-	12,15,15	2.17	1 (8%)	14,17,17	1.25	2 (14%)
3	LDA	D	1309	-	12,15,15	1.98	1 (8%)	14,17,17	0.54	0
3	LDA	D	1311	-	12,15,15	1.99	1 (8%)	14,17,17	0.66	0
3	LDA	D	1295	-	12,15,15	2.05	1 (8%)	14,17,17	0.69	0
3	LDA	C	413	-	12,15,15	1.97	1 (8%)	14,17,17	0.56	0
3	LDA	B	1291	-	12,15,15	1.86	1 (8%)	14,17,17	0.73	0
3	LDA	C	1305	-	12,15,15	2.10	1 (8%)	14,17,17	0.52	0
3	LDA	B	1313	-	12,15,15	1.94	1 (8%)	14,17,17	0.50	0
3	LDA	B	1329	-	12,15,15	2.11	1 (8%)	14,17,17	0.59	0
3	LDA	B	1297	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
3	LDA	A	1314	-	12,15,15	2.05	1 (8%)	14,17,17	0.49	0
3	LDA	C	1298	-	12,15,15	2.08	1 (8%)	14,17,17	0.93	1 (7%)
3	LDA	A	1318	-	12,15,15	1.74	1 (8%)	14,17,17	0.68	0
3	LDA	A	1306	-	12,15,15	2.18	1 (8%)	14,17,17	0.53	0
3	LDA	C	1293	-	12,15,15	2.02	1 (8%)	14,17,17	0.60	0
3	LDA	A	1308	-	12,15,15	2.14	1 (8%)	14,17,17	1.07	1 (7%)
3	LDA	C	1312	-	12,15,15	2.04	1 (8%)	14,17,17	0.44	0
3	LDA	D	1298	-	12,15,15	1.86	1 (8%)	14,17,17	0.49	0
3	LDA	A	1290	-	12,15,15	1.98	1 (8%)	14,17,17	0.85	0
3	LDA	D	1304	-	12,15,15	2.57	1 (8%)	14,17,17	1.43	1 (7%)
3	LDA	B	482	-	12,15,15	1.99	1 (8%)	14,17,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LDA	B	1319	-	12,15,15	1.94	1 (8%)	14,17,17	0.69	0
3	LDA	C	1327	-	12,15,15	2.11	1 (8%)	14,17,17	0.58	0
3	LDA	C	1296	-	12,15,15	2.09	1 (8%)	14,17,17	0.51	0
3	LDA	C	1306	-	12,15,15	2.04	1 (8%)	14,17,17	0.89	0
3	LDA	D	1302	-	12,15,15	2.05	1 (8%)	14,17,17	0.50	0
3	LDA	B	1295	-	12,15,15	2.01	1 (8%)	14,17,17	0.85	0
3	LDA	D	1290	-	12,15,15	2.11	1 (8%)	14,17,17	0.72	1 (7%)
3	LDA	A	1302	-	12,15,15	2.04	1 (8%)	14,17,17	0.47	0
3	LDA	C	1316	-	12,15,15	1.98	1 (8%)	14,17,17	0.55	0
3	LDA	C	1289	-	12,15,15	1.97	1 (8%)	14,17,17	0.66	0
3	LDA	A	1323	-	12,15,15	1.97	1 (8%)	14,17,17	0.59	0
3	LDA	D	1293	-	12,15,15	2.10	1 (8%)	14,17,17	0.55	0
3	LDA	B	1326	-	12,15,15	2.02	1 (8%)	14,17,17	0.51	0
3	LDA	C	1323	-	12,15,15	1.99	1 (8%)	14,17,17	0.50	0
3	LDA	B	1322	-	12,15,15	2.05	1 (8%)	14,17,17	0.60	0
3	LDA	A	1311	-	12,15,15	2.07	1 (8%)	14,17,17	0.57	0
3	LDA	B	1303	-	12,15,15	2.02	1 (8%)	14,17,17	0.47	0
3	LDA	B	1310	-	12,15,15	2.05	1 (8%)	14,17,17	0.51	0
3	LDA	B	1302	-	12,15,15	2.02	1 (8%)	14,17,17	0.47	0
3	LDA	B	1301	-	12,15,15	2.10	1 (8%)	14,17,17	0.49	0
3	LDA	C	1297	-	12,15,15	1.87	1 (8%)	14,17,17	0.51	0
3	LDA	B	1308	-	12,15,15	2.02	1 (8%)	14,17,17	0.56	0
3	LDA	C	1317	-	12,15,15	2.00	1 (8%)	14,17,17	0.58	0
3	LDA	C	1313	-	12,15,15	2.04	1 (8%)	14,17,17	0.58	0
3	LDA	C	1302	-	12,15,15	2.13	1 (8%)	14,17,17	0.48	0
3	LDA	C	1322	-	12,15,15	2.01	1 (8%)	14,17,17	0.69	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	LDA	B	1316	-	-	9/13/13/13	-
3	LDA	D	1297	-	-	7/13/13/13	-
3	LDA	A	1303	-	-	8/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	D	1282	-	-	7/13/13/13	-
3	LDA	C	1318	-	-	11/13/13/13	-
3	LDA	C	1300	-	-	9/13/13/13	-
3	LDA	B	1294	-	-	8/13/13/13	-
3	LDA	A	1299	-	-	7/13/13/13	-
3	LDA	C	1320	-	-	8/13/13/13	-
3	LDA	A	1324	-	-	11/13/13/13	-
3	LDA	B	1325	-	-	6/13/13/13	-
3	LDA	A	1305	-	-	5/13/13/13	-
3	LDA	B	1307	-	-	8/13/13/13	-
3	LDA	C	1294	-	-	9/13/13/13	-
3	LDA	B	1300	-	-	7/13/13/13	-
3	LDA	B	1312	-	-	6/13/13/13	-
3	LDA	C	1311	-	-	9/13/13/13	-
3	LDA	D	1281	-	-	7/13/13/13	-
3	LDA	B	1296	-	-	6/13/13/13	-
3	LDA	B	1293	-	-	7/13/13/13	-
3	LDA	A	1300	-	-	11/13/13/13	-
3	LDA	B	1304	-	-	10/13/13/13	-
3	LDA	B	1330	-	-	8/13/13/13	-
3	LDA	A	1301	-	-	7/13/13/13	-
3	LDA	A	1295	-	-	6/13/13/13	-
3	LDA	A	1291	-	-	8/13/13/13	-
3	LDA	B	1321	-	-	7/13/13/13	-
3	LDA	B	1292	-	-	8/13/13/13	-
3	LDA	D	1310	-	-	4/13/13/13	-
3	LDA	A	1304	-	-	10/13/13/13	-
3	LDA	C	1281	-	-	12/13/13/13	-
3	LDA	B	413	-	-	5/13/13/13	-
3	LDA	D	1294	-	-	8/13/13/13	-
3	LDA	B	1327	-	-	8/13/13/13	-
3	LDA	C	1324	-	-	3/13/13/13	-
3	LDA	B	1305	-	-	5/13/13/13	-
3	LDA	A	1307	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	A	1319	-	-	3/13/13/13	-
3	LDA	A	1313	-	-	7/13/13/13	-
3	LDA	B	1311	-	-	10/13/13/13	-
3	LDA	B	1309	-	-	9/13/13/13	-
4	TAM	B	1289	-	-	10/12/12/12	-
3	LDA	A	1312	-	-	12/13/13/13	-
3	LDA	A	1316	-	-	6/13/13/13	-
3	LDA	A	1309	-	-	10/13/13/13	-
3	LDA	B	1317	-	-	10/13/13/13	-
3	LDA	A	1296	-	-	7/13/13/13	-
3	LDA	D	1296	-	-	6/13/13/13	-
3	LDA	D	1303	-	-	6/13/13/13	-
3	LDA	A	1317	-	-	5/13/13/13	-
3	LDA	B	1315	-	-	8/13/13/13	-
3	LDA	A	413	-	-	5/13/13/13	-
3	LDA	C	1304	-	-	4/13/13/13	-
3	LDA	B	1299	-	-	5/13/13/13	-
3	LDA	B	1318	-	-	9/13/13/13	-
3	LDA	B	1306	-	-	11/13/13/13	-
3	LDA	A	1028	-	-	9/13/13/13	-
3	LDA	B	1298	-	-	5/13/13/13	-
3	LDA	A	1325	-	-	5/13/13/13	-
3	LDA	A	1320	-	-	10/13/13/13	-
3	LDA	B	1328	-	-	8/13/13/13	-
3	LDA	A	1326	-	-	4/13/13/13	-
3	LDA	C	1307	-	-	8/13/13/13	-
3	LDA	B	1324	-	-	9/13/13/13	-
3	LDA	A	1289	-	-	11/13/13/13	-
3	LDA	A	1327	-	-	10/13/13/13	-
3	LDA	D	1299	-	-	6/13/13/13	-
3	LDA	C	1315	-	-	8/13/13/13	-
3	LDA	C	1308	-	-	10/13/13/13	-
3	LDA	A	1292	-	-	7/13/13/13	-
3	LDA	A	1321	-	-	5/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	D	1307	-	-	10/13/13/13	-
3	LDA	D	1308	-	-	9/13/13/13	-
3	LDA	A	1322	-	-	6/13/13/13	-
3	LDA	B	1320	-	-	8/13/13/13	-
3	LDA	A	1294	-	-	7/13/13/13	-
3	LDA	C	1303	-	-	5/13/13/13	-
3	LDA	C	1314	-	-	5/13/13/13	-
3	LDA	C	1292	-	-	7/13/13/13	-
3	LDA	D	1312	-	-	1/13/13/13	-
3	LDA	C	1295	-	-	6/13/13/13	-
3	LDA	D	1313	-	-	10/13/13/13	-
3	LDA	B	1314	-	-	10/13/13/13	-
3	LDA	C	1299	-	-	7/13/13/13	-
3	LDA	A	1298	-	-	5/13/13/13	-
3	LDA	C	1290	-	-	9/13/13/13	-
3	LDA	C	1309	-	-	9/13/13/13	-
3	LDA	B	1323	-	-	11/13/13/13	-
3	LDA	C	1291	-	-	8/13/13/13	-
3	LDA	C	1310	-	-	6/13/13/13	-
3	LDA	C	1321	-	-	11/13/13/13	-
3	LDA	A	1297	-	-	5/13/13/13	-
3	LDA	D	1305	-	-	8/13/13/13	-
3	LDA	D	1301	-	-	10/13/13/13	-
3	LDA	B	1290	-	-	11/13/13/13	-
3	LDA	D	1300	-	-	7/13/13/13	-
3	LDA	C	1319	-	-	8/13/13/13	-
3	LDA	D	1292	-	-	8/13/13/13	-
3	LDA	D	1291	-	-	8/13/13/13	-
3	LDA	A	1293	-	-	8/13/13/13	-
3	LDA	C	1301	-	-	7/13/13/13	-
3	LDA	C	1326	-	-	7/13/13/13	-
3	LDA	C	1328	-	-	7/13/13/13	-
3	LDA	A	1310	-	-	9/13/13/13	-
3	LDA	A	1315	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	C	1325	-	-	6/13/13/13	-
3	LDA	D	1306	-	-	7/13/13/13	-
3	LDA	D	1309	-	-	10/13/13/13	-
3	LDA	D	1311	-	-	11/13/13/13	-
3	LDA	D	1295	-	-	8/13/13/13	-
3	LDA	C	413	-	-	5/13/13/13	-
3	LDA	B	1291	-	-	7/13/13/13	-
3	LDA	C	1305	-	-	8/13/13/13	-
3	LDA	B	1313	-	-	7/13/13/13	-
3	LDA	B	1329	-	-	10/13/13/13	-
3	LDA	B	1297	-	-	6/13/13/13	-
3	LDA	A	1314	-	-	7/13/13/13	-
3	LDA	C	1298	-	-	6/13/13/13	-
3	LDA	A	1318	-	-	6/13/13/13	-
3	LDA	A	1306	-	-	4/13/13/13	-
3	LDA	C	1293	-	-	8/13/13/13	-
3	LDA	A	1308	-	-	7/13/13/13	-
3	LDA	C	1312	-	-	7/13/13/13	-
3	LDA	D	1298	-	-	5/13/13/13	-
3	LDA	A	1290	-	-	7/13/13/13	-
3	LDA	D	1304	-	-	7/13/13/13	-
3	LDA	B	482	-	-	7/13/13/13	-
3	LDA	B	1319	-	-	6/13/13/13	-
3	LDA	C	1327	-	-	8/13/13/13	-
3	LDA	C	1296	-	-	7/13/13/13	-
3	LDA	C	1306	-	-	6/13/13/13	-
3	LDA	D	1302	-	-	7/13/13/13	-
3	LDA	B	1295	-	-	7/13/13/13	-
3	LDA	D	1290	-	-	11/13/13/13	-
3	LDA	A	1302	-	-	6/13/13/13	-
3	LDA	C	1316	-	-	7/13/13/13	-
3	LDA	C	1289	-	-	11/13/13/13	-
3	LDA	A	1323	-	-	10/13/13/13	-
3	LDA	D	1293	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LDA	B	1326	-	-	7/13/13/13	-
3	LDA	C	1323	-	-	8/13/13/13	-
3	LDA	B	1322	-	-	4/13/13/13	-
3	LDA	A	1311	-	-	7/13/13/13	-
3	LDA	B	1303	-	-	6/13/13/13	-
3	LDA	B	1310	-	-	6/13/13/13	-
3	LDA	B	1302	-	-	7/13/13/13	-
3	LDA	B	1301	-	-	9/13/13/13	-
3	LDA	C	1297	-	-	5/13/13/13	-
3	LDA	B	1308	-	-	9/13/13/13	-
3	LDA	C	1317	-	-	10/13/13/13	-
3	LDA	C	1313	-	-	9/13/13/13	-
3	LDA	C	1302	-	-	6/13/13/13	-
3	LDA	C	1322	-	-	7/13/13/13	-

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1309	LDA	O1-N1	-10.04	1.18	1.42
3	A	1312	LDA	O1-N1	-9.86	1.19	1.42
3	A	1304	LDA	O1-N1	-9.15	1.20	1.42
3	A	1303	LDA	O1-N1	-9.00	1.21	1.42
3	B	1304	LDA	O1-N1	-8.99	1.21	1.42

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1308	LDA	CM2-N1-C1	7.24	125.45	110.23
3	A	1315	LDA	CM2-N1-C1	7.23	125.43	110.23
3	D	1304	LDA	CM1-N1-C1	5.09	120.93	110.23
3	A	1307	LDA	CM1-N1-C1	4.97	120.67	110.23
3	A	1312	LDA	CM1-N1-C1	4.74	120.19	110.23

There are no chirality outliers.

5 of 1151 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1316	LDA	C2-C1-N1-CM2

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Mol	Chain	Res	Type	Atoms
3	C	1318	LDA	C2-C1-N1-CM1
3	C	1318	LDA	C2-C1-N1-CM2
3	C	1318	LDA	N1-C1-C2-C3
3	C	1300	LDA	C2-C1-N1-O1

There are no ring outliers.

117 monomers are involved in 299 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1303	LDA	4	0
3	D	1282	LDA	2	0
3	C	1318	LDA	4	0
3	C	1300	LDA	3	0
3	B	1294	LDA	6	0
3	A	1299	LDA	1	0
3	C	1320	LDA	2	0
3	A	1324	LDA	3	0
3	B	1307	LDA	4	0
3	C	1294	LDA	4	0
3	B	1300	LDA	1	0
3	B	1312	LDA	2	0
3	C	1311	LDA	1	0
3	D	1281	LDA	1	0
3	B	1293	LDA	4	0
3	A	1300	LDA	8	0
3	B	1304	LDA	5	0
3	B	1330	LDA	6	0
3	A	1301	LDA	1	0
3	A	1291	LDA	7	0
3	B	1292	LDA	12	0
3	D	1310	LDA	1	0
3	A	1304	LDA	4	0
3	C	1281	LDA	4	0
3	B	413	LDA	2	0
3	B	1327	LDA	1	0
3	C	1324	LDA	1	0
3	A	1307	LDA	2	0
3	A	1319	LDA	13	0
3	A	1313	LDA	10	0
3	B	1311	LDA	3	0
3	B	1309	LDA	1	0
4	B	1289	TAM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1316	LDA	2	0
3	A	1309	LDA	6	0
3	B	1315	LDA	2	0
3	A	413	LDA	9	0
3	C	1304	LDA	1	0
3	B	1299	LDA	5	0
3	B	1306	LDA	3	0
3	B	1298	LDA	1	0
3	A	1325	LDA	4	0
3	A	1320	LDA	6	0
3	B	1328	LDA	5	0
3	A	1326	LDA	2	0
3	C	1307	LDA	7	0
3	B	1324	LDA	1	0
3	A	1327	LDA	2	0
3	D	1299	LDA	6	0
3	C	1315	LDA	4	0
3	C	1308	LDA	7	0
3	A	1292	LDA	4	0
3	A	1321	LDA	1	0
3	D	1307	LDA	10	0
3	D	1308	LDA	5	0
3	A	1322	LDA	5	0
3	B	1320	LDA	1	0
3	A	1294	LDA	2	0
3	C	1303	LDA	2	0
3	C	1314	LDA	2	0
3	C	1292	LDA	4	0
3	D	1312	LDA	1	0
3	D	1313	LDA	3	0
3	B	1314	LDA	1	0
3	C	1299	LDA	2	0
3	A	1298	LDA	4	0
3	C	1290	LDA	6	0
3	C	1309	LDA	2	0
3	B	1323	LDA	1	0
3	C	1291	LDA	11	0
3	C	1310	LDA	1	0
3	C	1321	LDA	3	0
3	A	1297	LDA	2	0
3	D	1305	LDA	2	0
3	D	1301	LDA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1319	LDA	4	0
3	D	1292	LDA	6	0
3	D	1291	LDA	6	0
3	A	1293	LDA	1	0
3	C	1326	LDA	2	0
3	C	1328	LDA	2	0
3	A	1310	LDA	6	0
3	A	1315	LDA	9	0
3	C	1325	LDA	1	0
3	D	1306	LDA	4	0
3	D	1309	LDA	1	0
3	D	1311	LDA	2	0
3	D	1295	LDA	3	0
3	C	413	LDA	3	0
3	B	1291	LDA	3	0
3	C	1305	LDA	1	0
3	B	1313	LDA	5	0
3	B	1329	LDA	6	0
3	C	1298	LDA	5	0
3	A	1318	LDA	9	0
3	A	1306	LDA	2	0
3	A	1308	LDA	6	0
3	C	1312	LDA	1	0
3	D	1298	LDA	2	0
3	A	1290	LDA	4	0
3	D	1304	LDA	1	0
3	B	482	LDA	1	0
3	B	1319	LDA	4	0
3	C	1327	LDA	3	0
3	B	1295	LDA	1	0
3	A	1302	LDA	1	0
3	C	1316	LDA	1	0
3	A	1323	LDA	1	0
3	D	1293	LDA	4	0
3	B	1326	LDA	8	0
3	C	1323	LDA	7	0
3	B	1322	LDA	4	0
3	B	1310	LDA	4	0
3	B	1301	LDA	8	0
3	C	1297	LDA	1	0
3	C	1313	LDA	4	0
3	C	1302	LDA	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.