wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:02 AM GMT

PDB ID	:	3NSG
Title	:	Crystal Structure of OmpF, an Outer Membrane Protein from Salmonella typhi
Authors	:	Balasubramaniam, D.; Arockiasamy, A.; Sharma, A.; Krishnaswamy, S.
Deposited on	:	2010-07-01
Resolution	:	2.79 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

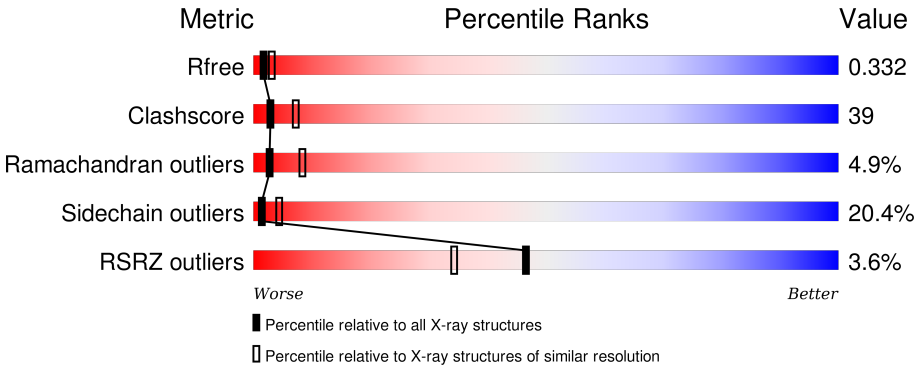
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.79 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 <=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	341	5% 35% 48% 16%
1	B	341	3% 39% 52% 9%
1	C	341	3% 39% 49% 11%

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
2	SO4	A	353	-	-	-	X
2	SO4	A	354	-	-	-	X
2	SO4	A	358	-	-	-	X
2	SO4	A	361	-	-	X	-
2	SO4	A	366	-	-	-	X
2	SO4	B	345	-	-	X	-
2	SO4	B	349	-	-	-	X
2	SO4	C	343	-	-	-	X
2	SO4	C	348	-	-	-	X
2	SO4	C	362	-	-	-	X
2	SO4	C	363	-	-	-	X
2	SO4	C	364	-	-	-	X
2	SO4	C	368	-	-	-	X
2	SO4	C	370	-	-	X	-
3	GOL	A	370	-	-	-	X
3	GOL	A	371	-	-	-	X
3	GOL	A	375	-	-	-	X
3	GOL	B	365	-	-	X	-
3	GOL	B	373	-	-	-	X
3	GOL	C	1325	-	-	-	X
3	GOL	C	375	-	-	X	-
4	LDA	A	384	-	-	-	X
4	LDA	A	386	-	-	-	X
4	LDA	A	387	-	-	-	X
4	LDA	A	388	-	-	-	X
4	LDA	C	385	-	-	-	X
5	TAM	A	390	-	-	X	X
6	FLC	C	388	-	-	X	-

2 Entry composition

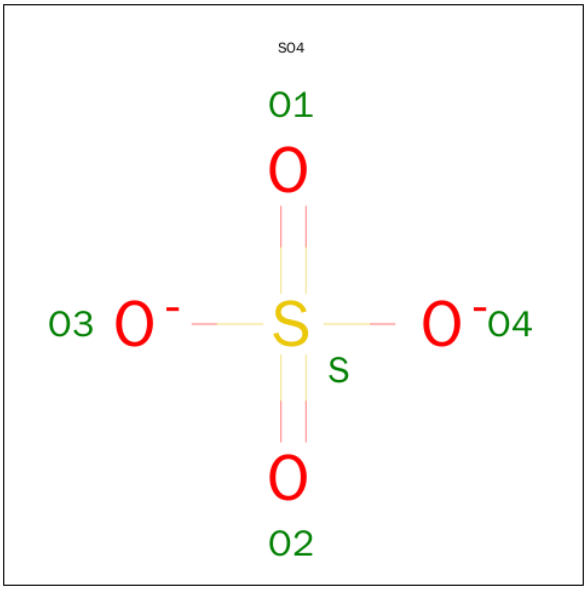
There are 8 unique types of molecules in this entry. The entry contains 9432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	Se	0	0	0
			2669	1662	453	547	7			
1	B	341	Total	C	N	O	Se	0	0	0
			2669	1662	453	547	7			
1	C	341	Total	C	N	O	Se	0	0	0
			2669	1662	453	547	7			

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



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	A	1	Total	O	S	0	0
			5	4	1		

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

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

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

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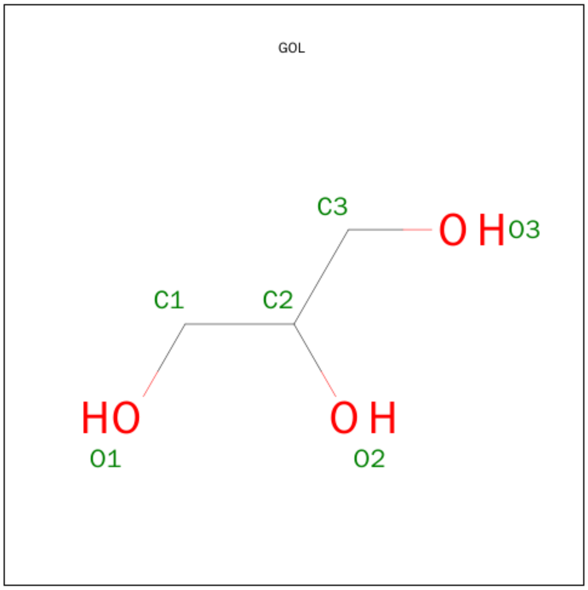
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

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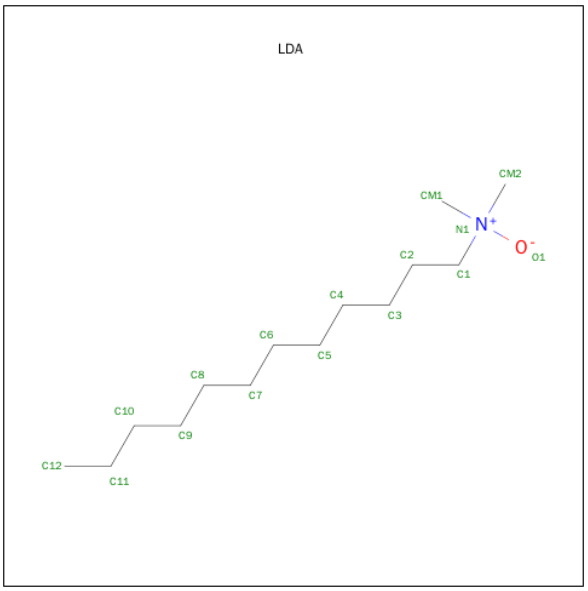
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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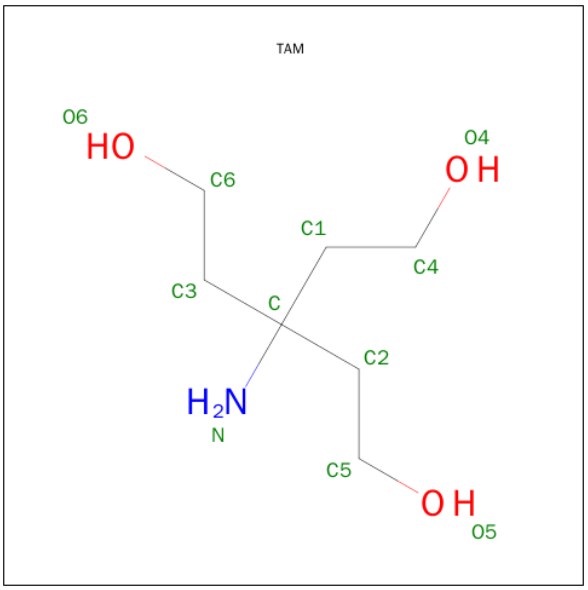
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 16 14 1 1	0	0
4	B	1	Total C N O 16 14 1 1	0	0
4	B	1	Total C N O 16 14 1 1	0	0
4	B	1	Total C N O 16 14 1 1	0	0
4	B	1	Total C N O 16 14 1 1	0	0
4	C	1	Total C N O 16 14 1 1	0	0
4	C	1	Total C N O 16 14 1 1	0	0
4	C	1	Total C N O 16 14 1 1	0	0
4	C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

- Molecule 5 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 11 7 1 3	0	0
5	A	1	Total C N O 11 7 1 3	0	0

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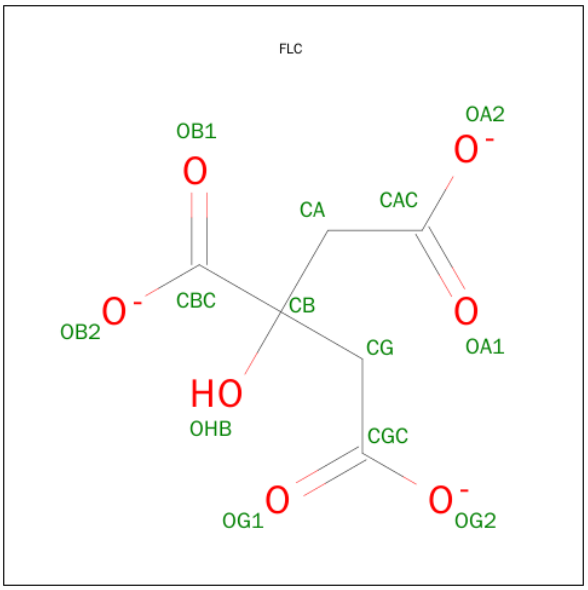
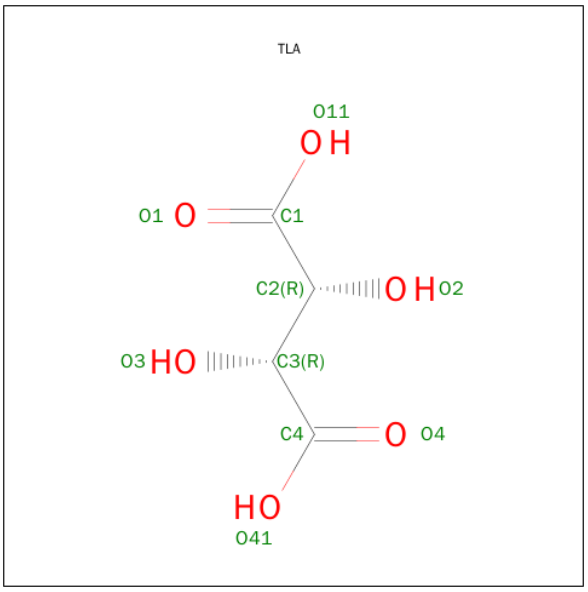
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 11 7 1 3	0	0
5	C	1	Total C N O 11 7 1 3	0	0
5	C	1	Total C N O 11 7 1 3	0	0
5	C	1	Total C N O 11 7 1 3	0	0

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 6 7	0	0
6	C	1	Total C O 13 6 7	0	0
6	C	1	Total C O 13 6 7	0	0
6	C	1	Total C O 13 6 7	0	0

- Molecule 7 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 10 4 6	0	0
7	B	1	Total C O 10 4 6	0	0

- Molecule 8 is water.

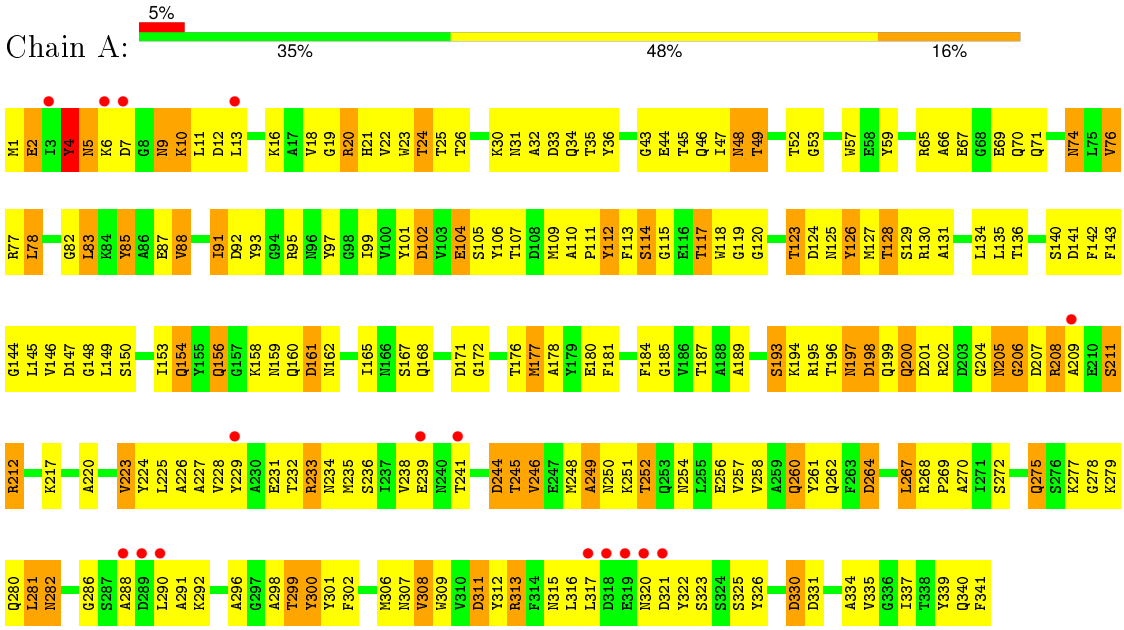
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	134	Total O 134 134	0	0
8	B	115	Total O 115 115	0	0
8	C	138	Total O 138 138	0	0

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 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.

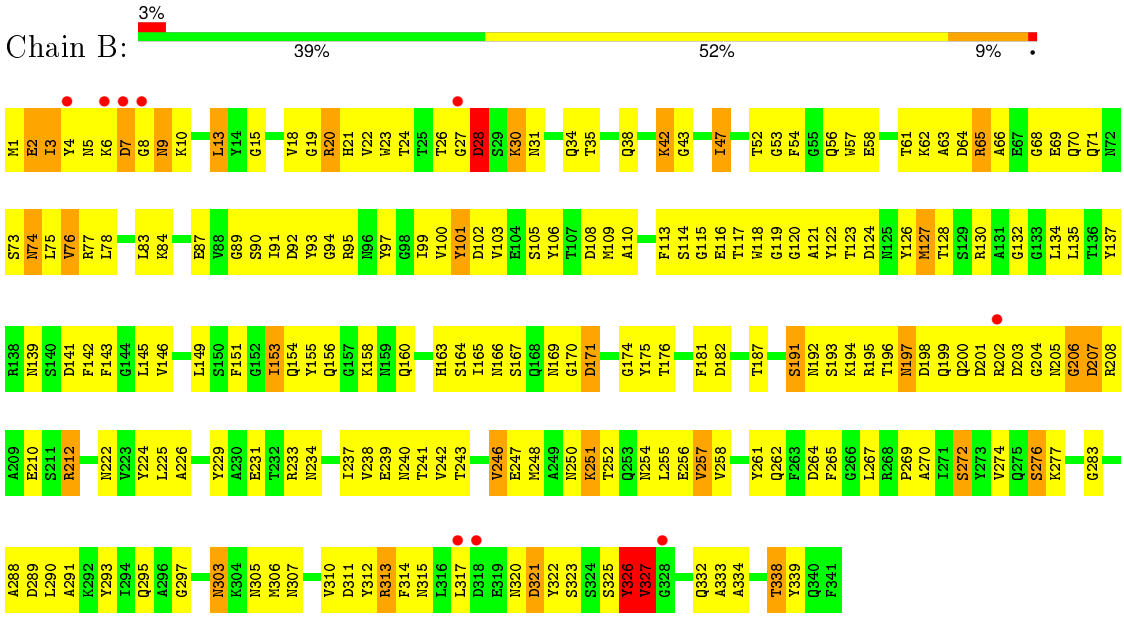
- Molecule 1: Outer membrane protein F

Chain A:



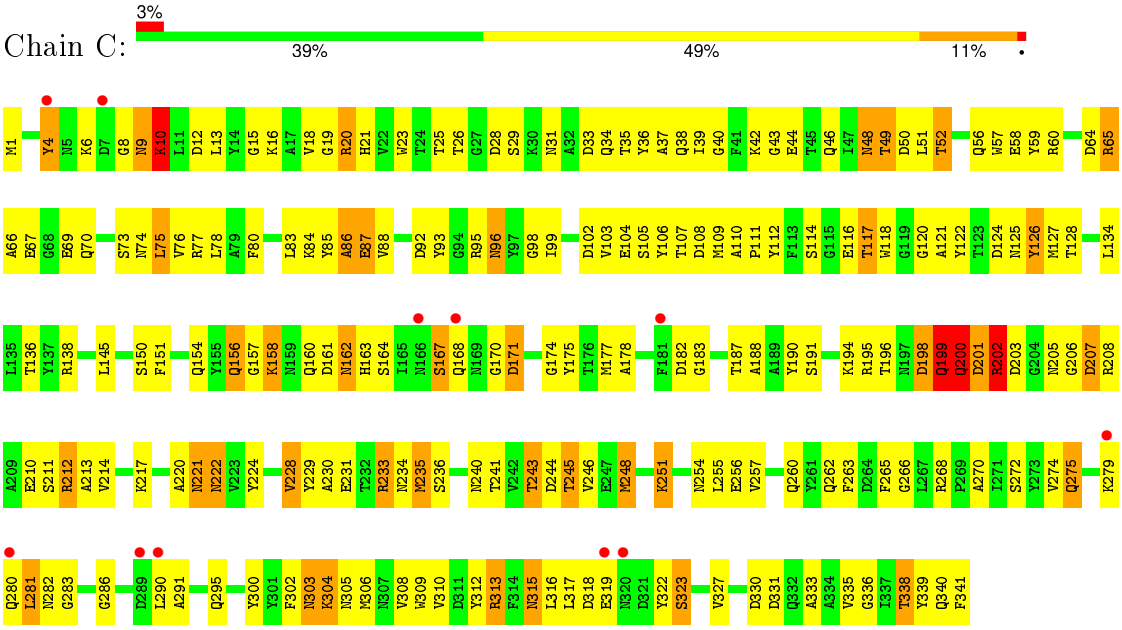
- Molecule 1: Outer membrane protein F

Chain B:



• Molecule 1: Outer membrane protein F

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.19Å 139.34Å 150.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.59 – 2.79 42.59 – 2.79	Depositor EDS
% Data completeness (in resolution range)	84.1 (42.59-2.79) 84.1 (42.59-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.255 , 0.337 0.253 , 0.332	Depositor DCC
R_{free} test set	1898 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	1.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 54.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	1 of 38016 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, LDA, TLA, SO4, TAM, FLC

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	0.60	0/2717	0.75	0/3668
1	B	0.61	0/2717	0.75	0/3668
1	C	0.59	0/2717	0.73	0/3668
All	All	0.60	0/8151	0.74	0/11004

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	2669	0	2464	246	0
1	B	2669	0	2464	219	0
1	C	2669	0	2464	231	0
2	A	135	0	0	6	0
2	B	110	0	0	4	0
2	C	155	0	0	6	0
3	A	84	0	112	4	0
3	B	66	0	88	6	0
3	C	78	0	104	8	0
4	A	96	0	186	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	112	0	217	10	0
4	C	64	0	124	15	0
5	A	22	0	34	11	0
5	B	11	0	17	0	0
5	C	33	0	51	12	0
6	A	13	0	5	0	0
6	C	39	0	15	6	0
7	A	10	0	4	0	0
7	B	10	0	4	1	0
8	A	134	0	0	11	0
8	B	115	0	0	7	0
8	C	138	0	0	11	0
All	All	9432	0	8353	687	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 39.

The worst 5 of 687 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:198:ASP:HA	1:A:200:GLN:NE2	1.61	1.13
1:A:21:HIS:CE1	1:A:31:ASN:OD1	2.04	1.11
1:A:107:THR:HG21	1:A:256:GLU:OE1	1.56	1.05
1:A:117:THR:HG23	1:A:118:TRP:H	1.22	1.04
4:B:375:LDA:HM13	4:C:382:LDA:H21	1.38	1.03

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	339/341 (99%)	286 (84%)	39 (12%)	14 (4%)	3 11
1	B	339/341 (99%)	285 (84%)	37 (11%)	17 (5%)	3 8
1	C	339/341 (99%)	279 (82%)	41 (12%)	19 (6%)	2 6
All	All	1017/1023 (99%)	850 (84%)	117 (12%)	50 (5%)	3 8

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	PHE
1	A	205	ASN
1	A	208	ARG
1	A	245	THR
1	A	249	ALA

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	271/265 (102%)	208 (77%)	63 (23%)	1 3
1	B	271/265 (102%)	223 (82%)	48 (18%)	2 7
1	C	271/265 (102%)	216 (80%)	55 (20%)	1 4
All	All	813/795 (102%)	647 (80%)	166 (20%)	1 4

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	65	ARG
1	B	225	LEU
1	C	274	VAL
1	B	74	ASN
1	B	171	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	154	GLN
1	B	315	ASN
1	C	282	ASN
1	B	159	ASN
1	B	282	ASN

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

147 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	342	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	A	343	-	4,4,4	0.21	0	6,6,6	0.20	0
2	SO4	A	344	-	4,4,4	0.09	0	6,6,6	0.16	0
2	SO4	A	345	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	A	346	-	4,4,4	0.09	0	6,6,6	0.13	0
2	SO4	A	347	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	A	348	-	4,4,4	0.09	0	6,6,6	0.17	0
2	SO4	A	349	-	4,4,4	0.19	0	6,6,6	0.13	0
2	SO4	A	350	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	A	351	-	4,4,4	0.14	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	352	-	4,4,4	0.09	0	6,6,6	0.20	0
2	SO4	A	353	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	A	354	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	A	355	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	A	356	-	4,4,4	0.10	0	6,6,6	0.27	0
2	SO4	A	357	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO4	A	358	-	4,4,4	0.16	0	6,6,6	0.23	0
2	SO4	A	359	-	4,4,4	0.11	0	6,6,6	0.16	0
2	SO4	A	360	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	361	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	A	362	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	A	363	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	A	364	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	A	365	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	366	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	A	367	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	369	-	4,4,4	0.16	0	6,6,6	0.11	0
3	GOL	A	370	-	5,5,5	0.35	0	5,5,5	0.24	0
3	GOL	A	371	-	5,5,5	0.41	0	5,5,5	0.21	0
3	GOL	A	372	-	5,5,5	0.34	0	5,5,5	0.25	0
3	GOL	A	373	-	5,5,5	0.30	0	5,5,5	0.24	0
3	GOL	A	374	-	5,5,5	0.36	0	5,5,5	0.09	0
3	GOL	A	375	-	5,5,5	0.33	0	5,5,5	0.59	0
3	GOL	A	376	-	5,5,5	0.33	0	5,5,5	0.34	0
3	GOL	A	377	-	5,5,5	0.33	0	5,5,5	0.35	0
3	GOL	A	378	-	5,5,5	0.24	0	5,5,5	0.27	0
3	GOL	A	379	-	5,5,5	0.33	0	5,5,5	0.27	0
3	GOL	A	380	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	A	381	-	5,5,5	0.31	0	5,5,5	0.32	0
3	GOL	A	382	-	5,5,5	0.30	0	5,5,5	0.17	0
3	GOL	A	383	-	5,5,5	0.34	0	5,5,5	0.35	0
4	LDA	A	384	-	15,15,15	3.63	2 (13%)	16,17,17	0.99	0
4	LDA	A	385	-	15,15,15	3.79	2 (13%)	16,17,17	0.54	0
4	LDA	A	386	-	15,15,15	3.71	2 (13%)	16,17,17	0.86	0
4	LDA	A	387	-	15,15,15	3.66	1 (6%)	16,17,17	0.75	0
4	LDA	A	388	-	15,15,15	3.71	2 (13%)	16,17,17	0.65	0
4	LDA	A	389	-	15,15,15	3.57	1 (6%)	16,17,17	0.74	0
5	TAM	A	390	-	7,10,10	0.46	0	9,12,12	0.45	0
5	TAM	A	391	-	7,10,10	0.53	0	9,12,12	0.57	0
6	FLC	A	392	-	3,12,12	1.97	1 (33%)	3,17,17	2.90	2 (66%)
7	TLA	A	393	-	3,9,9	0.63	0	6,12,12	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	342	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	B	343	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	B	344	-	4,4,4	0.13	0	6,6,6	0.24	0
2	SO4	B	345	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	B	346	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	B	347	-	4,4,4	0.09	0	6,6,6	0.42	0
2	SO4	B	348	-	4,4,4	0.15	0	6,6,6	0.37	0
2	SO4	B	349	-	4,4,4	0.20	0	6,6,6	0.24	0
2	SO4	B	350	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	B	351	-	4,4,4	0.65	0	6,6,6	0.39	0
2	SO4	B	352	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	B	353	-	4,4,4	0.20	0	6,6,6	0.23	0
2	SO4	B	354	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	B	355	-	4,4,4	0.10	0	6,6,6	0.14	0
2	SO4	B	356	-	4,4,4	0.11	0	6,6,6	0.06	0
2	SO4	B	357	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	B	358	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	B	359	-	4,4,4	0.22	0	6,6,6	0.19	0
2	SO4	B	360	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	B	361	-	4,4,4	0.08	0	6,6,6	0.20	0
2	SO4	B	362	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	B	363	-	4,4,4	0.16	0	6,6,6	0.18	0
3	GOL	B	364	-	5,5,5	0.42	0	5,5,5	0.22	0
3	GOL	B	365	-	5,5,5	0.22	0	5,5,5	0.47	0
3	GOL	B	366	-	5,5,5	0.44	0	5,5,5	0.70	0
3	GOL	B	367	-	5,5,5	0.33	0	5,5,5	0.35	0
3	GOL	B	368	-	5,5,5	0.38	0	5,5,5	0.19	0
3	GOL	B	369	-	5,5,5	0.37	0	5,5,5	0.42	0
3	GOL	B	370	-	5,5,5	0.31	0	5,5,5	0.29	0
3	GOL	B	371	-	5,5,5	0.37	0	5,5,5	0.48	0
3	GOL	B	372	-	5,5,5	0.36	0	5,5,5	0.46	0
3	GOL	B	373	-	5,5,5	0.36	0	5,5,5	0.19	0
3	GOL	B	374	-	5,5,5	0.37	0	5,5,5	0.19	0
4	LDA	B	375	-	15,15,15	4.05	2 (13%)	16,17,17	1.16	2 (12%)
4	LDA	B	376	-	15,15,15	3.83	2 (13%)	16,17,17	0.71	0
4	LDA	B	377	-	15,15,15	3.43	1 (6%)	16,17,17	0.90	1 (6%)
4	LDA	B	378	-	15,15,15	3.79	1 (6%)	16,17,17	0.84	0
4	LDA	B	379	-	15,15,15	3.73	1 (6%)	16,17,17	0.65	0
4	LDA	B	380	-	15,15,15	3.80	2 (13%)	16,17,17	0.67	0
4	LDA	B	381	-	15,15,15	3.37	2 (13%)	16,17,17	0.77	0
5	TAM	B	382	-	7,10,10	0.54	0	9,12,12	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	TLA	B	383	-	3,9,9	0.55	0	6,12,12	1.49	1 (16%)
3	GOL	C	1325	-	5,5,5	0.27	0	5,5,5	0.27	0
2	SO4	C	342	-	4,4,4	0.12	0	6,6,6	0.27	0
2	SO4	C	343	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	C	344	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	C	345	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	C	346	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	C	347	-	4,4,4	0.11	0	6,6,6	0.22	0
2	SO4	C	348	-	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	C	349	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	C	350	-	4,4,4	0.06	0	6,6,6	0.14	0
2	SO4	C	351	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	C	352	-	4,4,4	0.10	0	6,6,6	0.25	0
2	SO4	C	353	-	4,4,4	0.08	0	6,6,6	0.13	0
2	SO4	C	354	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	C	355	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	C	356	-	4,4,4	0.05	0	6,6,6	0.16	0
2	SO4	C	357	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	C	358	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	C	359	-	4,4,4	0.09	0	6,6,6	0.05	0
2	SO4	C	360	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	C	361	-	4,4,4	0.08	0	6,6,6	0.10	0
2	SO4	C	362	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	C	363	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	C	364	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SO4	C	365	-	4,4,4	0.09	0	6,6,6	0.14	0
2	SO4	C	366	-	4,4,4	0.09	0	6,6,6	0.16	0
2	SO4	C	367	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	C	368	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	C	369	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	C	370	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	C	371	-	4,4,4	0.11	0	6,6,6	0.12	0
2	SO4	C	372	-	4,4,4	0.11	0	6,6,6	0.11	0
3	GOL	C	373	-	5,5,5	0.33	0	5,5,5	0.19	0
3	GOL	C	374	-	5,5,5	0.34	0	5,5,5	0.50	0
3	GOL	C	375	-	5,5,5	0.28	0	5,5,5	0.31	0
3	GOL	C	376	-	5,5,5	0.38	0	5,5,5	0.13	0
3	GOL	C	377	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	C	378	-	5,5,5	0.37	0	5,5,5	0.36	0
3	GOL	C	379	-	5,5,5	0.32	0	5,5,5	0.28	0
3	GOL	C	380	-	5,5,5	0.35	0	5,5,5	0.20	0
3	GOL	C	381	-	5,5,5	0.38	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LDA	C	382	-	15,15,15	3.69	2 (13%)	16,17,17	0.88	0
4	LDA	C	383	-	15,15,15	3.70	2 (13%)	16,17,17	0.78	0
4	LDA	C	384	-	15,15,15	3.88	2 (13%)	16,17,17	0.79	0
4	LDA	C	385	-	15,15,15	3.73	2 (13%)	16,17,17	0.65	0
5	TAM	C	386	-	7,10,10	0.52	0	9,12,12	0.75	0
5	TAM	C	387	-	7,10,10	0.63	0	9,12,12	0.71	0
6	FLC	C	388	-	3,12,12	1.90	1 (33%)	3,17,17	1.99	1 (33%)
6	FLC	C	389	-	3,12,12	0.62	0	3,17,17	2.86	1 (33%)
3	GOL	C	390	-	5,5,5	0.34	0	5,5,5	0.28	0
6	FLC	C	391	-	3,12,12	0.91	0	3,17,17	4.43	3 (100%)
3	GOL	C	392	-	5,5,5	0.34	0	5,5,5	0.17	0
5	TAM	C	393	-	7,10,10	0.46	0	9,12,12	0.76	0
3	GOL	C	394	-	5,5,5	0.30	0	5,5,5	0.61	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	342	-	-	0/0/0/0	0/0/0/0
2	SO4	A	343	-	-	0/0/0/0	0/0/0/0
2	SO4	A	344	-	-	0/0/0/0	0/0/0/0
2	SO4	A	345	-	-	0/0/0/0	0/0/0/0
2	SO4	A	346	-	-	0/0/0/0	0/0/0/0
2	SO4	A	347	-	-	0/0/0/0	0/0/0/0
2	SO4	A	348	-	-	0/0/0/0	0/0/0/0
2	SO4	A	349	-	-	0/0/0/0	0/0/0/0
2	SO4	A	350	-	-	0/0/0/0	0/0/0/0
2	SO4	A	351	-	-	0/0/0/0	0/0/0/0
2	SO4	A	352	-	-	0/0/0/0	0/0/0/0
2	SO4	A	353	-	-	0/0/0/0	0/0/0/0
2	SO4	A	354	-	-	0/0/0/0	0/0/0/0
2	SO4	A	355	-	-	0/0/0/0	0/0/0/0
2	SO4	A	356	-	-	0/0/0/0	0/0/0/0
2	SO4	A	357	-	-	0/0/0/0	0/0/0/0
2	SO4	A	358	-	-	0/0/0/0	0/0/0/0
2	SO4	A	359	-	-	0/0/0/0	0/0/0/0
2	SO4	A	360	-	-	0/0/0/0	0/0/0/0
2	SO4	A	361	-	-	0/0/0/0	0/0/0/0
2	SO4	A	362	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	363	-	-	0/0/0/0	0/0/0/0
2	SO4	A	364	-	-	0/0/0/0	0/0/0/0
2	SO4	A	365	-	-	0/0/0/0	0/0/0/0
2	SO4	A	366	-	-	0/0/0/0	0/0/0/0
2	SO4	A	367	-	-	0/0/0/0	0/0/0/0
2	SO4	A	369	-	-	0/0/0/0	0/0/0/0
3	GOL	A	370	-	-	0/4/4/4	0/0/0/0
3	GOL	A	371	-	-	0/4/4/4	0/0/0/0
3	GOL	A	372	-	-	0/4/4/4	0/0/0/0
3	GOL	A	373	-	-	0/4/4/4	0/0/0/0
3	GOL	A	374	-	-	0/4/4/4	0/0/0/0
3	GOL	A	375	-	-	0/4/4/4	0/0/0/0
3	GOL	A	376	-	-	0/4/4/4	0/0/0/0
3	GOL	A	377	-	-	0/4/4/4	0/0/0/0
3	GOL	A	378	-	-	0/4/4/4	0/0/0/0
3	GOL	A	379	-	-	0/4/4/4	0/0/0/0
3	GOL	A	380	-	-	0/4/4/4	0/0/0/0
3	GOL	A	381	-	-	0/4/4/4	0/0/0/0
3	GOL	A	382	-	-	0/4/4/4	0/0/0/0
3	GOL	A	383	-	-	0/4/4/4	0/0/0/0
4	LDA	A	384	-	-	0/13/13/13	0/0/0/0
4	LDA	A	385	-	-	0/13/13/13	0/0/0/0
4	LDA	A	386	-	-	0/13/13/13	0/0/0/0
4	LDA	A	387	-	-	0/13/13/13	0/0/0/0
4	LDA	A	388	-	-	0/13/13/13	0/0/0/0
4	LDA	A	389	-	-	0/13/13/13	0/0/0/0
5	TAM	A	390	-	-	0/12/12/12	0/0/0/0
5	TAM	A	391	-	-	0/12/12/12	0/0/0/0
6	FLC	A	392	-	-	0/6/16/16	0/0/0/0
7	TLA	A	393	-	-	0/4/12/12	0/0/0/0
2	SO4	B	342	-	-	0/0/0/0	0/0/0/0
2	SO4	B	343	-	-	0/0/0/0	0/0/0/0
2	SO4	B	344	-	-	0/0/0/0	0/0/0/0
2	SO4	B	345	-	-	0/0/0/0	0/0/0/0
2	SO4	B	346	-	-	0/0/0/0	0/0/0/0
2	SO4	B	347	-	-	0/0/0/0	0/0/0/0
2	SO4	B	348	-	-	0/0/0/0	0/0/0/0
2	SO4	B	349	-	-	0/0/0/0	0/0/0/0
2	SO4	B	350	-	-	0/0/0/0	0/0/0/0
2	SO4	B	351	-	-	0/0/0/0	0/0/0/0
2	SO4	B	352	-	-	0/0/0/0	0/0/0/0
2	SO4	B	353	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	354	-	-	0/0/0/0	0/0/0/0
2	SO4	B	355	-	-	0/0/0/0	0/0/0/0
2	SO4	B	356	-	-	0/0/0/0	0/0/0/0
2	SO4	B	357	-	-	0/0/0/0	0/0/0/0
2	SO4	B	358	-	-	0/0/0/0	0/0/0/0
2	SO4	B	359	-	-	0/0/0/0	0/0/0/0
2	SO4	B	360	-	-	0/0/0/0	0/0/0/0
2	SO4	B	361	-	-	0/0/0/0	0/0/0/0
2	SO4	B	362	-	-	0/0/0/0	0/0/0/0
2	SO4	B	363	-	-	0/0/0/0	0/0/0/0
3	GOL	B	364	-	-	0/4/4/4	0/0/0/0
3	GOL	B	365	-	-	0/4/4/4	0/0/0/0
3	GOL	B	366	-	-	0/4/4/4	0/0/0/0
3	GOL	B	367	-	-	0/4/4/4	0/0/0/0
3	GOL	B	368	-	-	0/4/4/4	0/0/0/0
3	GOL	B	369	-	-	0/4/4/4	0/0/0/0
3	GOL	B	370	-	-	0/4/4/4	0/0/0/0
3	GOL	B	371	-	-	0/4/4/4	0/0/0/0
3	GOL	B	372	-	-	0/4/4/4	0/0/0/0
3	GOL	B	373	-	-	0/4/4/4	0/0/0/0
3	GOL	B	374	-	-	0/4/4/4	0/0/0/0
4	LDA	B	375	-	-	0/13/13/13	0/0/0/0
4	LDA	B	376	-	-	0/13/13/13	0/0/0/0
4	LDA	B	377	-	-	0/13/13/13	0/0/0/0
4	LDA	B	378	-	-	0/13/13/13	0/0/0/0
4	LDA	B	379	-	-	0/13/13/13	0/0/0/0
4	LDA	B	380	-	-	0/13/13/13	0/0/0/0
4	LDA	B	381	-	-	0/13/13/13	0/0/0/0
5	TAM	B	382	-	-	0/12/12/12	0/0/0/0
7	TLA	B	383	-	-	0/4/12/12	0/0/0/0
3	GOL	C	1325	-	-	0/4/4/4	0/0/0/0
2	SO4	C	342	-	-	0/0/0/0	0/0/0/0
2	SO4	C	343	-	-	0/0/0/0	0/0/0/0
2	SO4	C	344	-	-	0/0/0/0	0/0/0/0
2	SO4	C	345	-	-	0/0/0/0	0/0/0/0
2	SO4	C	346	-	-	0/0/0/0	0/0/0/0
2	SO4	C	347	-	-	0/0/0/0	0/0/0/0
2	SO4	C	348	-	-	0/0/0/0	0/0/0/0
2	SO4	C	349	-	-	0/0/0/0	0/0/0/0
2	SO4	C	350	-	-	0/0/0/0	0/0/0/0
2	SO4	C	351	-	-	0/0/0/0	0/0/0/0
2	SO4	C	352	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	353	-	-	0/0/0/0	0/0/0/0
2	SO4	C	354	-	-	0/0/0/0	0/0/0/0
2	SO4	C	355	-	-	0/0/0/0	0/0/0/0
2	SO4	C	356	-	-	0/0/0/0	0/0/0/0
2	SO4	C	357	-	-	0/0/0/0	0/0/0/0
2	SO4	C	358	-	-	0/0/0/0	0/0/0/0
2	SO4	C	359	-	-	0/0/0/0	0/0/0/0
2	SO4	C	360	-	-	0/0/0/0	0/0/0/0
2	SO4	C	361	-	-	0/0/0/0	0/0/0/0
2	SO4	C	362	-	-	0/0/0/0	0/0/0/0
2	SO4	C	363	-	-	0/0/0/0	0/0/0/0
2	SO4	C	364	-	-	0/0/0/0	0/0/0/0
2	SO4	C	365	-	-	0/0/0/0	0/0/0/0
2	SO4	C	366	-	-	0/0/0/0	0/0/0/0
2	SO4	C	367	-	-	0/0/0/0	0/0/0/0
2	SO4	C	368	-	-	0/0/0/0	0/0/0/0
2	SO4	C	369	-	-	0/0/0/0	0/0/0/0
2	SO4	C	370	-	-	0/0/0/0	0/0/0/0
2	SO4	C	371	-	-	0/0/0/0	0/0/0/0
2	SO4	C	372	-	-	0/0/0/0	0/0/0/0
3	GOL	C	373	-	-	0/4/4/4	0/0/0/0
3	GOL	C	374	-	-	0/4/4/4	0/0/0/0
3	GOL	C	375	-	-	0/4/4/4	0/0/0/0
3	GOL	C	376	-	-	0/4/4/4	0/0/0/0
3	GOL	C	377	-	-	0/4/4/4	0/0/0/0
3	GOL	C	378	-	-	0/4/4/4	0/0/0/0
3	GOL	C	379	-	-	0/4/4/4	0/0/0/0
3	GOL	C	380	-	-	0/4/4/4	0/0/0/0
3	GOL	C	381	-	-	0/4/4/4	0/0/0/0
4	LDA	C	382	-	-	0/13/13/13	0/0/0/0
4	LDA	C	383	-	-	0/13/13/13	0/0/0/0
4	LDA	C	384	-	-	0/13/13/13	0/0/0/0
4	LDA	C	385	-	-	0/13/13/13	0/0/0/0
5	TAM	C	386	-	-	0/12/12/12	0/0/0/0
5	TAM	C	387	-	-	0/12/12/12	0/0/0/0
6	FLC	C	388	-	-	0/6/16/16	0/0/0/0
6	FLC	C	389	-	-	0/6/16/16	0/0/0/0
3	GOL	C	390	-	-	0/4/4/4	0/0/0/0
6	FLC	C	391	-	-	0/6/16/16	0/0/0/0
3	GOL	C	392	-	-	0/4/4/4	0/0/0/0
5	TAM	C	393	-	-	0/12/12/12	0/0/0/0
3	GOL	C	394	-	-	0/4/4/4	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	375	LDA	O1-N1	-15.34	1.24	1.39
4	C	384	LDA	O1-N1	-14.60	1.25	1.39
4	B	376	LDA	O1-N1	-14.57	1.25	1.39
4	B	378	LDA	O1-N1	-14.47	1.25	1.39
4	B	380	LDA	O1-N1	-14.42	1.25	1.39

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	383	TLA	C1-C2-C3	-3.45	106.28	113.35
6	A	392	FLC	CB-CA-CAC	-3.42	109.49	114.96
6	C	388	FLC	CB-CG-CGC	-3.34	109.62	114.96
4	B	375	LDA	O1-N1-C1	-2.96	106.94	110.27
4	B	375	LDA	CM2-N1-CM1	-2.10	106.46	108.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

42 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	350	SO4	1	0
2	A	358	SO4	1	0
2	A	361	SO4	3	0
2	A	363	SO4	1	0
3	A	370	GOL	2	0
3	A	375	GOL	1	0
3	A	380	GOL	1	0
4	A	384	LDA	4	0
4	A	386	LDA	1	0
4	A	388	LDA	1	0
5	A	390	TAM	10	0
5	A	391	TAM	1	0
2	B	345	SO4	2	0
2	B	348	SO4	1	0
2	B	354	SO4	1	0
3	B	364	GOL	1	0
3	B	365	GOL	4	0
3	B	368	GOL	1	0
4	B	375	LDA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	376	LDA	1	0
4	B	377	LDA	2	0
4	B	379	LDA	2	0
4	B	380	LDA	3	0
4	B	381	LDA	1	0
7	B	383	TLA	1	0
2	C	343	SO4	1	0
2	C	348	SO4	1	0
2	C	364	SO4	1	0
2	C	365	SO4	1	0
2	C	370	SO4	2	0
3	C	375	GOL	6	0
4	C	382	LDA	4	0
4	C	383	LDA	4	0
4	C	384	LDA	4	0
4	C	385	LDA	4	0
5	C	386	TAM	4	0
5	C	387	TAM	5	0
6	C	388	FLC	5	0
6	C	391	FLC	1	0
3	C	392	GOL	1	0
5	C	393	TAM	3	0
3	C	394	GOL	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/341 (97%)	0.21	16 (4%) 34 23	34, 57, 80, 91	0
1	B	334/341 (97%)	0.16	9 (2%) 58 45	34, 56, 68, 88	0
1	C	334/341 (97%)	0.24	11 (3%) 50 38	34, 58, 81, 92	0
All	All	1002/1023 (97%)	0.20	36 (3%) 46 34	34, 57, 79, 92	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASP	5.9
1	A	320	ASN	5.4
1	B	7	ASP	4.7
1	A	288	ALA	4.6
1	B	4	TYR	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 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, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	TAM	A	390	11/11	0.73	0.79	29.25	19,21,22,22	11
3	GOL	B	373	6/6	0.63	0.71	10.89	107,108,109,109	0
2	SO4	C	343	5/5	0.89	0.34	7.83	126,126,127,127	0
3	GOL	C	1325	6/6	0.79	0.48	7.31	113,114,115,115	0
2	SO4	C	364	5/5	0.81	0.59	6.86	143,143,144,144	0
2	SO4	A	353	5/5	0.93	0.32	6.78	129,130,130,130	0
3	GOL	A	370	6/6	0.86	0.31	6.16	82,83,84,84	0
4	LDA	A	384	16/16	0.92	0.42	5.99	51,59,71,71	0
4	LDA	A	388	16/16	0.83	0.32	5.61	101,107,115,115	0
4	LDA	A	387	16/16	0.75	0.39	5.03	65,82,95,96	0
2	SO4	C	368	5/5	0.88	0.45	4.60	114,114,114,114	0
4	LDA	C	385	16/16	0.73	0.40	3.80	91,97,103,103	0
2	SO4	A	366	5/5	0.77	0.35	3.64	167,167,167,167	0
2	SO4	A	358	5/5	0.83	0.32	3.63	126,126,126,126	0
3	GOL	A	371	6/6	0.78	0.35	3.51	85,85,86,86	0
2	SO4	B	349	5/5	0.90	0.30	3.04	104,105,105,105	0
3	GOL	A	375	6/6	0.86	0.35	2.99	81,81,82,82	0
2	SO4	A	354	5/5	0.87	0.24	2.69	122,122,123,123	0
2	SO4	C	348	5/5	0.85	0.27	2.65	98,98,99,99	0
2	SO4	C	362	5/5	0.88	0.36	2.34	148,149,149,149	0
2	SO4	C	363	5/5	0.81	0.23	2.26	144,144,145,145	0
4	LDA	A	386	16/16	0.94	0.28	2.22	46,49,61,62	0
2	SO4	A	360	5/5	0.90	0.23	1.80	120,120,121,121	0
2	SO4	C	367	5/5	0.96	0.39	1.67	99,100,100,100	0
2	SO4	B	348	5/5	0.94	0.21	1.52	107,107,107,108	0
2	SO4	C	365	5/5	0.96	0.35	1.45	100,100,101,101	0
4	LDA	C	383	16/16	0.90	0.24	1.45	35,48,68,69	0
2	SO4	A	349	5/5	0.91	0.19	1.26	113,113,113,114	0
4	LDA	B	380	16/16	0.89	0.22	0.89	80,84,86,86	0
2	SO4	B	346	5/5	0.88	0.19	0.53	144,144,144,144	0
3	GOL	B	365	6/6	0.92	0.16	0.28	78,78,79,80	0
4	LDA	C	384	16/16	0.96	0.19	-0.17	41,45,58,58	0
4	LDA	B	379	16/16	0.81	0.22	-	73,87,96,96	0
5	TAM	C	386	11/11	0.73	0.28	-	50,51,51,52	11
3	GOL	A	372	6/6	0.65	0.35	-	86,88,88,88	0
2	SO4	B	356	5/5	0.89	0.33	-	139,139,139,139	0
2	SO4	C	350	5/5	0.89	0.25	-	146,146,147,147	0
2	SO4	B	354	5/5	0.90	0.26	-	153,153,153,153	0
2	SO4	C	371	5/5	0.84	0.17	-	137,137,137,137	0
2	SO4	B	350	5/5	0.80	0.28	-	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	357	5/5	0.85	0.32	-	113,113,113,114	0
2	SO4	B	359	5/5	0.96	0.29	-	108,108,108,108	0
3	GOL	B	366	6/6	0.83	0.39	-	56,60,61,63	0
2	SO4	B	351	5/5	0.69	0.59	-	174,174,175,175	0
2	SO4	C	347	5/5	0.85	0.31	-	119,119,119,119	0
2	SO4	C	344	5/5	0.97	0.10	-	82,82,83,84	0
3	GOL	B	367	6/6	0.67	0.31	-	85,85,86,86	0
2	SO4	A	352	5/5	0.93	0.43	-	113,113,113,114	0
3	GOL	A	383	6/6	0.78	0.31	-	90,91,91,92	0
2	SO4	A	367	5/5	0.90	0.25	-	114,114,115,115	0
2	SO4	A	355	5/5	0.92	0.18	-	133,133,133,133	0
6	FLC	C	388	13/13	0.81	0.45	-	42,44,46,46	0
5	TAM	C	387	11/11	0.88	0.24	-	21,23,24,26	11
2	SO4	C	359	5/5	0.79	0.57	-	143,144,144,144	0
3	GOL	A	378	6/6	0.50	0.89	-	118,119,119,119	0
2	SO4	B	353	5/5	0.86	0.33	-	121,121,121,121	0
3	GOL	A	382	6/6	0.77	0.25	-	82,84,84,86	0
2	SO4	C	352	5/5	0.85	0.14	-	112,112,112,112	0
3	GOL	C	392	6/6	0.77	0.36	-	104,105,105,105	0
3	GOL	C	376	6/6	0.32	0.47	-	134,135,135,135	0
3	GOL	A	380	6/6	0.91	0.19	-	76,77,77,77	0
2	SO4	C	356	5/5	0.86	0.43	-	113,113,114,114	0
2	SO4	A	369	5/5	0.33	0.71	-	164,164,164,164	0
2	SO4	A	364	5/5	0.81	0.24	-	145,145,145,145	0
2	SO4	A	342	5/5	0.90	0.30	-	132,132,132,132	0
3	GOL	B	372	6/6	0.82	0.43	-	74,75,76,76	0
2	SO4	A	344	5/5	0.91	0.26	-	105,105,106,106	0
2	SO4	C	345	5/5	0.89	0.17	-	113,113,113,114	0
4	LDA	A	389	16/16	0.71	0.48	-	75,93,105,106	0
2	SO4	B	355	5/5	0.78	0.38	-	142,142,142,142	0
7	TLA	A	393	10/10	0.79	0.32	-	125,126,126,127	0
2	SO4	C	360	5/5	0.48	0.36	-	170,170,170,170	0
3	GOL	A	379	6/6	0.82	0.18	-	82,84,85,85	0
2	SO4	B	361	5/5	0.77	0.22	-	143,143,144,144	0
3	GOL	C	379	6/6	0.44	0.86	-	122,123,124,124	0
3	GOL	C	373	6/6	0.86	0.33	-	70,72,72,73	0
3	GOL	B	364	6/6	0.81	0.30	-	99,100,101,101	0
3	GOL	C	375	6/6	0.75	0.22	-	117,119,119,120	0
2	SO4	A	346	5/5	0.92	0.16	-	105,105,105,106	0
2	SO4	B	352	5/5	0.96	0.18	-	102,102,102,102	0
4	LDA	C	382	16/16	0.90	0.33	-	43,56,67,67	0
2	SO4	A	357	5/5	0.94	0.25	-	106,106,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	C	361	5/5	0.85	0.24	-	122,123,123,123	0
2	SO4	A	356	5/5	0.90	0.28	-	104,104,104,104	0
2	SO4	C	342	5/5	0.95	0.23	-	83,83,84,86	0
2	SO4	B	363	5/5	0.88	0.29	-	123,123,123,123	0
3	GOL	B	369	6/6	0.72	0.28	-	80,82,84,85	0
2	SO4	C	346	5/5	0.88	0.43	-	124,125,125,125	0
6	FLC	C	389	13/13	0.79	0.33	-	95,97,98,99	0
2	SO4	B	343	5/5	0.66	0.45	-	151,151,151,151	0
3	GOL	A	374	6/6	0.88	0.40	-	81,83,83,84	0
2	SO4	A	347	5/5	0.90	0.31	-	103,104,104,104	0
2	SO4	B	347	5/5	0.88	0.21	-	98,99,99,100	0
3	GOL	C	394	6/6	0.59	0.24	-	67,69,70,70	0
2	SO4	C	366	5/5	0.70	0.35	-	148,148,148,148	0
2	SO4	A	362	5/5	0.88	0.24	-	133,134,134,134	0
2	SO4	A	365	5/5	0.77	0.37	-	131,131,132,132	0
2	SO4	A	363	5/5	0.81	0.18	-	138,138,138,139	0
2	SO4	A	343	5/5	0.88	0.24	-	142,142,142,142	0
2	SO4	C	369	5/5	0.80	0.34	-	114,114,114,114	0
3	GOL	C	390	6/6	0.79	0.26	-	94,96,97,97	0
3	GOL	B	374	6/6	0.79	0.69	-	84,85,86,87	0
2	SO4	B	344	5/5	0.78	0.41	-	134,134,134,134	0
3	GOL	C	374	6/6	0.86	0.17	-	91,91,92,92	0
2	SO4	B	360	5/5	0.92	0.16	-	113,113,113,113	0
2	SO4	C	355	5/5	0.93	0.19	-	109,110,110,110	0
2	SO4	C	351	5/5	0.87	0.29	-	105,106,107,107	0
2	SO4	A	351	5/5	0.86	0.44	-	128,128,128,128	0
3	GOL	C	377	6/6	0.76	0.29	-	97,97,99,99	0
4	LDA	A	385	16/16	0.57	0.75	-	106,112,117,117	0
2	SO4	A	361	5/5	0.94	0.30	-	126,127,127,127	0
3	GOL	B	368	6/6	0.80	0.33	-	87,88,88,89	0
6	FLC	C	391	13/13	0.81	0.15	-	85,87,87,88	0
4	LDA	B	377	16/16	0.72	0.33	-	87,101,108,108	0
3	GOL	A	377	6/6	0.48	0.33	-	82,83,84,84	0
3	GOL	A	376	6/6	0.71	0.26	-	101,102,102,102	0
5	TAM	C	393	11/11	0.67	0.21	-	60,61,61,61	11
3	GOL	C	381	6/6	0.94	0.31	-	77,78,78,79	0
2	SO4	A	350	5/5	0.73	0.70	-	143,144,144,144	0
2	SO4	A	359	5/5	0.80	0.35	-	136,136,136,136	0
3	GOL	A	381	6/6	0.77	0.35	-	95,96,96,97	0
3	GOL	C	378	6/6	0.69	0.37	-	83,85,85,86	0
2	SO4	C	372	5/5	0.82	0.28	-	134,134,134,135	0
7	TLA	B	383	10/10	0.87	0.23	-	76,79,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GOL	B	370	6/6	0.88	0.31	-	85,85,86,86	0
3	GOL	C	380	6/6	0.86	0.23	-	96,96,97,97	0
4	LDA	B	375	16/16	0.94	0.31	-	57,60,62,62	0
6	FLC	A	392	13/13	0.73	0.45	-	120,120,121,121	0
2	SO4	C	370	5/5	0.86	0.21	-	139,139,139,139	0
2	SO4	B	358	5/5	0.86	0.45	-	110,110,110,110	0
4	LDA	B	378	16/16	0.85	0.34	-	73,84,95,95	0
2	SO4	C	358	5/5	0.93	0.12	-	120,120,120,120	0
2	SO4	A	348	5/5	0.90	0.16	-	141,141,141,141	0
3	GOL	A	373	6/6	0.88	0.24	-	89,90,90,90	0
3	GOL	B	371	6/6	0.76	0.43	-	88,89,89,89	0
2	SO4	B	342	5/5	0.94	0.35	-	101,101,101,101	0
2	SO4	B	362	5/5	0.80	0.54	-	148,148,148,149	0
2	SO4	B	345	5/5	0.80	0.35	-	106,106,107,107	0
2	SO4	C	354	5/5	0.81	0.60	-	152,152,152,153	0
5	TAM	A	391	11/11	0.71	0.30	-	62,63,63,64	11
4	LDA	B	376	16/16	0.91	0.37	-	72,76,81,81	0
2	SO4	C	357	5/5	0.88	0.18	-	119,120,120,120	0
4	LDA	B	381	16/16	0.56	0.47	-	83,90,105,105	0
2	SO4	C	353	5/5	0.78	0.31	-	128,128,128,128	0
2	SO4	A	345	5/5	0.87	0.18	-	112,112,112,112	0
5	TAM	B	382	11/11	0.73	0.19	-	52,54,55,55	11
2	SO4	C	349	5/5	0.92	0.28	-	96,97,97,97	0

6.5 Other polymers

There are no such residues in this entry.