wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 03:57 AM EDT

PDB ID	:	4IXX
Title	:	Crystal structure of S213G variant DAH7PS without Tyr bound from Neisseria meningitidis
Authors	:	Cross, P.J.; Pietersma, A.L.; Allison, T.M.; Wilson-Coutts, S.M.; Cochrane, F.C.; Parker, E.J.
Deposited on	:	2013-01-28
Resolution	:	2.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

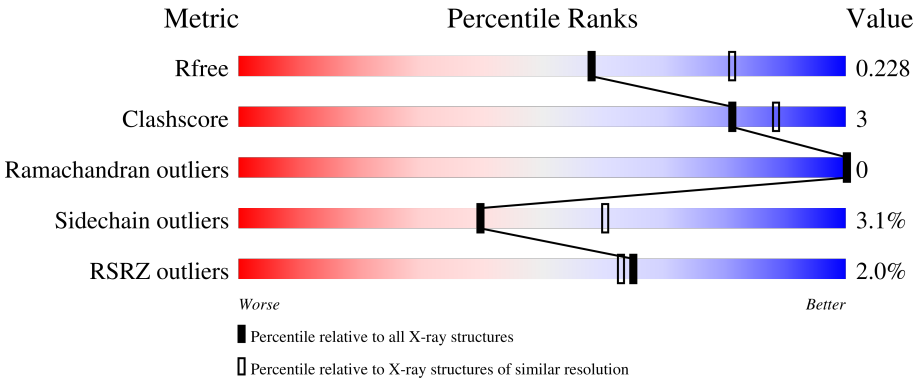
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	351	2% 89% 7% .
1	B	351	2% 90% 6% . .
1	C	351	3% 88% 8% . .
1	D	351	% 91% 7% .

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	SO4	B	402	-	-	X	-
3	SO4	C	403	-	-	X	-
3	SO4	D	403	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10543 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 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2608	1632	470	492	14			
1	B	339	Total	C	N	O	S	0	0	0
			2582	1618	465	485	14			
1	C	340	Total	C	N	O	S	0	0	0
			2596	1625	468	489	14			
1	D	342	Total	C	N	O	S	0	0	0
			2618	1641	471	492	14			

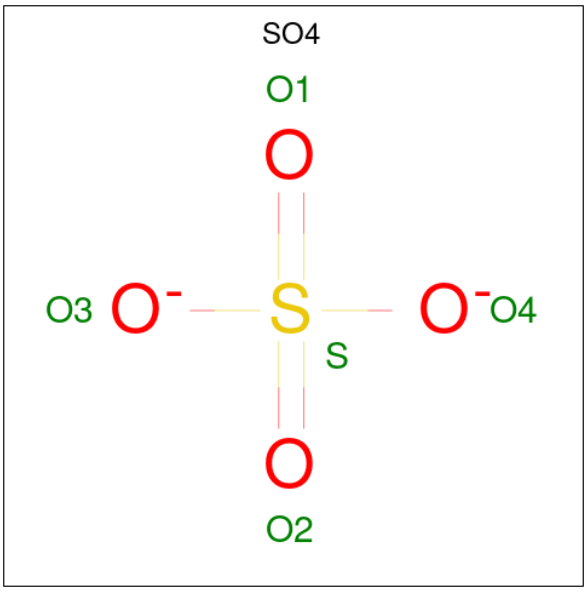
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLY	SER	engineered mutation	UNP Q9K169
B	213	GLY	SER	engineered mutation	UNP Q9K169
C	213	GLY	SER	engineered mutation	UNP Q9K169
D	213	GLY	SER	engineered mutation	UNP Q9K169

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

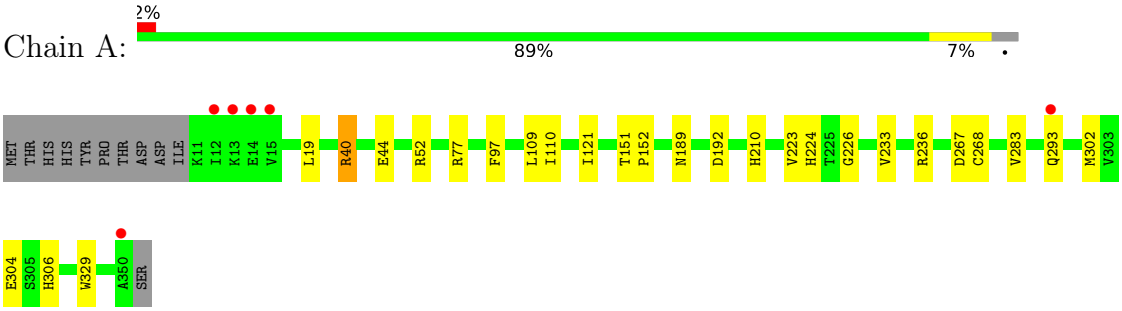
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0
4	B	16	Total O 16 16	0	0
4	C	17	Total O 17 17	0	0
4	D	27	Total O 27 27	0	0

3 Residue-property plots (i)

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 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.

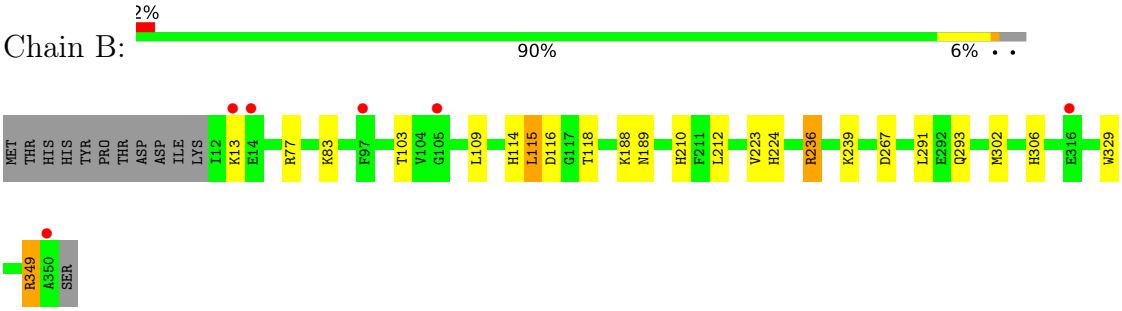
• Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase

Chain A:



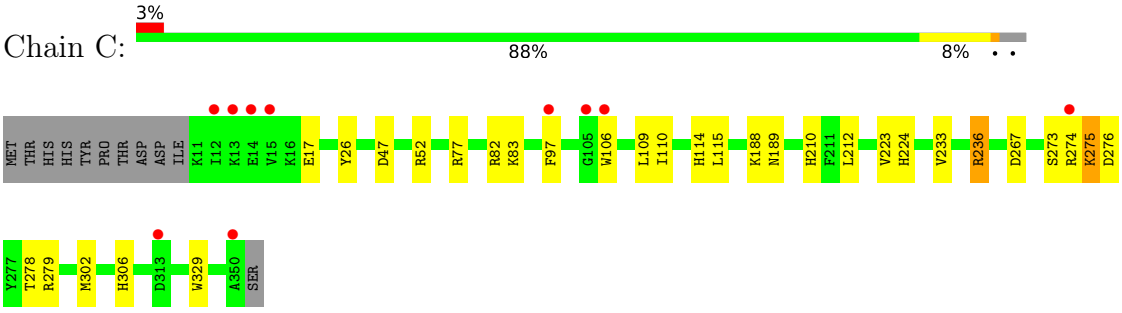
• Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase

Chain B:



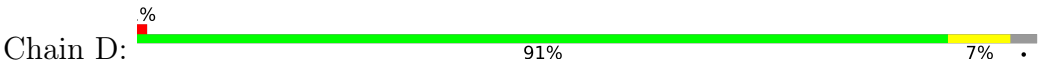
• Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase

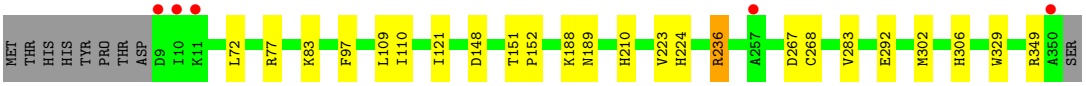
Chain C:



• Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase

Chain D:




MET
THR
HIS
HIS
TYR
PRO
THR
ASP
D9
I10
K11
L72
R77
K83
F97
L109
I110
I121
D148
T151
P152
K188
N189
H210
V223
H224
R236
A257
D267
C268
V283
E292
M302
H306
W329
R349
A350
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.06Å 132.43Å 75.03Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	19.59 – 2.40 19.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.59-2.40) 99.5 (19.59-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.225 0.195 , 0.228	Depositor DCC
R_{free} test set	3384 reflections (6.14%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 23.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10543	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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, 0.333 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, MN

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	0.71	1/2656 (0.0%)	0.79	1/3592 (0.0%)
1	B	0.65	0/2630	0.74	0/3560
1	C	0.69	0/2644	0.75	1/3578 (0.0%)
1	D	0.68	0/2666	0.74	0/3605
All	All	0.68	1/10596 (0.0%)	0.75	2/14335 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	GLU	CA-CB	5.62	1.66	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	82	ARG	NE-CZ-NH1	-5.56	117.52	120.30

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	2608	0	2594	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2582	0	2560	16	0
1	C	2596	0	2573	15	0
1	D	2618	0	2612	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	4	0
3	C	10	0	0	2	0
3	D	10	0	0	4	0
4	A	40	0	0	1	0
4	B	16	0	0	0	0
4	C	17	0	0	0	0
4	D	27	0	0	1	0
All	All	10543	0	10339	53	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 3.

The worst 5 of 53 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:114:HIS:C	1:B:115:LEU:HD12	1.56	1.26
1:D:188:LYS:HD3	3:D:403:SO4:O1	1.60	1.00
1:D:292:GLU:O	1:D:349:ARG:NH1	1.93	1.00
1:D:188:LYS:CD	3:D:403:SO4:O1	2.24	0.86
1:B:114:HIS:C	1:B:115:LEU:CD1	2.45	0.82

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	338/351 (96%)	330 (98%)	8 (2%)	0	100	100
1	B	337/351 (96%)	328 (97%)	9 (3%)	0	100	100
1	C	338/351 (96%)	329 (97%)	9 (3%)	0	100	100
1	D	340/351 (97%)	332 (98%)	8 (2%)	0	100	100
All	All	1353/1404 (96%)	1319 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	274/288 (95%)	266 (97%)	8 (3%)	42	62
1	B	269/288 (93%)	258 (96%)	11 (4%)	30	48
1	C	271/288 (94%)	262 (97%)	9 (3%)	38	57
1	D	275/288 (96%)	269 (98%)	6 (2%)	52	71
All	All	1089/1152 (94%)	1055 (97%)	34 (3%)	40	60

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	83	LYS
1	D	109	LEU
1	D	236	ARG
1	B	189	ASN
1	B	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	C	210	HIS
1	D	210	HIS

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

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	SO4	B	402	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	A	403	-	4,4,4	0.51	0	6,6,6	1.06	1 (16%)
3	SO4	A	402	-	4,4,4	0.40	0	6,6,6	0.27	0
3	SO4	C	402	-	4,4,4	0.34	0	6,6,6	0.33	0
3	SO4	D	402	-	4,4,4	0.33	0	6,6,6	0.51	0
3	SO4	C	403	-	4,4,4	0.32	0	6,6,6	0.05	0
3	SO4	D	403	-	4,4,4	0.32	0	6,6,6	0.04	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	SO4	O3-S-O2	2.13	120.45	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SO4	4	0
3	C	403	SO4	2	0
3	D	403	SO4	4	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

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	340/351 (96%)	-0.41	6 (1%)	68	66	26, 41, 73, 134	0
1	B	339/351 (96%)	-0.30	6 (1%)	68	66	28, 49, 86, 115	0
1	C	340/351 (96%)	-0.34	10 (2%)	51	50	27, 45, 92, 113	0
1	D	342/351 (97%)	-0.39	5 (1%)	73	72	29, 43, 73, 106	0
All	All	1361/1404 (96%)	-0.36	27 (1%)	65	63	26, 44, 84, 134	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	LYS	4.6
1	C	350	ALA	4.4
1	A	350	ALA	4.3
1	D	10	ILE	3.6
1	B	350	ALA	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.

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, 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	B-factors(Å^2)	Q<0.9
3	SO4	C	402	5/5	0.70	0.35	98,106,118,119	0
3	SO4	B	402	5/5	0.83	0.28	46,46,49,51	5
3	SO4	D	403	5/5	0.85	0.30	31,33,42,45	5
3	SO4	C	403	5/5	0.88	0.28	26,28,35,35	5
3	SO4	A	403	5/5	0.93	0.22	21,23,33,36	5
3	SO4	A	402	5/5	0.95	0.27	76,77,84,86	0
3	SO4	D	402	5/5	0.96	0.21	68,71,75,82	0
2	MN	C	401	1/1	0.97	0.06	48,48,48,48	0
2	MN	B	401	1/1	0.97	0.06	59,59,59,59	0
2	MN	A	401	1/1	0.98	0.09	35,35,35,35	0
2	MN	D	401	1/1	0.99	0.05	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.