wwPDB X-ray Structure Validation Summary Report (i)

Feb 13, 2017 – 07:17 am GMT

PDB ID	:	4E8N
Title	:	Structure of Oceanobacillus iheyensis group II intron in a ligand-free state in the presence of NH4+ and Mg2+
Authors	:	Marcia, M.; Pyle, A.M.
Deposited on	:	2012-03-20
Resolution	:	2.96 Å(reported)

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

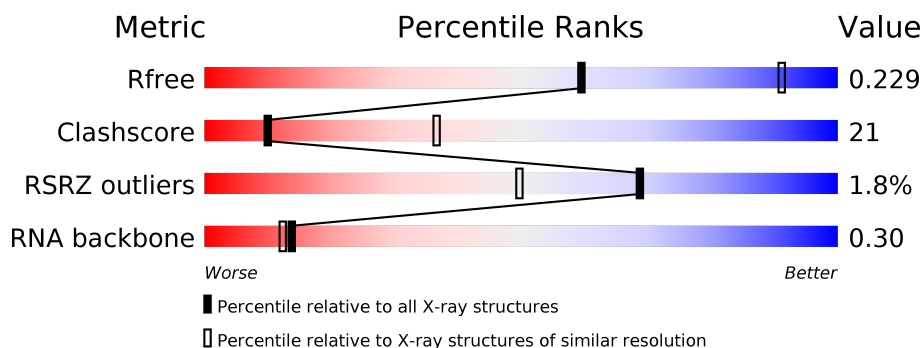|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.229
Clashscore		21
RSRZ outliers		1.8%
RNA backbone		0.30

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)
RNA backbone	2435	1008 (3.30-2.62)

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	393	2% · 21% · 34% · 33% · 12%

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	MG	A	409	-	-	-	X
2	MG	A	424	-	-	-	X
3	NH4	A	435	-	-	-	X

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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NH4	A	439	-	-	-	X
4	SPM	A	446	-	-	-	X
5	EPE	A	448	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8537 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.
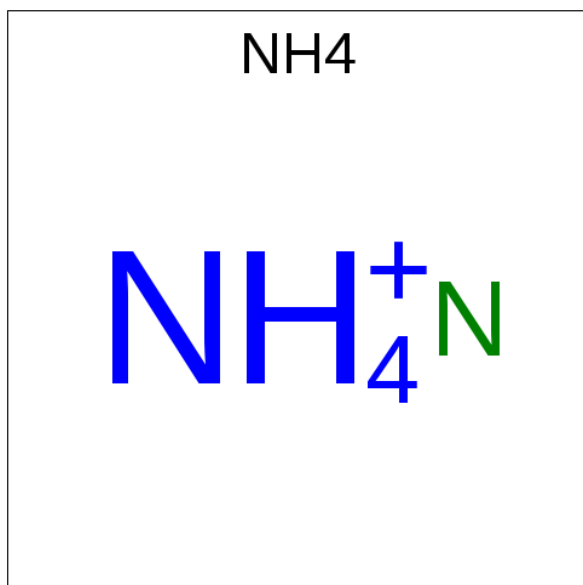
- Molecule 1 is a RNA chain called Group IIC intron.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total 8412	C 3754	N 1559	O 2707	P 392	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total 31	Mg 31	0	0

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0
3	A	1	Total 1	N 1	0	0

- Molecule 4 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).
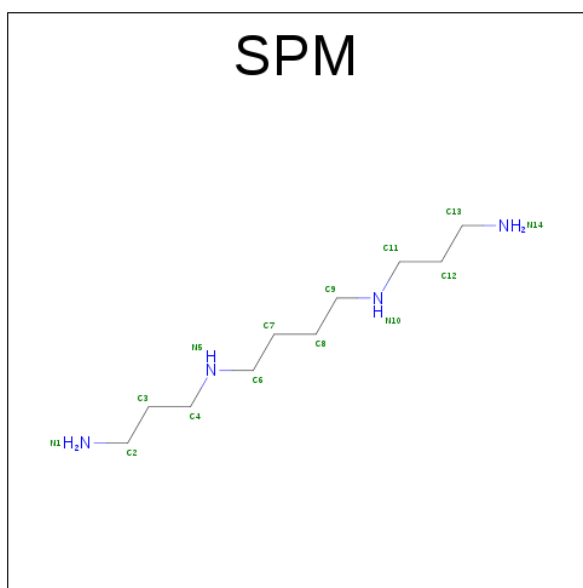
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 14	C 10	N 4	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
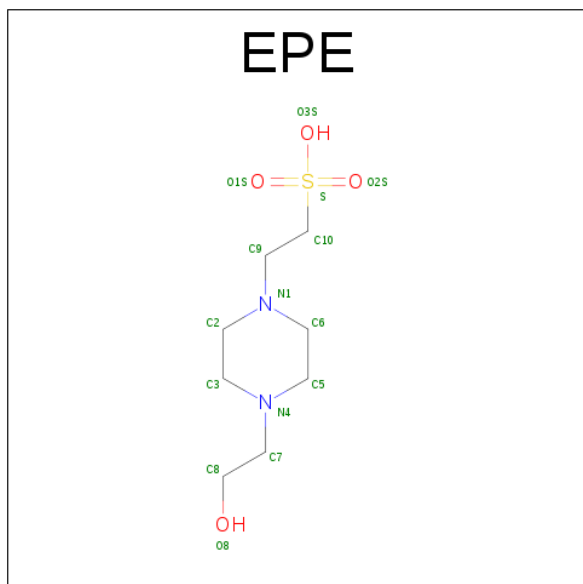
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 4	O 3	S 1			0	0
5	A	1	Total 12	C 6	N 2	O 3	S 1	0	0
5	A	1	Total 4	O 3	S 1			0	0
5	A	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total 31	O 31	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Group IIC intron
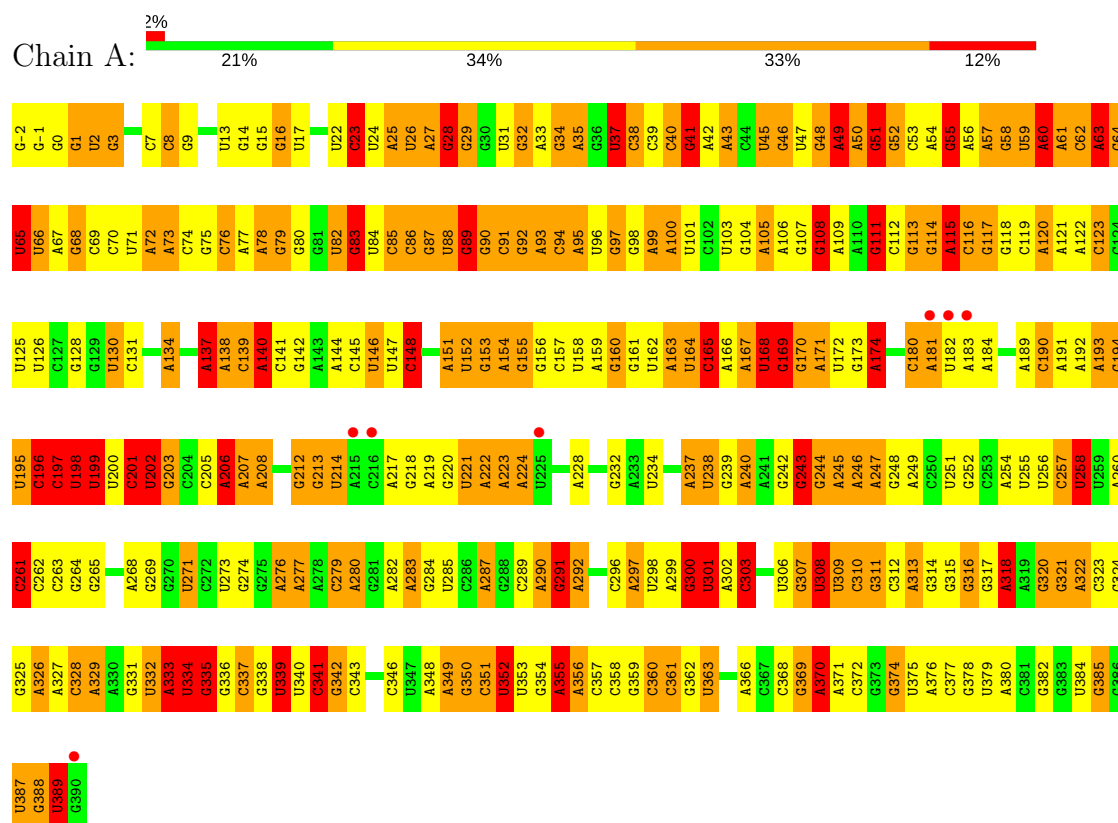
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.89Å 95.43Å 224.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.96 49.10 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.10-2.96) 98.9 (49.10-2.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.235 0.193 , 0.229	Depositor DCC
R_{free} test set	2013 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	91.4	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 62.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8537	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, MG, EPE, SPM

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	0.64	4/9427 (0.0%)	1.55	305/14705 (2.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	A	O3'-P	-7.01	1.52	1.61
1	A	168	U	O3'-P	-6.66	1.53	1.61
1	A	60	A	C3'-O3'	-5.38	1.34	1.42
1	A	245	A	O3'-P	-5.31	1.54	1.61

The worst 5 of 305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	A	O5'-P-OP2	-18.57	88.42	110.70
1	A	198	U	O5'-P-OP2	-17.04	90.25	110.70
1	A	171	A	O5'-P-OP1	-17.01	90.28	110.70
1	A	47	U	O5'-P-OP1	-16.80	90.54	110.70
1	A	197	C	O5'-P-OP1	-15.81	91.47	105.70

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	8412	0	4224	262	0
2	A	31	0	0	0	0
3	A	14	0	0	4	0
4	A	14	0	26	1	0
5	A	35	0	31	6	0
6	A	31	0	0	1	0
All	All	8537	0	4281	263	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 21.

The worst 5 of 263 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:39:C:H2'	1:A:40:C:H5"	1.26	1.13
1:A:334:U:H5'	1:A:334:U:H6	1.18	1.05
1:A:334:U:C5'	1:A:334:U:H6	1.69	1.04
1:A:39:C:C2'	1:A:40:C:H5"	1.89	1.02
1:A:139:C:H2'	1:A:140:A:H8	1.25	0.99

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	391/393 (99%)	136 (34%)	0

5 of 136 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	G
1	A	0	G
1	A	1	G
1	A	2	U
1	A	13	U

There are no RNA pucker outliers to report.

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 ⓘ

Of 50 ligands modelled in this entry, 31 are monoatomic and 14 are modelled with single atom - leaving 5 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	$\#|Z| > 2$
4	SPM	A	446	-	13,13,13	0.59	0	12,12,12	1.29	1 (8%)
5	EPE	A	447	-	0,3,15	0.00	-	0,3,20	0.00	-
5	EPE	A	448	-	12,12,15	2.11	3 (25%)	14,16,20	2.78	4 (28%)
5	EPE	A	449	-	0,3,15	0.00	-	0,3,20	0.00	-
5	EPE	A	450	-	15,15,15	2.12	2 (13%)	18,20,20	1.69	2 (11%)

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
4	SPM	A	446	-	-	0/11/11/11	0/0/0/0
5	EPE	A	447	-	-	0/0/0/19	0/0/0/1
5	EPE	A	448	-	-	0/6/14/19	1/1/1/1
5	EPE	A	449	-	-	0/0/0/19	0/0/0/1
5	EPE	A	450	-	-	0/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	450	EPE	C10-S	-6.03	1.68	1.77
5	A	448	EPE	C10-S	-5.22	1.69	1.77
5	A	448	EPE	C9-N1	2.03	1.52	1.47
5	A	448	EPE	O3S-S	4.46	1.62	1.47
5	A	450	EPE	O3S-S	5.31	1.65	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	448	EPE	O3S-S-O1S	-2.44	105.77	111.37
5	A	448	EPE	O3S-S-O2S	-2.07	106.62	111.37
5	A	448	EPE	O2S-S-C10	2.15	108.64	106.79
4	A	446	SPM	C6-N5-C4	2.64	122.93	113.33
5	A	450	EPE	O2S-S-C10	4.06	110.28	106.79

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	448	EPE	C2-C3-C5-C6-N1-N4

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	446	SPM	1	0
5	A	450	EPE	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	393/393 (100%)	0.35	7 (1%)	69	50	45, 92, 218, 309	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	G	12.8
1	A	216	C	4.2
1	A	181	A	3.3
1	A	183	A	2.2
1	A	182	U	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SPM	A	446	14/14	0.74	0.79	29.17	28,64,73,76	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
5	EPE	A	448	12/15	0.85	0.63	20.64	54,67,79,80	12
2	MG	A	409	1/1	0.91	0.63	12.21	70,70,70,70	0
3	NH4	A	439	1/1	0.96	0.33	9.43	30,30,30,30	1
3	NH4	A	435	1/1	0.89	0.34	5.77	33,33,33,33	0
2	MG	A	424	1/1	0.72	0.39	5.20	85,85,85,85	0
5	EPE	A	447	4/15	0.88	0.15	1.30	92,95,101,112	4
2	MG	A	431	1/1	0.96	0.18	-0.95	94,94,94,94	0
2	MG	A	408	1/1	0.93	0.38	-	55,55,55,55	0
3	NH4	A	440	1/1	0.86	0.48	-	62,62,62,62	0
2	MG	A	415	1/1	0.90	0.61	-	59,59,59,59	0
3	NH4	A	433	1/1	0.91	0.27	-	56,56,56,56	0
2	MG	A	427	1/1	0.95	0.17	-	67,67,67,67	0
2	MG	A	405	1/1	0.96	0.14	-	90,90,90,90	0
3	NH4	A	437	1/1	0.45	0.73	-	24,24,24,24	1
2	MG	A	423	1/1	0.93	0.20	-	78,78,78,78	0
3	NH4	A	432	1/1	0.75	0.22	-	57,57,57,57	0
2	MG	A	412	1/1	0.90	0.20	-	70,70,70,70	0
2	MG	A	419	1/1	0.99	0.09	-	80,80,80,80	0
2	MG	A	421	1/1	0.92	1.30	-	94,94,94,94	0
3	NH4	A	434	1/1	0.86	0.14	-	87,87,87,87	0
2	MG	A	403	1/1	0.97	0.32	-	78,78,78,78	0
2	MG	A	422	1/1	0.82	0.60	-	96,96,96,96	0
2	MG	A	414	1/1	0.83	0.79	-	85,85,85,85	0
2	MG	A	428	1/1	0.96	0.34	-	75,75,75,75	0
2	MG	A	413	1/1	0.95	0.28	-	72,72,72,72	0
2	MG	A	429	1/1	0.94	0.84	-	86,86,86,86	0
5	EPE	A	449	4/15	0.91	0.49	-	56,57,62,77	4
2	MG	A	417	1/1	0.93	0.58	-	103,103,103,103	0
3	NH4	A	442	1/1	-0.07	2.63	-	48,48,48,48	1
2	MG	A	416	1/1	0.96	0.57	-	62,62,62,62	0
2	MG	A	418	1/1	0.88	0.27	-	47,47,47,47	0
3	NH4	A	441	1/1	0.93	0.28	-	66,66,66,66	0
2	MG	A	411	1/1	0.94	0.14	-	75,75,75,75	0
2	MG	A	425	1/1	0.92	0.42	-	141,141,141,141	0
2	MG	A	406	1/1	0.94	0.81	-	92,92,92,92	0
2	MG	A	426	1/1	0.77	0.16	-	92,92,92,92	0
2	MG	A	430	1/1	0.75	0.39	-	61,61,61,61	0
3	NH4	A	445	1/1	0.65	1.00	-	24,24,24,24	1
2	MG	A	401	1/1	0.94	0.47	-	74,74,74,74	0
2	MG	A	420	1/1	0.94	0.43	-	75,75,75,75	0
3	NH4	A	444	1/1	0.26	2.76	-	30,30,30,30	1
2	MG	A	410	1/1	0.90	0.41	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	MG	A	407	1/1	0.98	0.33	-	56,56,56,56	0
3	NH4	A	443	1/1	0.73	1.41	-	33,33,33,33	1
3	NH4	A	438	1/1	0.88	0.68	-	47,47,47,47	0
5	EPE	A	450	15/15	0.88	0.28	-	72,122,145,148	15
2	MG	A	404	1/1	0.98	0.41	-	97,97,97,97	0
2	MG	A	402	1/1	0.95	0.24	-	70,70,70,70	0
3	NH4	A	436	1/1	0.94	1.48	-	53,53,53,53	0

6.5   Other polymers ⓘ

There are no such residues in this entry.