



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 04:18 AM EST

PDB ID : 3OFK  
Title : Crystal structure of N-methyltransferase NodS from Bradyrhizobium japonicum WM9 in complex with S-adenosyl-l-homocysteine (SAH)  
Authors : Cakici, O.; Sikorski, M.; Stepkowski, T.; Bujacz, G.; Jaskolski, M.  
Deposited on : 2010-08-15  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
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) : 2.36

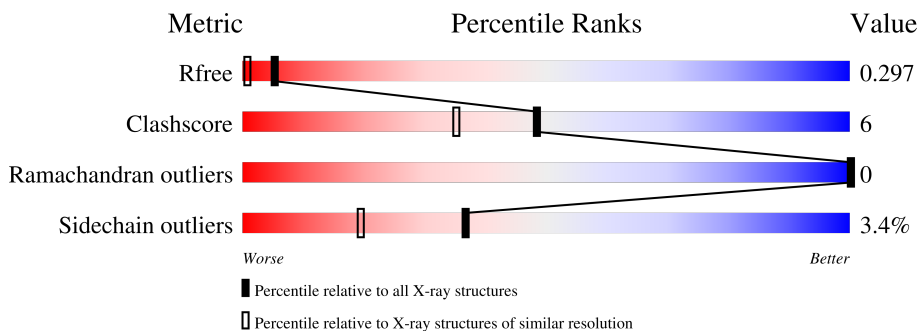
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	216	85% 8% • 6%
1	B	216	78% 11% • 9%
1	C	216	81% 11% • 6%
1	D	216	75% 9% 16%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7102 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 Nodulation protein S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	204	Total 1600	C 996	N 287	O 305	S 12	0	0	0
1	B	196	Total 1539	C 956	N 279	O 293	S 11	0	0	0
1	C	202	Total 1588	C 985	N 291	O 301	S 11	0	0	0
1	D	181	Total 1406	C 874	N 257	O 264	S 11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q9AQ22
A	-5	ILE	-	expression tag	UNP Q9AQ22
A	-4	ASP	-	expression tag	UNP Q9AQ22
A	-3	PRO	-	expression tag	UNP Q9AQ22
A	-2	PHE	-	expression tag	UNP Q9AQ22
A	-1	THR	-	expression tag	UNP Q9AQ22
A	0	MET	-	expression tag	UNP Q9AQ22
A	1	VAL	-	SEE REMARK 999	UNP Q9AQ22
B	-6	GLY	-	expression tag	UNP Q9AQ22
B	-5	ILE	-	expression tag	UNP Q9AQ22
B	-4	ASP	-	expression tag	UNP Q9AQ22
B	-3	PRO	-	expression tag	UNP Q9AQ22
B	-2	PHE	-	expression tag	UNP Q9AQ22
B	-1	THR	-	expression tag	UNP Q9AQ22
B	0	MET	-	expression tag	UNP Q9AQ22
B	1	VAL	-	SEE REMARK 999	UNP Q9AQ22
C	-6	GLY	-	expression tag	UNP Q9AQ22
C	-5	ILE	-	expression tag	UNP Q9AQ22
C	-4	ASP	-	expression tag	UNP Q9AQ22
C	-3	PRO	-	expression tag	UNP Q9AQ22
C	-2	PHE	-	expression tag	UNP Q9AQ22

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total 174	O 174	0	4
3	B	238	Total 244	O 244	0	6
3	C	259	Total 262	O 262	0	3
3	D	179	Total 185	O 185	0	6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.01Å 143.30Å 75.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 1.85 29.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.70-1.85) 94.4 (29.70-1.85)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.190 , 0.238 0.250 , 0.297	Depositor DCC
$R_{free}$ test set	1165 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtrriage
Anisotropy	0.166	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: SAH

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	0.67	1/1629 (0.1%)	0.75	1/2210 (0.0%)
1	B	1.01	2/1566 (0.1%)	0.94	3/2123 (0.1%)
1	C	0.97	2/1616 (0.1%)	0.91	0/2190
1	D	0.72	0/1429	0.78	0/1934
All	All	0.86	5/6240 (0.1%)	0.85	4/8457 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	83	CYS	CB-SG	-5.89	1.72	1.81
1	C	181	CYS	CB-SG	-5.59	1.72	1.81
1	B	181	CYS	C-N	-5.55	1.21	1.34
1	B	199	GLU	CD-OE2	5.51	1.31	1.25
1	A	181	CYS	CB-SG	-5.41	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	194	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	35	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	31	ARG	NE-CZ-NH1	5.11	122.86	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	1600	0	1573	17	0
1	B	1539	0	1510	14	0
1	C	1588	0	1565	29	0
1	D	1406	0	1399	14	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	174	0	0	1	0
3	B	244	0	0	4	0
3	C	262	0	0	11	0
3	D	185	0	0	5	0
All	All	7102	0	6123	74	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 6.

All (74) 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:D:159:VAL:HG22	3:D:231:HOH:O	1.50	1.08
1:C:133:MET:CE	1:C:143:LEU:HD11	1.89	1.02
1:C:133:MET:HE2	1:C:143:LEU:HD11	1.48	0.95
1:C:113:VAL:HG21	1:C:133:MET:CE	1.96	0.94
1:C:113:VAL:HG21	1:C:133:MET:HE1	1.50	0.93
1:A:123:MET:CE	1:A:159:VAL:HG12	2.01	0.90
1:D:123:MET:HE1	1:D:164:THR:HG21	1.55	0.89
1:A:123:MET:CE	1:A:159:VAL:CG1	2.54	0.86
1:D:123:MET:CE	1:D:164:THR:HG21	2.05	0.85
1:A:123:MET:HE3	1:A:159:VAL:HG12	1.60	0.82
1:C:133:MET:HE1	1:C:143:LEU:HD11	1.66	0.77
1:C:133:MET:HE2	1:C:143:LEU:CD1	2.17	0.75
1:C:149:ARG:CD	3:C:744:HOH:O	2.36	0.74
1:A:123:MET:HE3	1:A:159:VAL:CG1	2.18	0.71
1:C:11:GLU:HG2	3:C:825:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLU:HB2	3:C:838:HOH:O	1.92	0.68
1:D:142:HIS:HE1	3:D:236:HOH:O	1.77	0.68
1:D:132:ASN:HB3	3:D:638:HOH:O	2.00	0.62
1:B:4:ASP:N	3:B:535:HOH:O	2.33	0.61
1:C:133:MET:CE	1:C:143:LEU:CD1	2.72	0.60
1:C:113:VAL:CG2	1:C:133:MET:CE	2.76	0.60
1:C:24:ASP:HB2	3:C:766:HOH:O	2.02	0.59
1:A:105:ALA:HB3	3:A:745:HOH:O	2.03	0.57
1:A:190:CYS:SG	1:A:192:LEU:HD21	2.43	0.57
1:C:121:GLU:HB3	1:C:125:GLN:NE2	2.20	0.57
1:B:24:ASP:HB2	3:B:306[A]:HOH:O	2.04	0.57
1:B:4:ASP:N	3:B:763:HOH:O	2.38	0.57
1:A:123:MET:CE	1:A:159:VAL:HG11	2.35	0.56
1:C:21:ARG:HG2	3:C:268:HOH:O	2.05	0.56
1:D:123:MET:HE3	1:D:164:THR:HG21	1.86	0.55
1:D:123:MET:HE3	1:D:164:THR:CG2	2.37	0.55
1:D:142:HIS:CE1	3:D:236:HOH:O	2.58	0.54
1:C:132:ASN:HB3	3:C:833:HOH:O	2.09	0.53
1:D:123:MET:CE	1:D:164:THR:CG2	2.85	0.53
1:A:162:ALA:HB1	1:A:191:LEU:HB3	1.91	0.52
1:D:137:LEU:HD13	1:D:197:ASN:HB2	1.91	0.52
1:C:113:VAL:CG2	1:C:133:MET:HE3	2.39	0.51
1:A:146:GLY:HA3	1:A:192:LEU:HD22	1.93	0.50
1:C:150:ASP:OD1	1:C:164:THR:HG23	2.10	0.50
1:D:35:LEU:HD23	1:D:192:LEU:HD23	1.94	0.50
1:A:123:MET:HE1	1:A:159:VAL:HG12	1.90	0.50
1:A:179:VAL:HG23	1:A:192:LEU:HB2	1.93	0.49
1:C:111:ILE:HG21	1:C:133:MET:HE3	1.94	0.49
1:C:90:SER:C	3:C:235:HOH:O	2.51	0.48
1:C:149:ARG:HD3	3:C:744:HOH:O	2.05	0.48
1:C:21:ARG:HD2	3:C:822:HOH:O	2.15	0.47
1:C:30:GLU:HG2	1:C:181:CYS:SG	2.55	0.47
1:C:44:ALA:HB1	3:C:273:HOH:O	2.15	0.46
1:C:142:HIS:HA	1:C:195:PHE:O	2.14	0.46
1:A:137:LEU:HD13	1:A:197:ASN:HB2	1.97	0.46
1:A:190:CYS:SG	1:A:192:LEU:CD2	3.03	0.46
1:B:168:ILE:O	1:B:171:GLU:HB2	2.16	0.46
1:B:21:ARG:NH2	3:B:772:HOH:O	2.50	0.45
1:A:123:MET:HE2	1:A:159:VAL:CG1	2.45	0.45
1:B:34:GLN:HG3	1:B:181:CYS:SG	2.57	0.44
1:B:74:VAL:HG13	1:B:75:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:CG2	1:C:133:MET:HE3	2.48	0.44
1:B:35:LEU:HD11	1:B:114:ALA:CB	2.48	0.43
1:B:137:LEU:HD23	1:B:197:ASN:HB2	1.99	0.43
1:B:152:THR:HB	1:B:155:ARG:NH2	2.33	0.43
1:C:133:MET:HE2	1:C:133:MET:HB3	1.75	0.43
1:B:72:ILE:HG22	1:B:95:ALA:HB3	2.00	0.43
1:C:90:SER:HA	3:C:235:HOH:O	2.17	0.43
1:A:123:MET:HE2	1:A:159:VAL:HG11	2.01	0.43
1:A:73:ASP:O	1:A:96:ALA:HA	2.19	0.43
1:B:13:GLU:HG2	1:B:20:TRP:CE2	2.53	0.43
1:B:68:ARG:NH1	1:B:106:GLU:OE2	2.52	0.43
1:A:139:PRO:O	1:A:199:GLU:C	2.57	0.42
1:C:137:LEU:HD23	1:C:197:ASN:HB2	2.02	0.42
1:C:36:LEU:HA	1:C:36:LEU:HD12	1.86	0.41
1:D:25:ASN:HB3	1:D:28:GLU:HB2	2.01	0.41
1:B:35:LEU:HD23	1:B:192:LEU:HD23	2.03	0.41
1:D:60:GLU:HG3	1:D:85:ARG:HG2	2.02	0.41
1:D:151:ALA:HB3	3:D:747:HOH:O	2.21	0.41

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	202/216 (94%)	193 (96%)	9 (4%)	0	100	100
1	B	194/216 (90%)	188 (97%)	6 (3%)	0	100	100
1	C	200/216 (93%)	192 (96%)	8 (4%)	0	100	100
1	D	179/216 (83%)	173 (97%)	6 (3%)	0	100	100
All	All	775/864 (90%)	746 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	172/181 (95%)	165 (96%)	7 (4%)	30	13
1	B	164/181 (91%)	158 (96%)	6 (4%)	34	17
1	C	170/181 (94%)	166 (98%)	4 (2%)	49	33
1	D	150/181 (83%)	145 (97%)	5 (3%)	38	21
All	All	656/724 (91%)	634 (97%)	22 (3%)	37	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	77	ARG
1	A	104	THR
1	A	123	MET
1	A	179	VAL
1	A	181	CYS
1	A	184	GLN
1	B	30	GLU
1	B	35	LEU
1	B	41	SER
1	B	77	ARG
1	B	152	THR
1	B	182	GLN
1	C	4	ASP
1	C	5	ASN
1	C	83	CYS
1	C	164	THR
1	D	93	SER
1	D	103	SER
1	D	126	MET
1	D	180	GLN
1	D	184	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	B	184	GLN
1	C	5	ASN
1	D	142	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

4 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	SAH	D	217	-	24,28,28	1.29	2 (8%)	25,40,40	1.73	5 (20%)
2	SAH	A	217	-	24,28,28	1.38	3 (12%)	25,40,40	1.49	5 (20%)
2	SAH	B	217	-	24,28,28	1.13	3 (12%)	25,40,40	2.12	5 (20%)
2	SAH	C	217	-	24,28,28	1.31	2 (8%)	25,40,40	1.67	2 (8%)

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	SAH	D	217	-	-	0/11/31/31	0/3/3/3
2	SAH	A	217	-	-	0/11/31/31	0/3/3/3
2	SAH	B	217	-	-	0/11/31/31	0/3/3/3
2	SAH	C	217	-	-	0/11/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	217	SAH	C2-N3	4.81	1.39	1.32
2	A	217	SAH	C2-N3	4.64	1.39	1.32
2	C	217	SAH	C2-N3	3.59	1.37	1.32
2	B	217	SAH	C2-N3	3.47	1.37	1.32
2	A	217	SAH	C2-N1	3.04	1.39	1.33
2	D	217	SAH	C2-N1	2.52	1.38	1.33
2	C	217	SAH	O4'-C1'	2.48	1.44	1.41
2	A	217	SAH	OXT-C	-2.18	1.23	1.30
2	B	217	SAH	C2-N1	2.15	1.37	1.33
2	B	217	SAH	C2'-C1'	-2.10	1.50	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	217	SAH	N3-C2-N1	-7.82	116.46	128.68
2	C	217	SAH	N3-C2-N1	-6.11	119.13	128.68
2	D	217	SAH	N3-C2-N1	-5.08	120.74	128.68
2	A	217	SAH	N3-C2-N1	-4.95	120.95	128.68
2	B	217	SAH	OXT-C-O	-3.80	115.47	124.09
2	D	217	SAH	O4'-C1'-C2'	-3.07	102.44	106.93
2	D	217	SAH	OXT-C-CA	2.89	123.24	113.38
2	A	217	SAH	OXT-C-O	-2.52	118.36	124.09
2	B	217	SAH	C2-N1-C6	2.49	123.01	118.75
2	D	217	SAH	N6-C6-N1	2.44	123.63	118.57
2	B	217	SAH	O4'-C4'-C3'	2.38	109.83	105.11
2	B	217	SAH	OXT-C-CA	2.28	121.15	113.38
2	A	217	SAH	C5'-SD-CG	-2.19	95.68	102.27
2	D	217	SAH	OXT-C-O	-2.18	119.13	124.09
2	A	217	SAH	OXT-C-CA	2.06	120.42	113.38
2	A	217	SAH	N6-C6-N1	2.06	122.85	118.57
2	C	217	SAH	C3'-C2'-C1'	-2.03	97.93	100.98

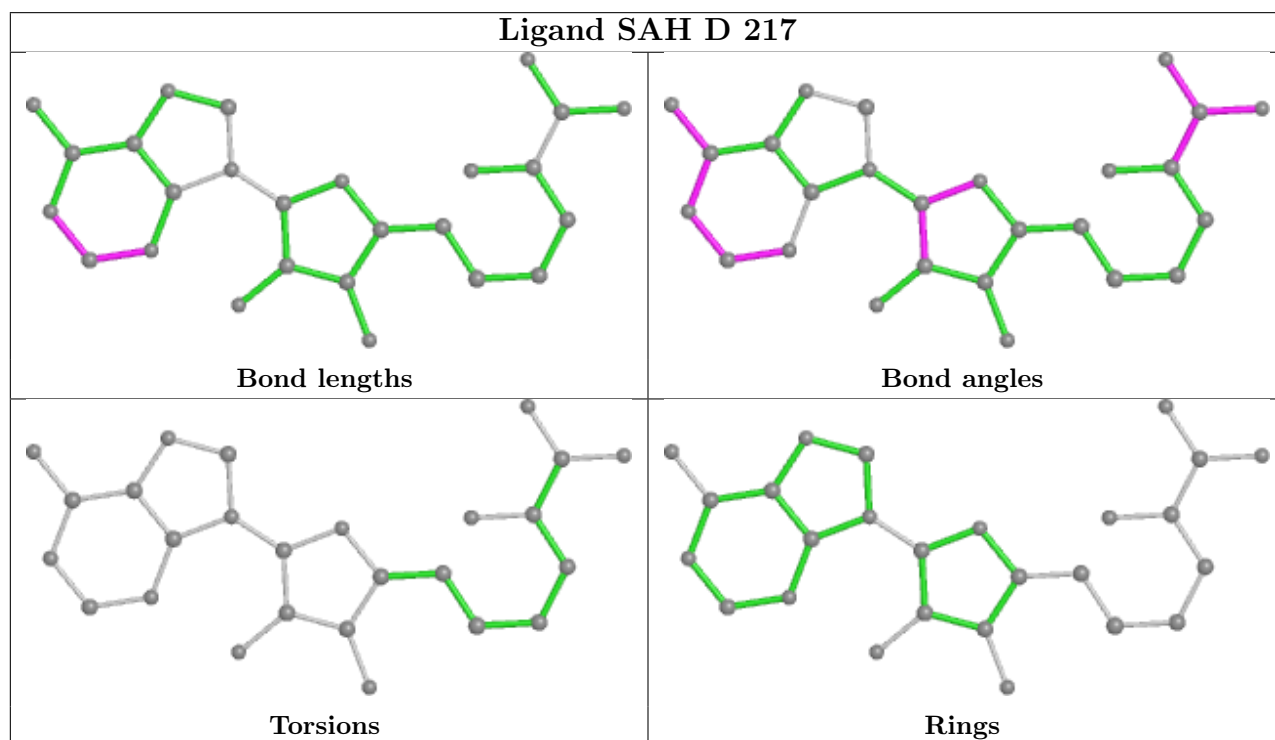
There are no chirality outliers.

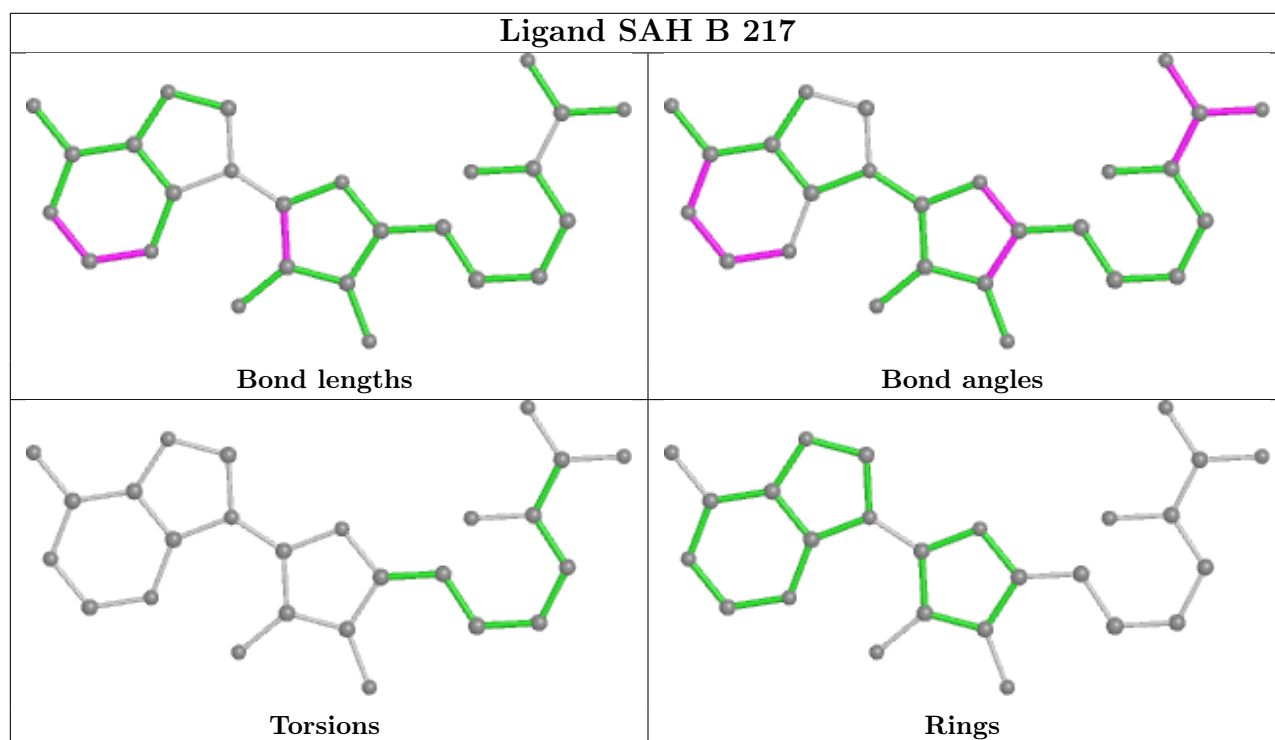
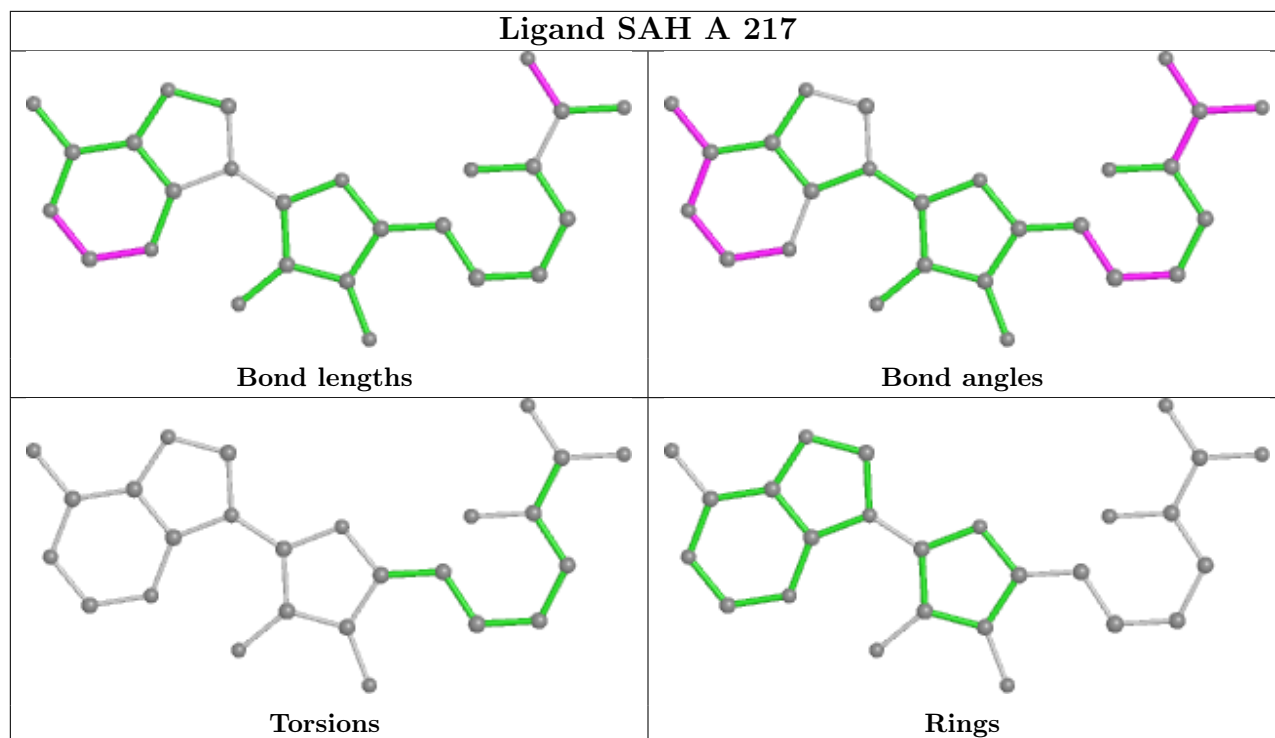
There are no torsion outliers.

There are no ring outliers.

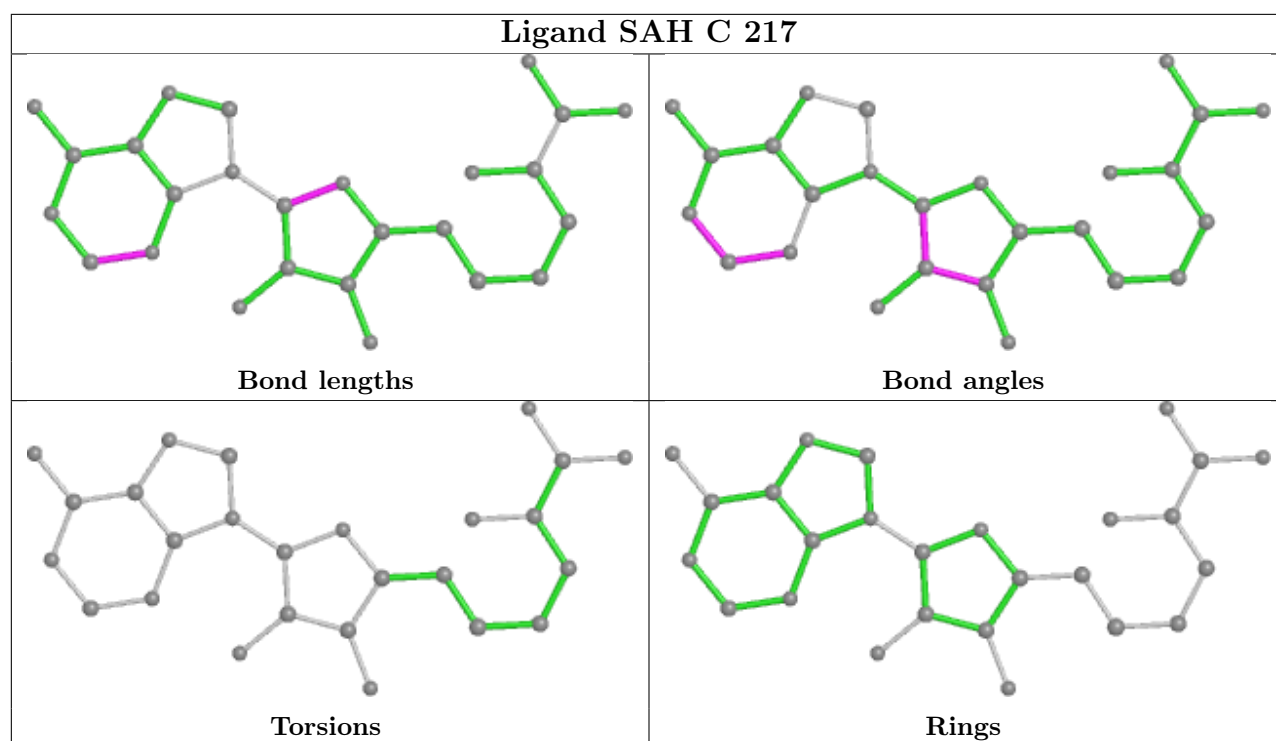
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

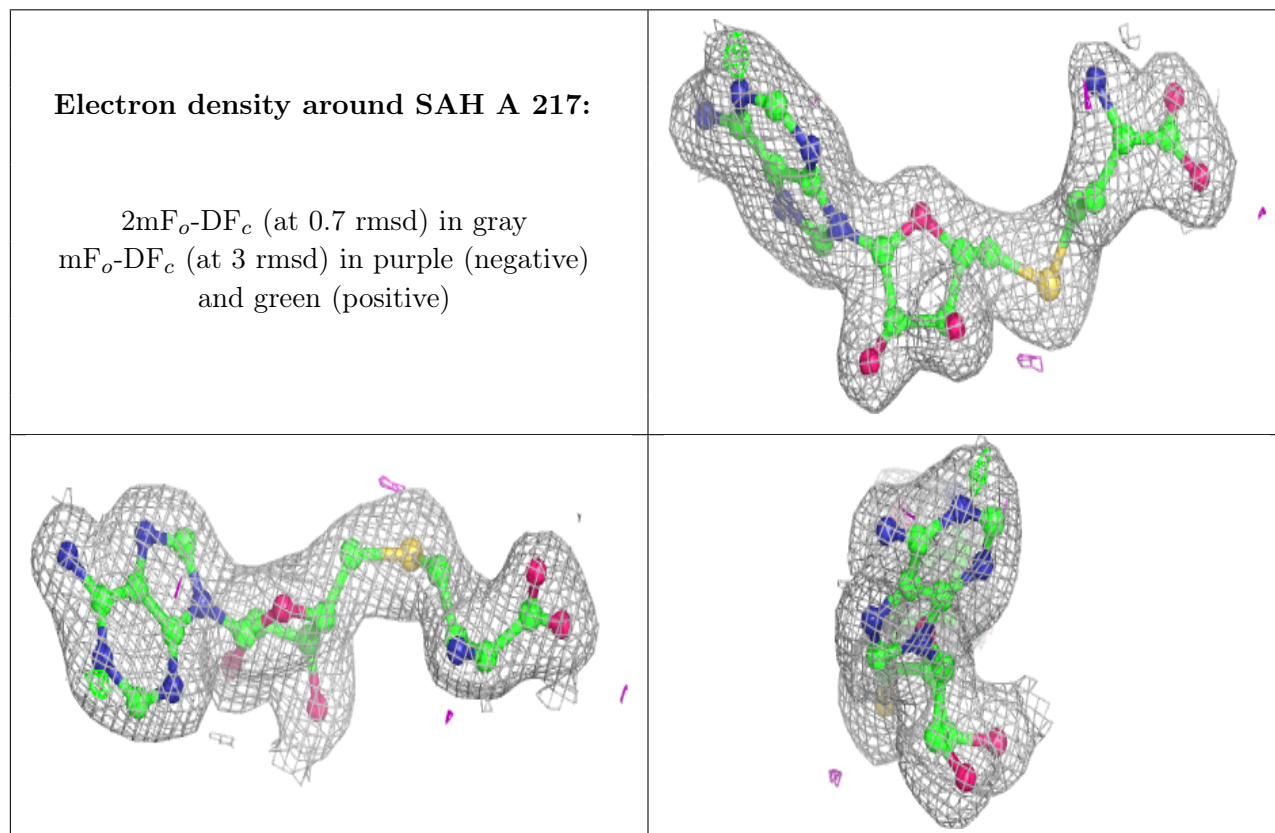
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

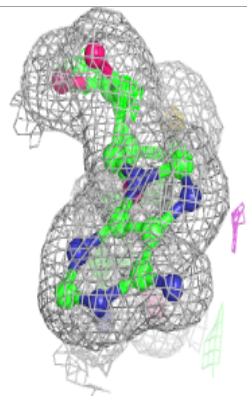
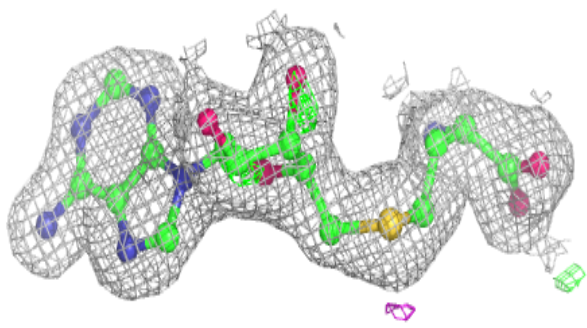
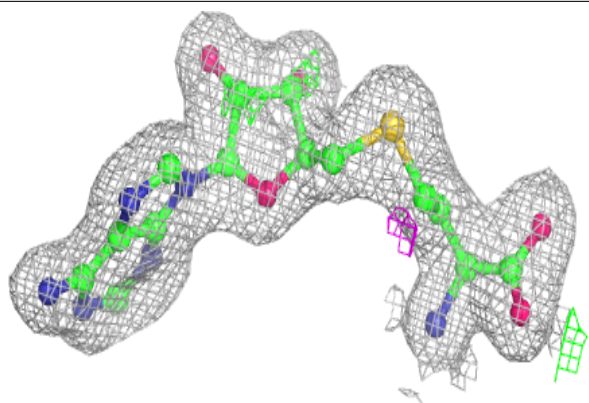
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

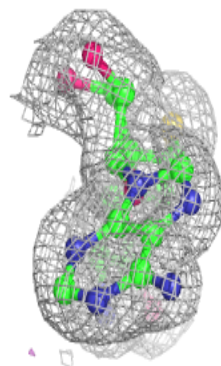
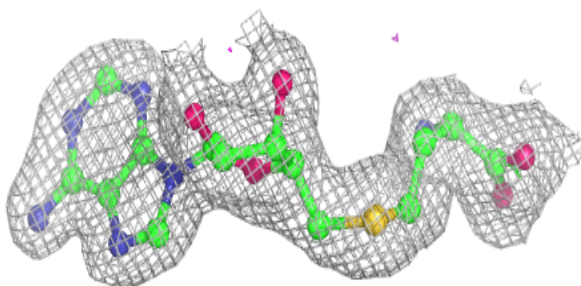
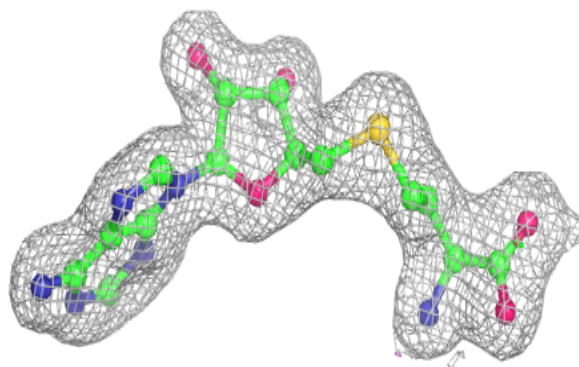


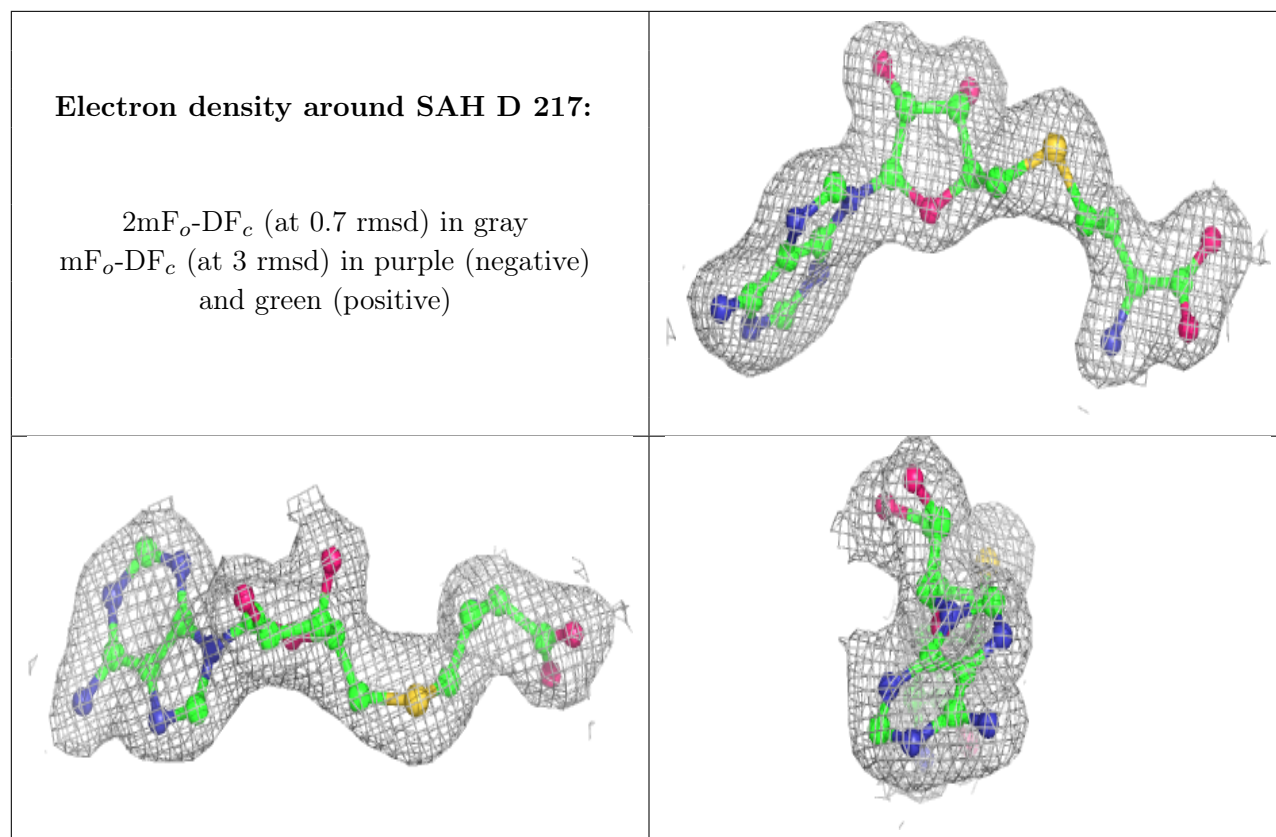
**Electron density around SAH B 217:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around SAH C 217:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.