wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:06 AM GMT

PDB ID	:	2FMT
Title	:	METHIONYL-TRNAFMET FORMYLTRANSFERASE COMPLEXED WITH FORMYL-METHIONYL-TRNAFMET
Authors	:	Schmitt, E.; Mechulam, Y.; Blanquet, S.
Deposited on	:	1998-07-29
Resolution	:	2.80 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 (i)) were used in the production of this report:

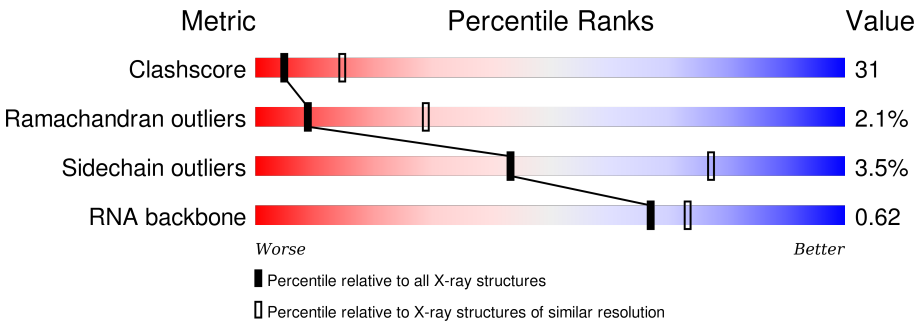
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	77	21% 60% 19%
1	D	77	19% 64% 17%
2	A	314	57% 40% •
2	B	314	52% 44% •

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
1	OMC	C	32	-	-	X	-
1	OMC	D	32	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8179 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 FORMYL-METHIONYL-TRNAFMET2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	C	77	1645	734	297	536	77	1	0	0	0
1	D	77	1645	734	297	536	77	1	0	0	0

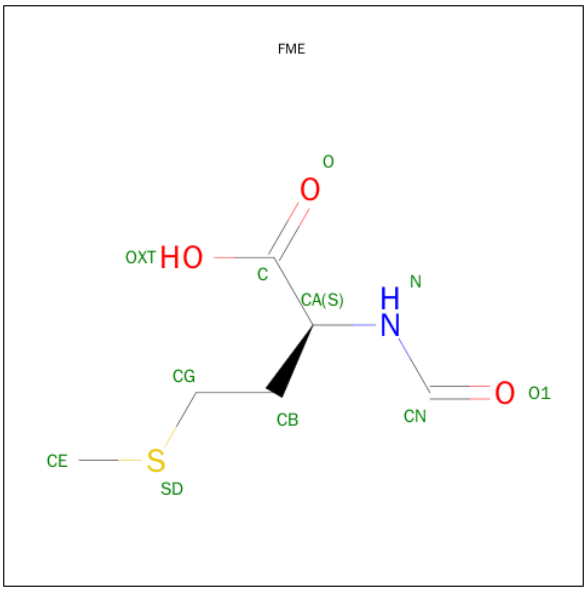
- Molecule 2 is a protein called METHIONYL-TRNA FMET FORMYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	314	2392	1517	414	450	11	0	0	0
2	B	314	2392	1517	414	450	11	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	D	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	10	6	1	2	1	0	0
			Total	C	N	O	S		
4	D	1	10	6	1	2	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	17	17	17	0	0
			Total	O		
5	D	13	13	13	0	0
			Total	O		
5	A	35	35	35	0	0
			Total	O		
5	B	18	18	18	0	0

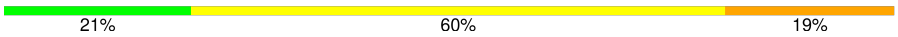
3 Residue-property plots (i)

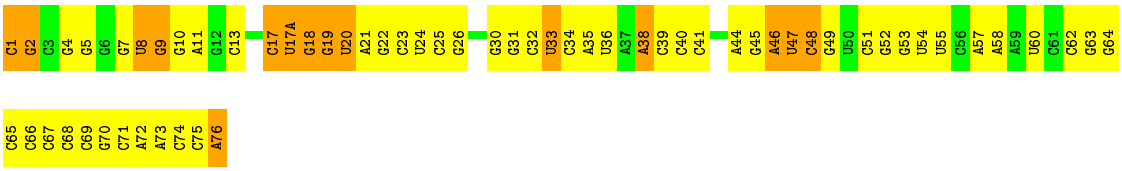
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: FORMYL-METHIONYL-TRNAFMET2

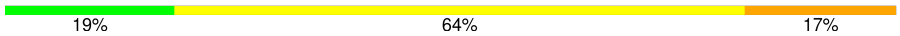
Chain C:

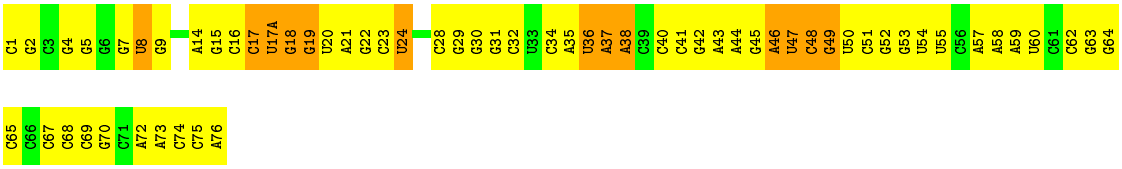




• Molecule 1: FORMYL-METHIONYL-TRNAFMET2

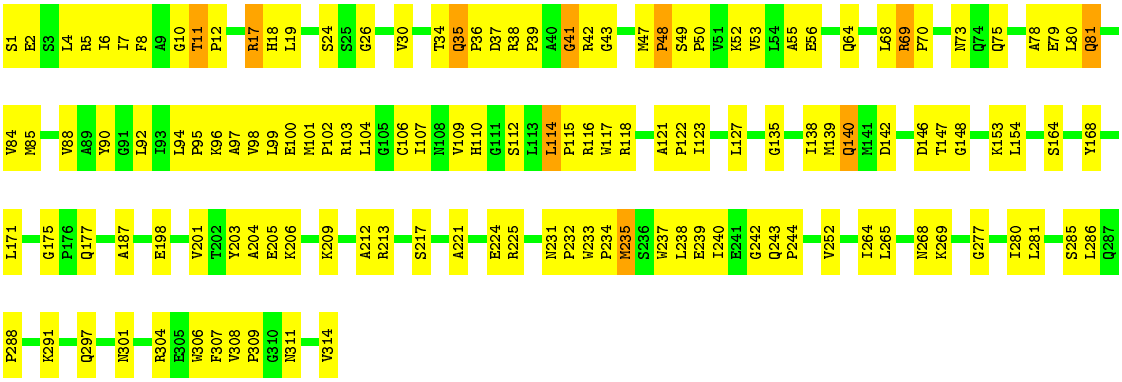
Chain D:





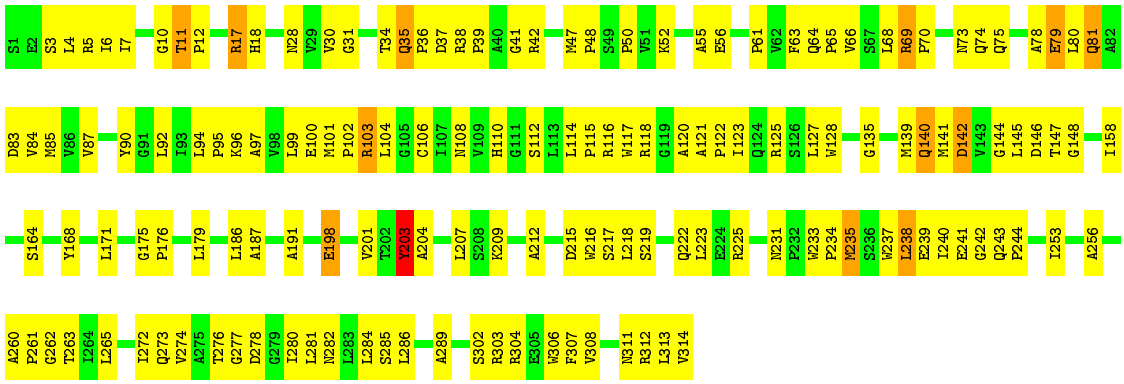
• Molecule 2: METHIONYL-TRNA FMET FORMYLTRANSFERASE

Chain A:



• Molecule 2: METHIONYL-TRNA FMET FORMYLTRANSFERASE

Chain B:


S1 E2 S3 L4 R5 I6 I7 G10 T11 P12 R17 H18 N28 V29 V30 G31 T34 Q35 P36 D37 R38 P39 A40 G41 R42 M47 P48 S49 P50 V51 K52 A55 E56 P61 V62 F63 Q64 P65 V66 S67 L68 R69 P70 N73 Q74 Q75 A78 E79 L80 Q81 A82
D83 V84 M85 V86 V87 Y90 G91 L92 I93 L94 P95 K96 A97 V98 L99 E100 M101 P102 R103 L104 G105 C106 I107 N108 V109 H110 G111 S112 L113 L114 P115 R116 W117 R118 G119 A120 A121 P122 I123 Q124 R125 S126 L127 W128 G135 M139 Q140 M141 D142 V143 G144 L145 D146 T147 G148 I158
S164 Y168 L171 G175 P176 L179 L186 A187 A191 E198 V201 T202 Y203 A204 L207 S208 K209 A212 D215 W216 S217 L218 S219 Q222 L223 E224 R225 N231 P232 W233 P234 M235 S236 W237 L238 E239 I240 E241 G242 Q243 P244 I253 A256
A260 P261 G262 T263 I264 L265 I272 Q273 V274 A275 T276 G277 D278 G279 I280 L281 N282 L283 L284 S285 L286 A289 S302 R303 R304 E305 W306 F307 V308 N311 R312 L313 V314

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	201.71Å 68.06Å 86.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 2.80	Depositor
% Data completeness (in resolution range)	87.2 (19.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 0.3C	Depositor
R, R_{free}	0.247 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8179	wwPDB-VP
Average B, all atoms ($Å^2$)	62.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, MG, FME, H2U, 4SU, PSU

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	C	0.52	2/1725 (0.1%)	0.73	2/2687 (0.1%)
1	D	0.51	1/1725 (0.1%)	0.76	2/2687 (0.1%)
2	A	0.49	0/2439	0.77	1/3317 (0.0%)
2	B	0.48	0/2439	0.76	2/3317 (0.1%)
All	All	0.50	3/8328 (0.0%)	0.76	7/12008 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	C	OP3-P	-7.45	1.52	1.61
1	C	1	C	OP3-P	-6.99	1.52	1.61
1	C	76	A	C3'-O3'	5.93	1.50	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1	C	OP2-P-O3'	6.52	119.53	105.20
1	C	1	C	OP1-P-O3'	6.11	118.64	105.20
2	B	41	GLY	N-CA-C	5.87	127.77	113.10
2	A	41	GLY	N-CA-C	5.70	127.34	113.10
1	D	2	G	O5'-P-OP2	-5.24	100.99	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	24	U	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1645	0	839	89	0
1	D	1645	0	839	75	0
2	A	2392	0	2442	140	0
2	B	2392	0	2442	176	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	10	0	10	1	0
4	D	10	0	10	1	0
5	A	35	0	0	0	0
5	B	18	0	0	0	0
5	C	17	0	0	0	0
5	D	13	0	0	0	0
All	All	8179	0	6582	459	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 31.

The worst 5 of 459 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:OMC:O2'	1:C:32:OMC:CM2	1.68	1.42
1:C:32:OMC:O2'	1:C:32:OMC:C2'	1.68	1.41
1:D:32:OMC:CM2	1:D:32:OMC:O2'	1.71	1.37
1:C:1:C:H3'	1:C:2:G:C5'	1.78	1.13
1:C:1:C:C3'	1:C:2:G:H5'	1.80	1.10

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
2	A	312/314 (99%)	262 (84%)	45 (14%)	5 (2%)	12 38
2	B	312/314 (99%)	264 (85%)	40 (13%)	8 (3%)	7 22
All	All	624/628 (99%)	526 (84%)	85 (14%)	13 (2%)	9 29

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	256	ALA
2	B	175	GLY
2	A	11	THR
2	B	42	ARG
2	A	235	MET

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
2	A	257/257 (100%)	248 (96%)	9 (4%)	43 77
2	B	257/257 (100%)	248 (96%)	9 (4%)	43 77
All	All	514/514 (100%)	496 (96%)	18 (4%)	43 77

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	268	ASN

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Mol	Chain	Res	Type
2	B	17	ARG
2	B	140	GLN
2	A	205	GLU
2	A	232	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	297	GLN
2	B	27	HIS
2	B	243	GLN
2	A	282	ASN
2	B	222	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	76/77 (98%)	14 (18%)	3 (3%)
1	D	76/77 (98%)	14 (18%)	4 (5%)
All	All	152/154 (98%)	28 (18%)	7 (4%)

5 of 28 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	G
1	C	8	4SU
1	C	9	G
1	C	17	C
1	C	17(A)	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	17	C
1	D	46	A
1	D	17(A)	U
1	C	17(A)	U
1	D	36	U

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	H2U	C	20	1	17,21,22	0.78	1 (5%)	23,30,33	1.36	1 (4%)
1	OMC	C	32	1	13,22,23	3.35	2 (15%)	20,31,34	1.19	2 (10%)
1	5MU	C	54	1	12,22,23	1.22	2 (16%)	14,32,35	4.41	3 (21%)
1	PSU	C	55	1	13,21,22	1.90	4 (30%)	18,30,33	5.98	4 (22%)
1	4SU	C	8	1	11,21,22	6.32	2 (18%)	13,30,33	2.74	1 (7%)
1	H2U	D	20	1	17,21,22	1.05	1 (5%)	23,30,33	1.30	1 (4%)
1	OMC	D	32	1	13,22,23	2.58	2 (15%)	20,31,34	1.04	2 (10%)
1	5MU	D	54	1	12,22,23	1.32	3 (25%)	14,32,35	4.46	3 (21%)
1	PSU	D	55	1	13,21,22	2.15	4 (30%)	18,30,33	5.99	4 (22%)
1	4SU	D	8	1	11,21,22	6.74	2 (18%)	13,30,33	2.59	1 (7%)

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
1	H2U	C	20	1	-	0/7/38/39	0/2/2/2
1	OMC	C	32	1	-	0/5/27/28	0/2/2/2
1	5MU	C	54	1	-	0/3/25/26	0/2/2/2
1	PSU	C	55	1	-	0/7/25/26	0/2/2/2
1	4SU	C	8	1	-	0/3/25/26	0/2/2/2
1	H2U	D	20	1	-	0/7/38/39	0/2/2/2
1	OMC	D	32	1	-	0/5/27/28	0/2/2/2
1	5MU	D	54	1	-	0/3/25/26	0/2/2/2
1	PSU	D	55	1	-	0/7/25/26	0/2/2/2
1	4SU	D	8	1	-	0/3/25/26	0/2/2/2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	4SU	C4-S4	-21.87	1.25	1.67
1	C	8	4SU	C4-S4	-20.46	1.27	1.67
1	D	55	PSU	C5-C1'	-4.70	1.48	1.52
1	D	55	PSU	C6-N1	-4.60	1.24	1.34
1	C	55	PSU	C6-N1	-4.52	1.24	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	55	PSU	N1-C2-N3	-21.72	114.48	128.33
1	C	55	PSU	N1-C2-N3	-21.58	114.56	128.33
1	C	8	4SU	C5-C4-N3	-9.80	114.03	123.63
1	D	8	4SU	C5-C4-N3	-9.26	114.55	123.63
1	D	54	5MU	C5-C4-N3	-9.02	115.10	125.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	20	H2U	4	0
1	C	32	OMC	11	0
1	C	54	5MU	3	0
1	C	55	PSU	4	0
1	C	8	4SU	3	0
1	D	32	OMC	9	0
1	D	54	5MU	2	0
1	D	55	PSU	4	0
1	D	8	4SU	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	FME	C	585	1	8,9,10	1.41	2 (25%)	6,9,11	1.68	2 (33%)
4	FME	D	586	1	8,9,10	1.00	0	6,9,11	1.75	2 (33%)

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	FME	C	585	1	-	1/6/9/11	0/0/0/0
4	FME	D	586	1	-	1/6/9/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	585	FME	O1-CN	-2.46	1.15	1.22
4	C	585	FME	CN-N	2.52	1.42	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	586	FME	O-C-CA	-3.25	116.84	125.44
4	C	585	FME	O-C-CA	-2.88	117.82	125.44
4	D	586	FME	O1-CN-N	-2.74	120.81	124.76
4	C	585	FME	O1-CN-N	-2.58	121.04	124.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	585	FME	O1-CN-N-CA
4	D	586	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	585	FME	1	0
4	D	586	FME	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.