wwPDB X-ray Structure Validation Summary Report (i)

Jul 14, 2021 – 11:10 am BST

PDB ID	:	6TW6
Title	:	Plasmodium vivax N-myristoyltransferase with bound indazole inhibitor IMP-923
Authors	:	Brannigan, J.A.
Deposited on	:	2020-01-12
Resolution	:	1.70 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 following versions of software and data (see references (i)) were used in the production of this report:

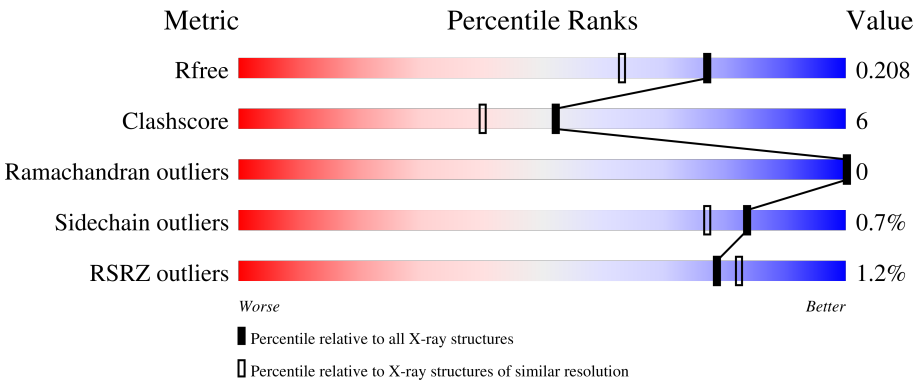
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

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

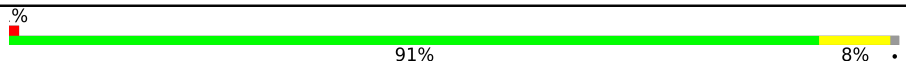
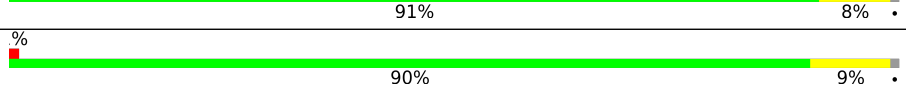
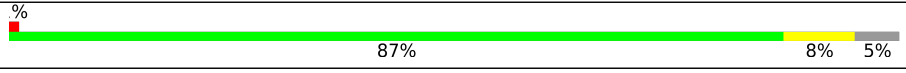
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	388	
1	BBB	388	
1	CCC	388	

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
7	DMS	AAA	506	-	-	X	-
7	DMS	BBB	505	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11986 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.

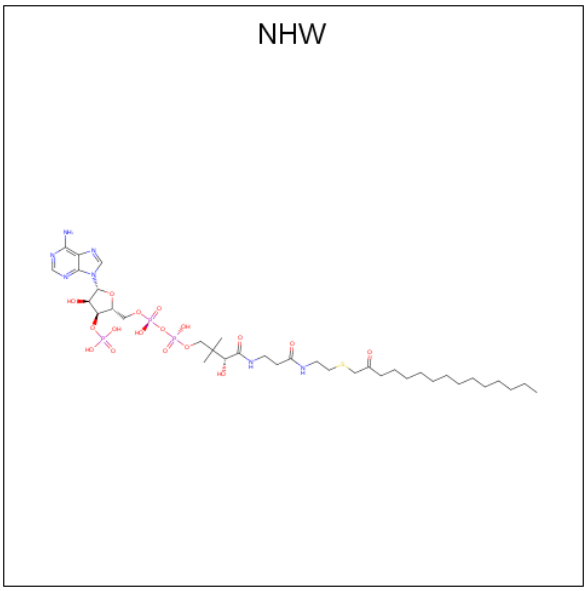
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	385	3427	2243	550	621	13	0	41	0
1	BBB	385	3408	2236	541	618	13	0	41	0
1	CCC	367	3233	2118	514	590	11	0	33	0

There are 12 discrepancies between the modelled and reference sequences:

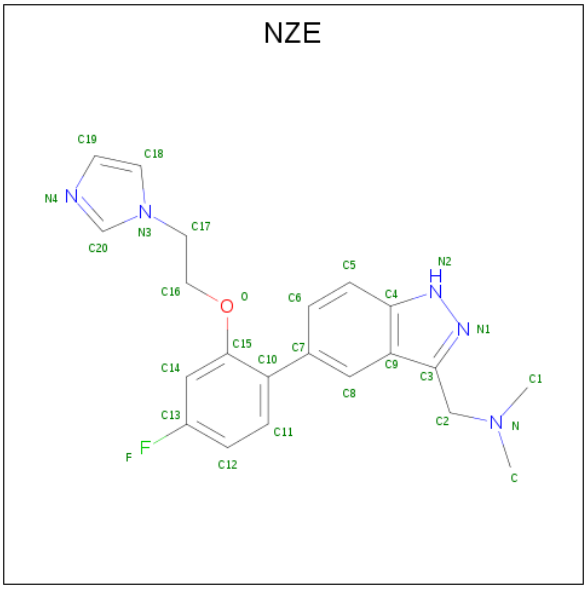
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	23	GLY	-	expression tag	UNP A5K1A2
AAA	24	PRO	-	expression tag	UNP A5K1A2
AAA	25	HIS	-	expression tag	UNP A5K1A2
AAA	26	MET	-	expression tag	UNP A5K1A2
BBB	23	GLY	-	expression tag	UNP A5K1A2
BBB	24	PRO	-	expression tag	UNP A5K1A2
BBB	25	HIS	-	expression tag	UNP A5K1A2
BBB	26	MET	-	expression tag	UNP A5K1A2
CCC	23	GLY	-	expression tag	UNP A5K1A2
CCC	24	PRO	-	expression tag	UNP A5K1A2
CCC	25	HIS	-	expression tag	UNP A5K1A2
CCC	26	MET	-	expression tag	UNP A5K1A2

- Molecule 2 is 2-oxopentadecyl-CoA (three-letter code: NHW) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	AAA	1	64	36	7	17	3	1	0	0
			Total	C	N	O	P	S		
2	BBB	1	64	36	7	17	3	1	0	0
			Total	C	N	O	P	S		
2	CCC	1	64	36	7	17	3	1	0	0

- Molecule 3 is [(5-{4-fluoro-2-[2-(1H-imidazol-1-yl)ethoxy]phenyl}-1H-indazol-3-yl)methyl]dimethylamine (three-letter code: NZE) (formula: $C_{21}H_{22}FN_5O$) (labeled as "Ligand of Interest" by depositor).

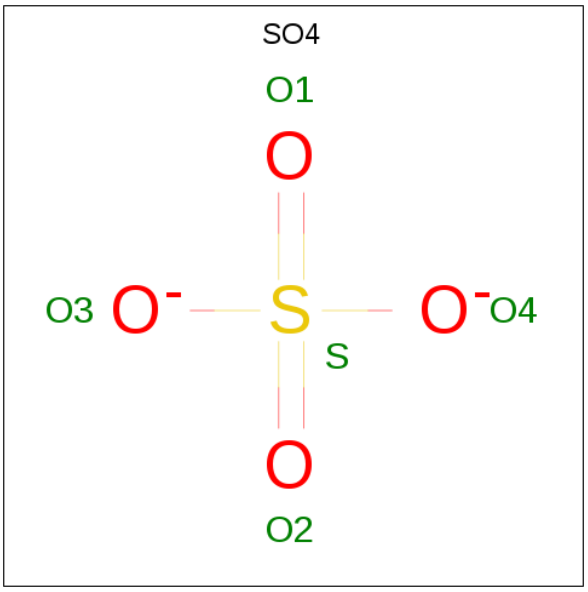


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	AAA	1	28	21	1	5	1	0	0
3	BBB	1	28	21	1	5	1	0	0
3	CCC	1	28	21	1	5	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	AAA	1	1	1	0	0
4	BBB	1	1	1	0	0
4	CCC	1	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

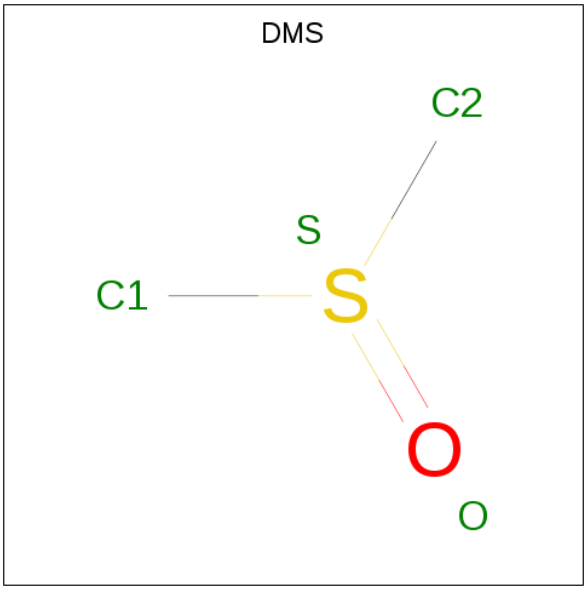


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	AAA	1	5	4	1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Cl 1 1	0	0
6	BBB	1	Total Cl 1 1	0	0
6	CCC	1	Total Cl 1 1	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C O S 4 2 1 1	0	0
7	BBB	1	Total C O S 4 2 1 1	0	0
7	CCC	1	Total C O S 4 2 1 1	0	0
7	CCC	1	Total C O S 4 2 1 1	0	0

- Molecule 8 is water.

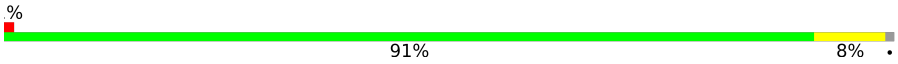
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	576	Total O 576 576	0	0
8	BBB	548	Total O 548 548	0	0
8	CCC	491	Total O 491 491	0	0

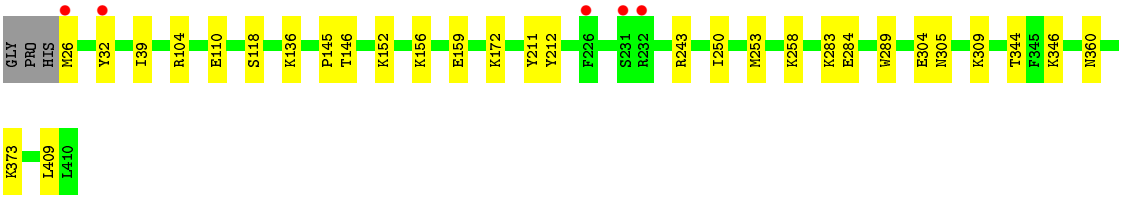
3 Residue-property plots (i)

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: Glycylpeptide N-tetradecanoyltransferase

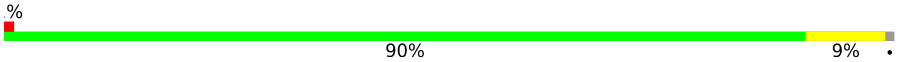
Chain AAA:

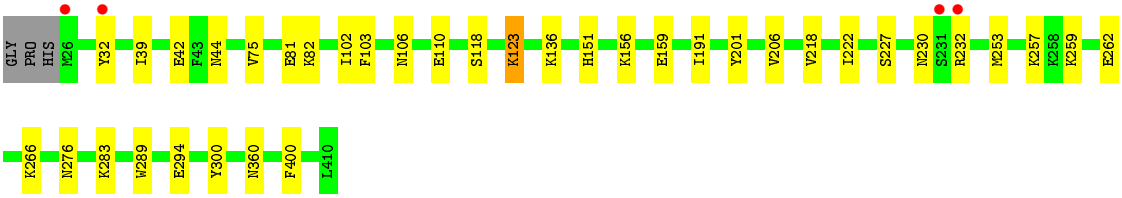




- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

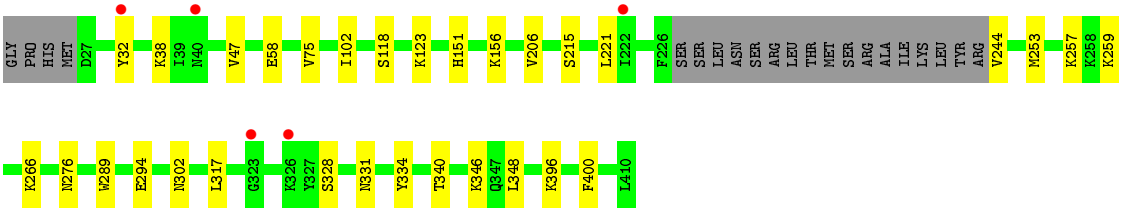
Chain BBB:





- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.61Å 121.78Å 178.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.38 – 1.70 50.33 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.38-1.70) 100.0 (50.33-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.168 , 0.208 0.168 , 0.208	Depositor DCC
R_{free} test set	6960 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11986	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NHW, MG, DMS, SO4, CL, NZE

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	AAA	0.49	0/3617	0.79	0/4884
1	BBB	0.50	0/3606	0.77	0/4869
1	CCC	0.50	0/3393	0.75	0/4586
All	All	0.50	0/10616	0.77	0/14339

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 (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	AAA	3427	0	3520	41	0
1	BBB	3408	0	3520	39	0
1	CCC	3233	0	3287	29	0
2	AAA	64	0	60	0	0
2	BBB	64	0	60	0	0
2	CCC	64	0	60	0	0
3	AAA	28	0	0	0	0
3	BBB	28	0	0	0	0
3	CCC	28	0	0	0	0
4	AAA	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
5	AAA	5	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
7	AAA	4	0	6	4	0
7	BBB	4	0	6	4	0
7	CCC	8	0	8	2	0
8	AAA	576	0	0	20	0
8	BBB	548	0	0	22	0
8	CCC	491	0	0	15	0
All	All	11986	0	10527	115	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.

The worst 5 of 115 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:CCC:123[B]:LYS:CG	8:CCC:646:HOH:O	1.65	1.29
7:BBB:505:DMS:H22	8:BBB:687:HOH:O	1.15	1.28
1:AAA:304[A]:GLU:OE1	1:AAA:309[A]:LYS:HE2	1.46	1.12
1:BBB:259[A]:LYS:NZ	8:BBB:602:HOH:O	1.80	1.11
1:CCC:331[A]:ASN:ND2	8:CCC:605:HOH:O	1.89	1.05

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	AAA	424/388 (109%)	415 (98%)	9 (2%)	0	100	100
1	BBB	424/388 (109%)	416 (98%)	8 (2%)	0	100	100
1	CCC	396/388 (102%)	385 (97%)	11 (3%)	0	100	100
All	All	1244/1164 (107%)	1216 (98%)	28 (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	AAA	392/353 (111%)	391 (100%)	1 (0%)	92	89
1	BBB	392/353 (111%)	388 (99%)	4 (1%)	76	67
1	CCC	367/353 (104%)	363 (99%)	4 (1%)	73	63
All	All	1151/1059 (109%)	1142 (99%)	9 (1%)	84	74

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	294[B]	GLU
1	CCC	328	SER
1	BBB	123[A]	LYS
1	BBB	123[B]	LYS
1	CCC	244	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	NZE	AAA	502	-	28,31,31	1.33	3 (10%)	34,43,43	2.17	14 (41%)
7	DMS	CCC	506	7	3,3,3	0.38	0	3,3,3	0.11	0
7	DMS	BBB	505	-	3,3,3	0.83	0	3,3,3	0.43	0
7	DMS	CCC	505	7	3,3,3	0.23	0	3,3,3	0.23	0
2	NHW	BBB	501	4	58,66,66	1.18	4 (6%)	70,92,92	1.29	6 (8%)
7	DMS	AAA	506	-	3,3,3	0.52	0	3,3,3	0.37	0
3	NZE	CCC	502	-	28,31,31	1.78	4 (14%)	34,43,43	1.80	11 (32%)
3	NZE	BBB	502	-	28,31,31	1.63	4 (14%)	34,43,43	2.05	12 (35%)
2	NHW	AAA	501	4	58,66,66	1.18	5 (8%)	70,92,92	1.53	11 (15%)
5	SO4	AAA	504	-	4,4,4	0.47	0	6,6,6	0.42	0
2	NHW	CCC	501	4	58,66,66	1.09	4 (6%)	70,92,92	1.65	8 (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
3	NZE	AAA	502	-	-	0/13/14/14	0/4/4/4
2	NHW	BBB	501	4	-	4/61/81/81	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NZE	CCC	502	-	-	0/13/14/14	0/4/4/4
3	NZE	BBB	502	-	-	0/13/14/14	0/4/4/4
2	NHW	AAA	501	4	-	1/61/81/81	0/3/3/3
2	NHW	CCC	501	4	-	2/61/81/81	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	502	NZE	C2-C3	6.11	1.53	1.51
3	BBB	502	NZE	C10-C15	5.60	1.52	1.40
3	CCC	502	NZE	C10-C15	4.39	1.49	1.40
2	BBB	501	NHW	P3X-O3X	3.27	1.65	1.59
3	AAA	502	NZE	C10-C15	3.21	1.47	1.40

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	CCC	501	NHW	O4X-C1X-C2X	-7.84	95.47	106.93
2	CCC	501	NHW	N3A-C2A-N1A	-5.88	119.48	128.68
2	BBB	501	NHW	N3A-C2A-N1A	-4.99	120.88	128.68
2	CCC	501	NHW	O4X-C4X-C5X	-4.77	93.67	109.37
3	BBB	502	NZE	C11-C10-C15	4.67	124.10	117.39

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	501	NHW	C4M-C5M-C6M-C7M
2	BBB	501	NHW	C6-C7-N8-C9
2	AAA	501	NHW	C4M-C5M-C6M-C7M
2	BBB	501	NHW	P2A-O3A-P1A-O1A
2	BBB	501	NHW	P2A-O3A-P1A-O2A

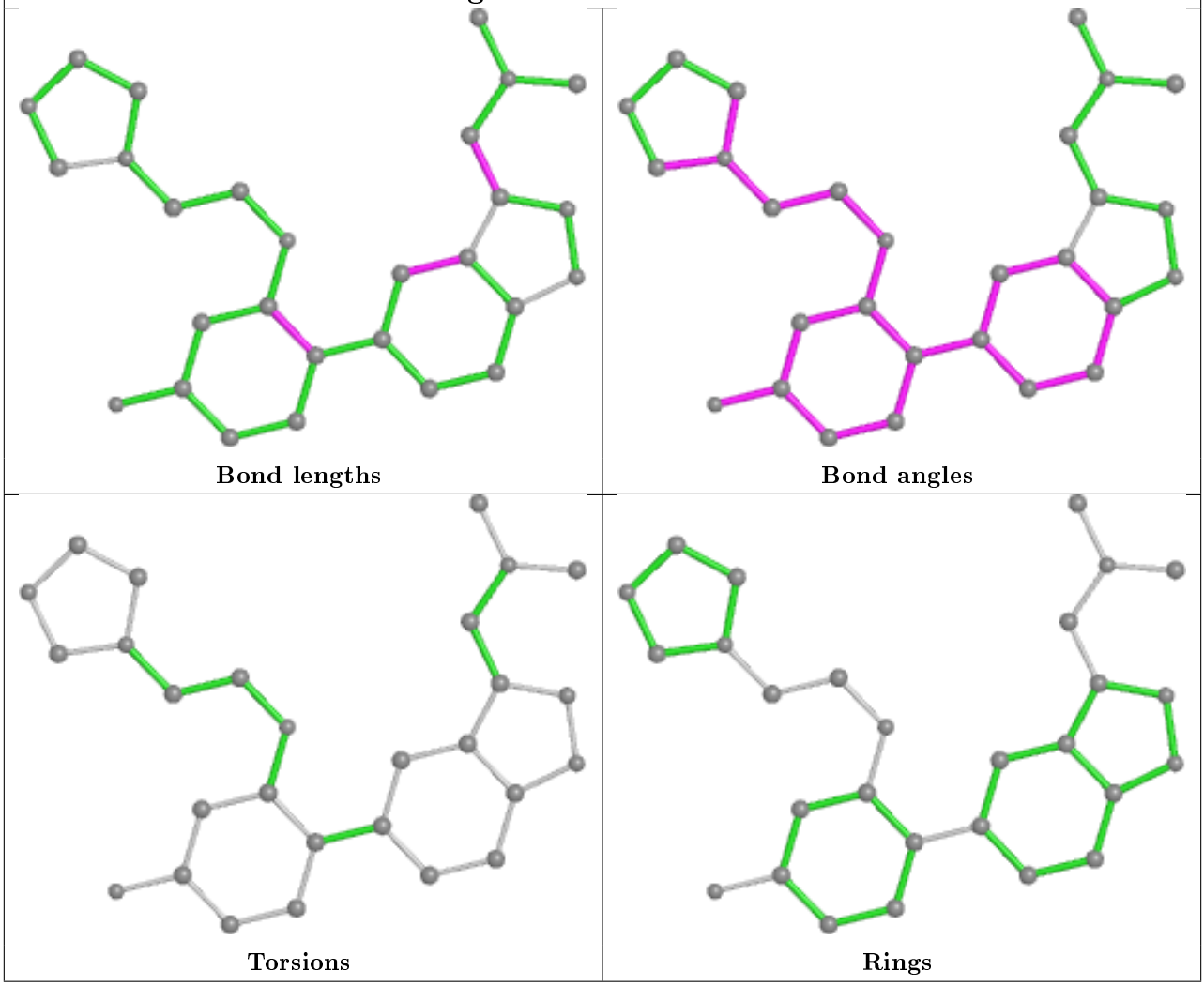
There are no ring outliers.

3 monomers are involved in 10 short contacts:

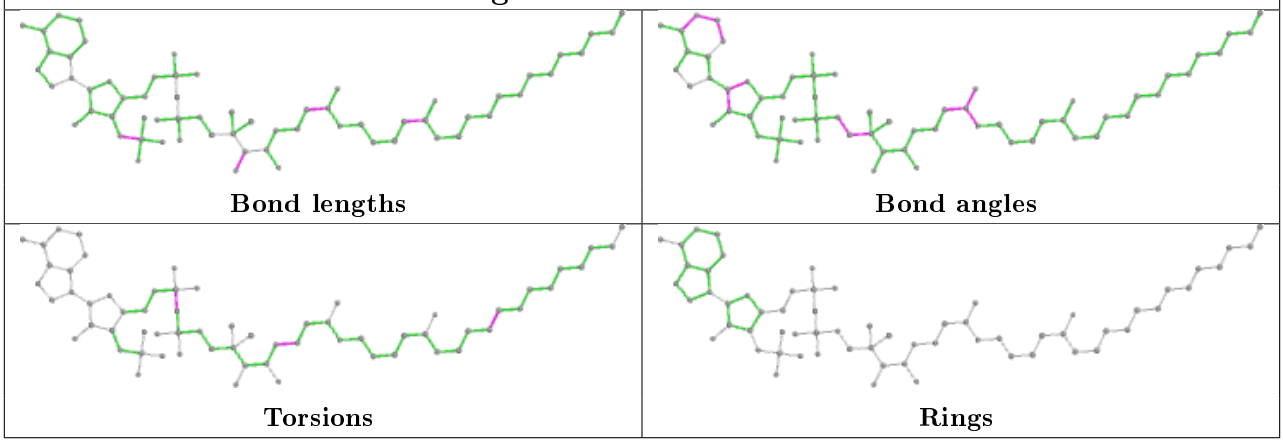
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	CCC	506	DMS	2	0
7	BBB	505	DMS	4	0
7	AAA	506	DMS	4	0

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 then 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.

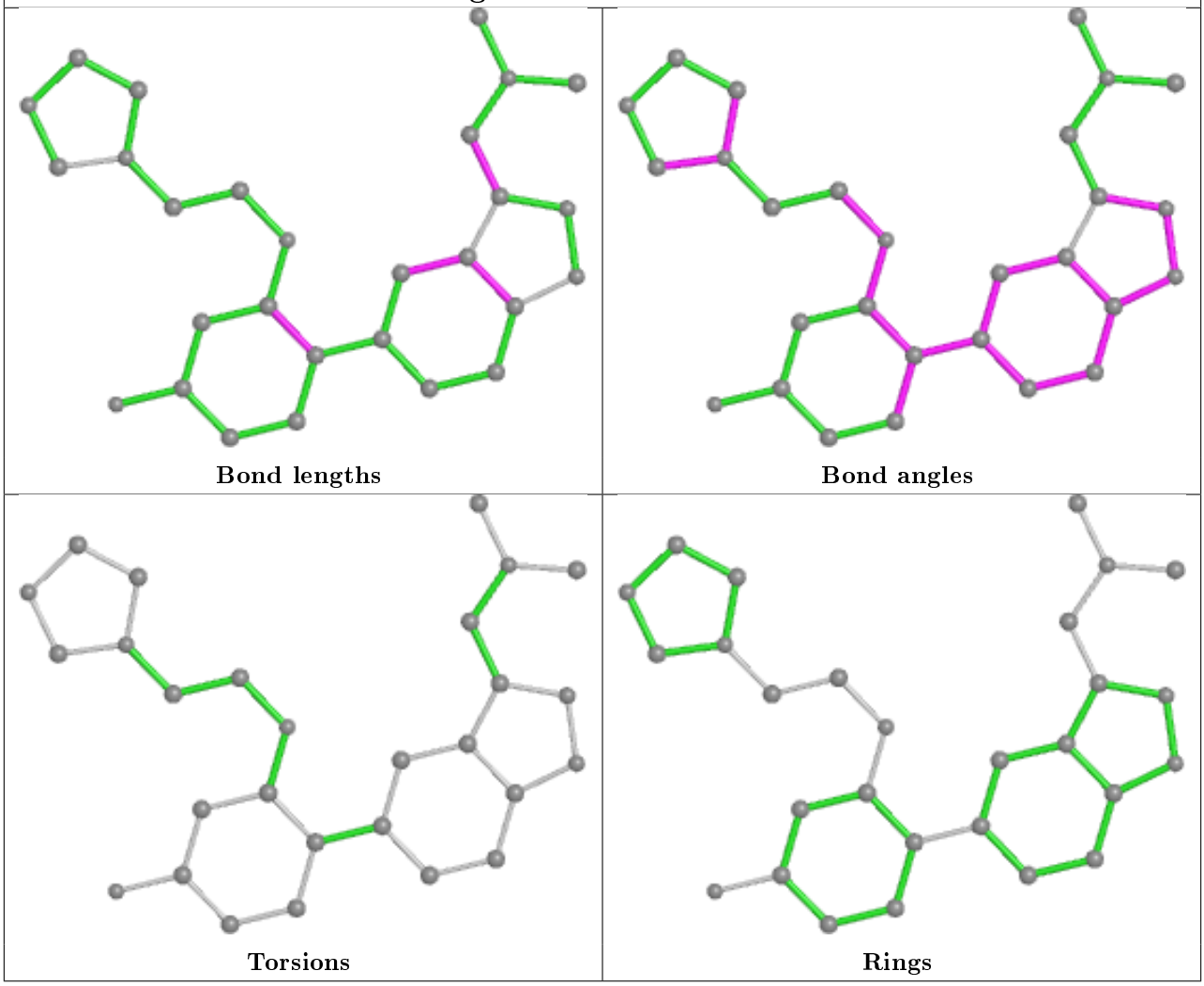
Ligand NZE AAA 502



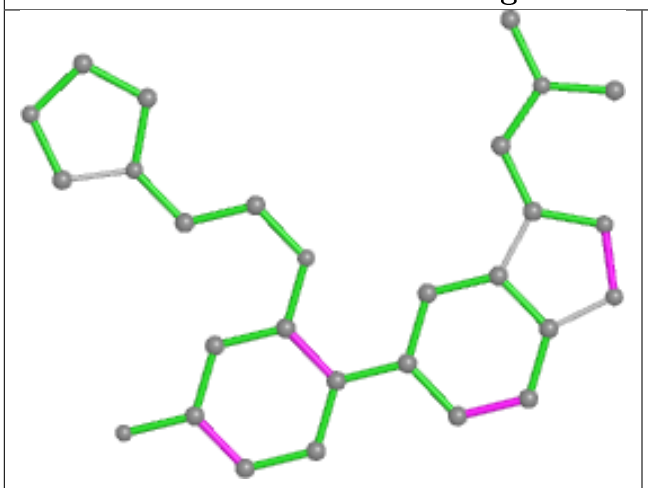
Ligand NHW BBB 501



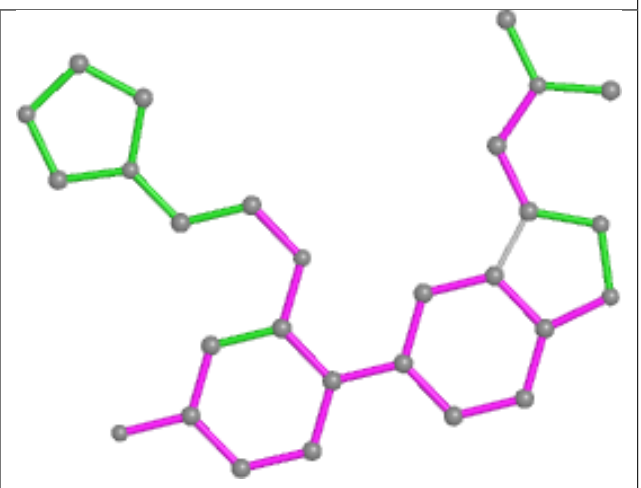
Ligand NZE CCC 502



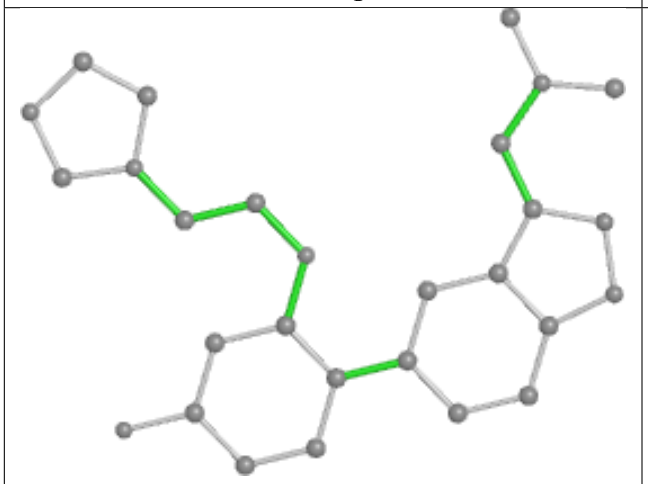
Ligand NZE BBB 502



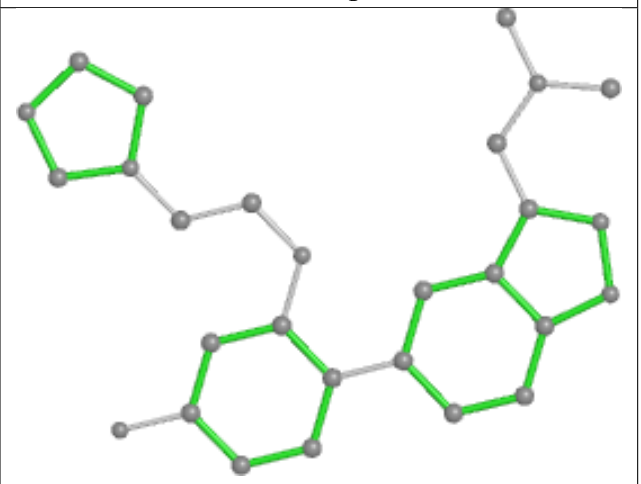
Bond lengths



Bond angles

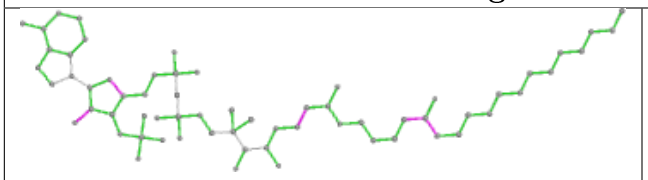


Torsions

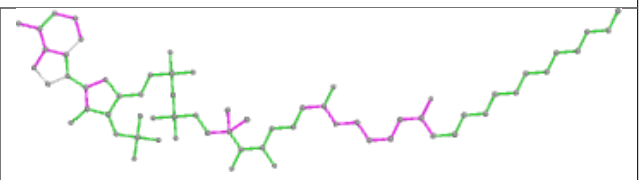


Rings

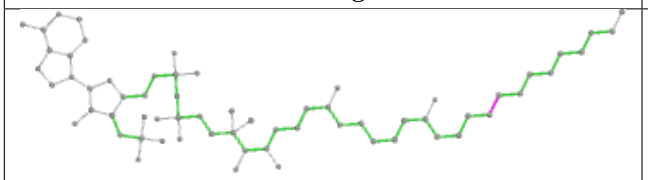
Ligand NHW AAA 501



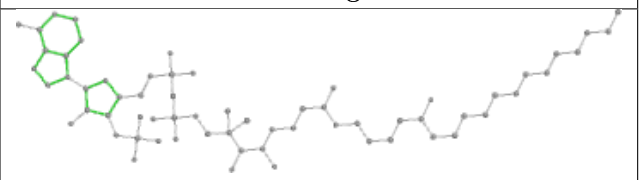
Bond lengths



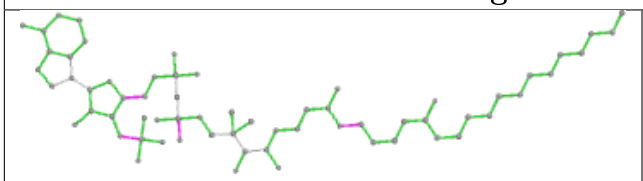
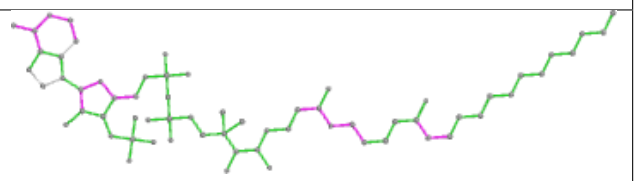
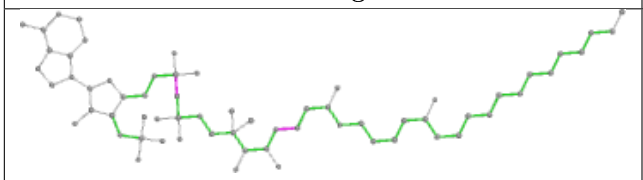
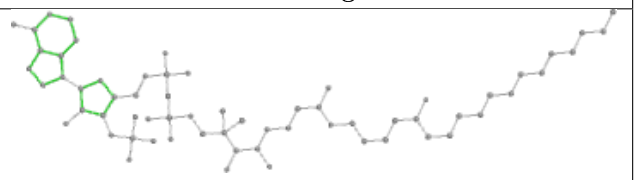
Bond angles



Torsions



Rings

Ligand NHW CCC 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	AAA	385/388 (99%)	-0.29	5 (1%)	77	81	8, 13, 26, 42	11 (2%)
1	BBB	385/388 (99%)	-0.30	4 (1%)	82	85	8, 12, 27, 44	14 (3%)
1	CCC	367/388 (94%)	-0.22	5 (1%)	75	79	9, 15, 29, 39	19 (5%)
All	All	1137/1164 (97%)	-0.27	14 (1%)	79	82	8, 13, 28, 44	44 (3%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	26	MET	6.1
1	BBB	26	MET	6.0
1	CCC	222	ILE	5.5
1	AAA	232	ARG	4.2
1	BBB	231[A]	SER	4.2

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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
7	DMS	CCC	505	4/4	0.72	0.26	23,28,33,35	4
7	DMS	AAA	506	4/4	0.78	0.32	12,13,15,23	4
7	DMS	CCC	506	4/4	0.86	0.27	30,32,32,38	4
7	DMS	BBB	505	4/4	0.88	0.26	13,14,17,23	4
3	NZE	BBB	502	28/28	0.92	0.10	11,13,28,29	0
5	SO4	AAA	504	5/5	0.92	0.14	42,43,43,50	0
3	NZE	CCC	502	28/28	0.93	0.09	14,19,32,35	0
3	NZE	AAA	502	28/28	0.94	0.10	12,15,27,31	0
2	NHW	AAA	501	64/64	0.97	0.07	7,11,13,15	0
2	NHW	BBB	501	64/64	0.98	0.07	7,10,13,14	0
2	NHW	CCC	501	64/64	0.98	0.07	8,12,16,18	0
4	MG	BBB	503	1/1	0.99	0.07	22,22,22,22	0
6	CL	AAA	505	1/1	0.99	0.07	12,12,12,12	0
4	MG	CCC	503	1/1	0.99	0.06	20,20,20,20	0
6	CL	BBB	504	1/1	1.00	0.07	11,11,11,11	0
6	CL	CCC	504	1/1	1.00	0.06	12,12,12,12	0
4	MG	AAA	503	1/1	1.00	0.06	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.