



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:23 PM GMT

PDB ID : 4CAE  
Title : Plasmodium vivax N-myristoyltransferase in complex with a benzothiophene inhibitor (compound 20b)  
Authors : Rackham, M.D.; Brannigan, J.A.; Rangachari, K.; Wilkinson, A.J.; Holder, A.A.; Tate, E.W.; Leatherbarrow, R.J.  
Deposited on : 2013-10-08  
Resolution : 1.46 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

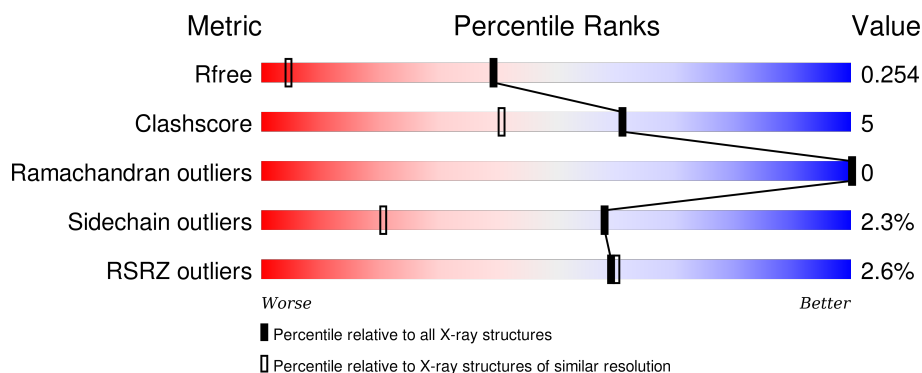
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.46 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))
$R_{free}$	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	384	<div> <div>2%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	B	384	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	C	384	<div> <div>3%</div> <div>88%</div> <div>6%</div> <div>.</div> </div>

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
5	DMS	B	1415	-	-	X	X
5	DMS	C	1414	-	-	-	X
7	SO4	B	1411	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11329 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
1	A	384	Total	C	N	O	S	0	25	0
			3321	2162	540	607	12			
1	B	384	Total	C	N	O	S	3	18	0
			3278	2139	531	596	12			
1	C	367	Total	C	N	O	S	1	17	0
			3133	2045	499	579	10			

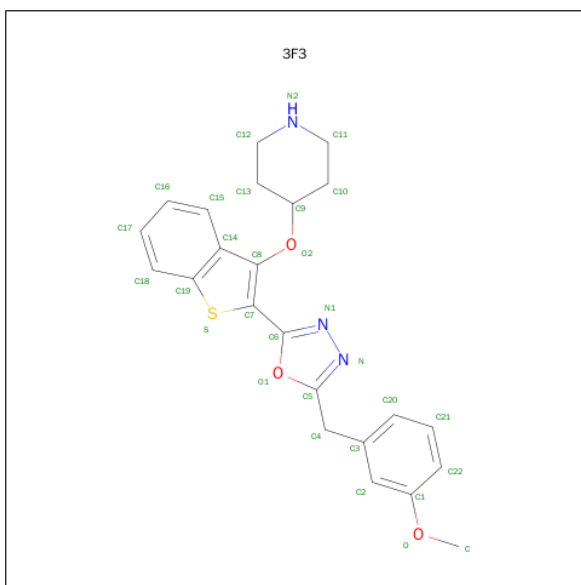
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

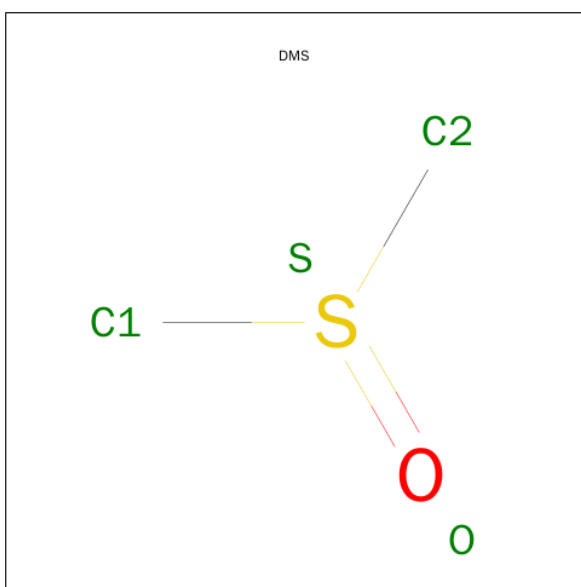
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 4-[(2-{5-[(3-METHOXYPHENYL)METHYL]-1,3,4-OXADIAZOL-2-YL}-1-BENZOTHIOPHEN-3-YL)OXY]PIPERIDINE (three-letter code: 3F3) (formula: C<sub>23</sub>H<sub>23</sub>N<sub>3</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			30	23	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			30	23	3	3	1		
4	C	1	Total	C	N	O	S	0	0
			30	23	3	3	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



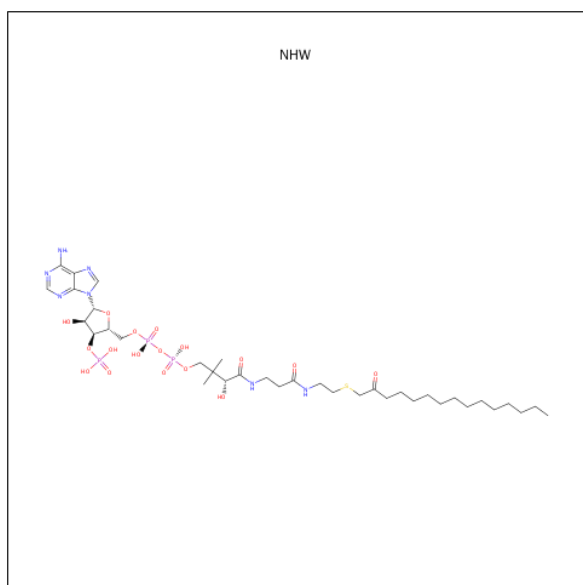
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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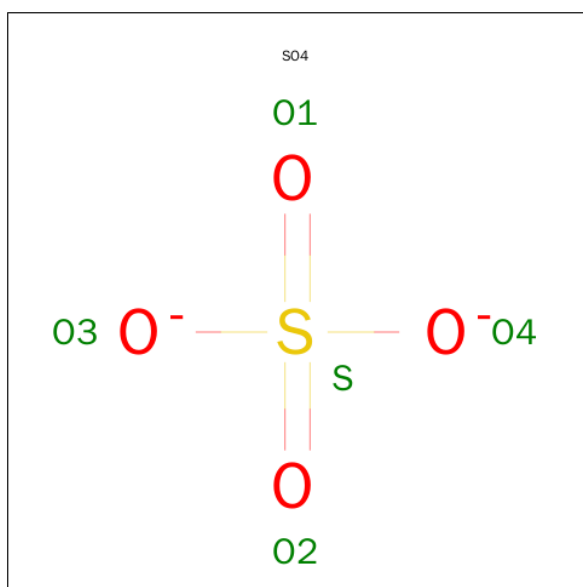
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 2-OXOPENTADECYL-COA (three-letter code: NHW) (formula:  $C_{36}H_{64}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
6	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
6	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

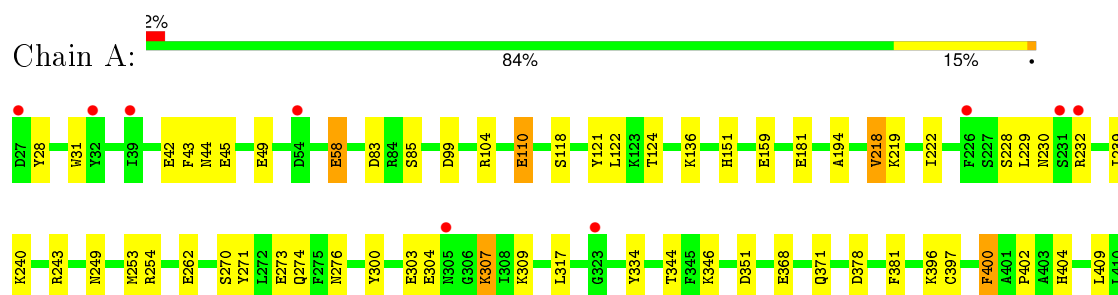
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	437	Total	O	0	0
			437	437		
8	B	453	Total	O	0	0
			453	453		
8	C	401	Total	O	0	0
			401	401		

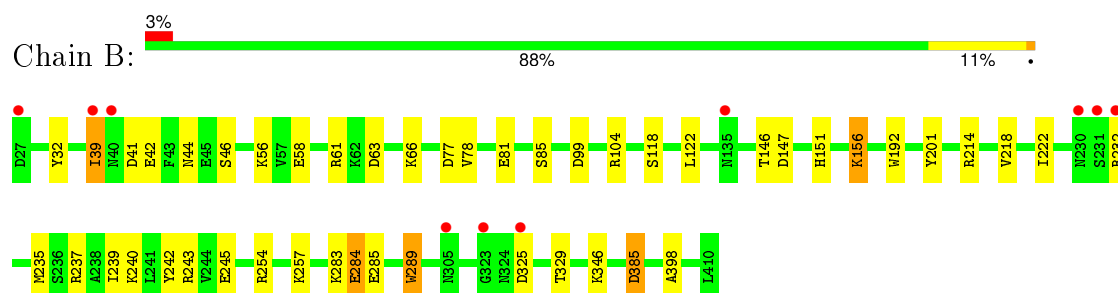
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

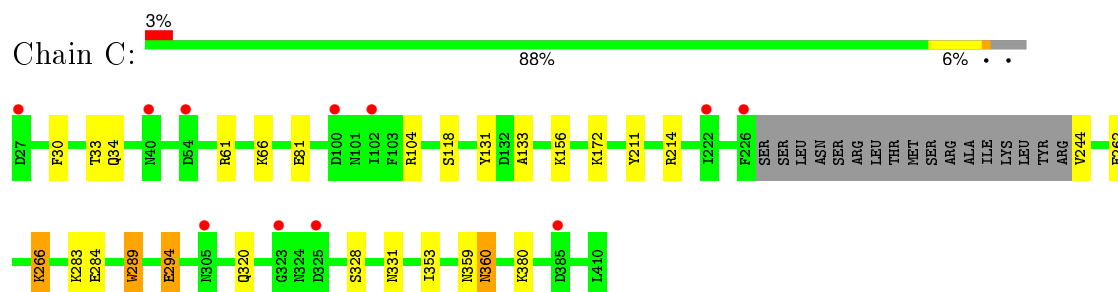
#### • Molecule 1: GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE



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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.50Å 121.05Å 178.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.22 – 1.46 24.43 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (100.22-1.46) 99.5 (24.43-1.46)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0029	Depositor
R, $R_{free}$	0.215 , 0.254 0.214 , 0.254	Depositor DCC
$R_{free}$ test set	10864 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.4	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 215168 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11329	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, CL, 3F3, NHW, DMS, SO4

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	0.99	2/3468 (0.1%)	1.03	4/4694 (0.1%)
1	B	0.99	3/3411 (0.1%)	1.04	10/4617 (0.2%)
1	C	1.08	5/3257 (0.2%)	1.00	3/4412 (0.1%)
All	All	1.02	10/10136 (0.1%)	1.02	17/13723 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66[A]	LYS	CE-NZ	-17.38	1.05	1.49
1	C	66[B]	LYS	CE-NZ	-17.38	1.05	1.49
1	C	66[A]	LYS	CD-CE	9.20	1.74	1.51
1	C	66[B]	LYS	CD-CE	9.20	1.74	1.51
1	A	181	GLU	CD-OE1	-7.25	1.17	1.25
1	B	192	TRP	CE3-CZ3	6.71	1.49	1.38
1	A	381	PHE	CG-CD1	5.27	1.46	1.38
1	B	289	TRP	CZ3-CH2	5.26	1.48	1.40
1	C	289	TRP	CE3-CZ3	5.24	1.47	1.38
1	B	245	GLU	CD-OE2	5.10	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284[A]	GLU	CB-CG-CD	11.19	144.41	114.20
1	B	284[B]	GLU	CB-CG-CD	11.19	144.41	114.20
1	B	104	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	A	104	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	B	61	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	C	61	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	104	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	C	104	ARG	NE-CZ-NH2	-6.92	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	214	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	77	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	63	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	104	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	351	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	385	ASP	CB-CA-C	-5.12	100.17	110.40
1	A	83	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	41	ASP	CB-CG-OD1	-5.08	113.73	118.30

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	3321	0	3353	52	0
1	B	3278	0	3310	43	0
1	C	3133	0	3128	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	30	0	23	1	0
4	B	30	0	23	0	0
4	C	30	0	23	0	0
5	A	4	0	6	0	0
5	B	4	0	6	4	0
5	C	4	0	6	0	0
6	A	64	0	60	1	0
6	B	64	0	60	0	0
6	C	64	0	60	0	0
7	B	5	0	0	0	0
8	A	437	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	453	0	0	13	0
8	C	401	0	0	6	0
All	All	11329	0	10058	110	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 5.

All (110) 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:32[A]:TYR:CD1	8:B:2007:HOH:O	1.83	1.25
1:C:30:PHE:O	1:C:33[A]:THR:HG22	1.42	1.19
1:A:218[B]:VAL:HG22	8:A:2269:HOH:O	1.43	1.13
1:C:331[A]:ASN:OD1	8:C:2338:HOH:O	1.80	0.97
1:B:289:TRP:CE2	5:B:1415:DMS:H23	2.05	0.92
1:A:344:THR:HG21	1:B:42[B]:GLU:HG2	1.53	0.87
1:A:344:THR:HG21	1:B:42[B]:GLU:CG	2.07	0.84
1:B:240:LYS:HG3	1:B:243[A]:ARG:NH2	1.93	0.84
1:B:289:TRP:NE1	5:B:1415:DMS:H23	1.95	0.82
1:A:262[B]:GLU:HG3	8:A:2318:HOH:O	1.81	0.81
1:A:121[A]:TYR:OH	8:A:2180:HOH:O	2.01	0.79
1:A:122:LEU:HB3	1:A:124:THR:HG22	1.65	0.78
1:B:32[A]:TYR:HD1	8:B:2007:HOH:O	1.36	0.76
1:B:151[B]:HIS:NE2	8:B:2028:HOH:O	1.73	0.72
1:A:276[B]:ASN:OD1	8:A:2336:HOH:O	2.08	0.70
1:B:257[B]:LYS:NZ	8:B:2321:HOH:O	2.26	0.69
1:B:32[A]:TYR:CE1	8:B:2007:HOH:O	2.23	0.68
1:A:159:GLU:CD	1:A:409:LEU:HD22	2.14	0.67
1:C:266:LYS:HG2	8:C:2285:HOH:O	1.96	0.64
1:C:262[B]:GLU:HG3	1:C:283:LYS:HE2	1.78	0.64
1:A:218[B]:VAL:CG2	1:A:239:ILE:HG12	2.28	0.63
1:A:42[A]:GLU:OE2	1:B:346:LYS:NZ	2.23	0.63
1:B:240:LYS:CG	1:B:243[A]:ARG:NH2	2.62	0.62
1:A:218[B]:VAL:HG21	1:A:239:ILE:HA	1.80	0.61
1:A:218[B]:VAL:HG21	1:A:239:ILE:HG12	1.82	0.61
1:B:257[B]:LYS:HD2	8:B:2322:HOH:O	1.99	0.61
1:A:85[A]:SER:OG	8:A:2110:HOH:O	2.16	0.58
1:A:194:ALA:HB2	6:A:1422:NHW:HDM	1.86	0.57
1:C:262[B]:GLU:HG3	1:C:283:LYS:CE	2.35	0.56
1:B:218:VAL:CG1	1:B:239[B]:ILE:HD13	2.35	0.56
1:A:42[A]:GLU:OE1	1:B:346:LYS:HE3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HB	1:B:239[B]:ILE:CD1	2.36	0.56
1:A:371:GLN:HG2	8:A:2337:HOH:O	2.05	0.56
1:A:317:LEU:HB3	1:A:334:TYR:CE1	2.43	0.53
1:C:156[B]:LYS:HB3	1:C:156[B]:LYS:NZ	2.24	0.53
1:B:235:MET:O	1:B:239[B]:ILE:HG12	2.07	0.53
1:C:156[B]:LYS:HB3	1:C:156[B]:LYS:HZ2	1.73	0.53
1:A:151[B]:HIS:CD2	8:A:2021:HOH:O	2.62	0.53
1:A:346:LYS:HE2	1:A:378:ASP:HB3	1.91	0.52
4:A:1414:3F3:C15	4:A:1414:3F3:H9	2.39	0.51
1:B:146[B]:THR:HG21	5:B:1415:DMS:H22	1.92	0.51
1:A:222[A]:ILE:HD12	1:A:229:LEU:HG	1.93	0.51
1:A:118:SER:O	1:A:121[A]:TYR:HB3	2.10	0.50
1:B:329:THR:HG23	8:B:2161:HOH:O	2.10	0.50
1:A:270[B]:SER:OG	8:A:2326:HOH:O	2.20	0.49
1:B:156[A]:LYS:HE2	1:B:156[A]:LYS:HA	1.95	0.49
1:A:230[B]:ASN:HD22	1:A:232:ARG:HD2	1.78	0.49
1:A:368:GLU:O	1:A:402:PRO:HB2	2.13	0.49
1:C:294:GLU:HG3	8:C:2157:HOH:O	2.12	0.49
1:C:284[B]:GLU:HG2	8:C:2305:HOH:O	2.12	0.48
1:B:283:LYS:HD2	8:B:2333:HOH:O	2.12	0.48
1:A:110[A]:GLU:HG3	8:A:2159:HOH:O	2.11	0.48
1:B:78:VAL:HG12	8:B:2094:HOH:O	2.12	0.48
1:B:254:ARG:NH1	1:B:257[B]:LYS:HD3	2.29	0.48
1:B:147:ASP:OD2	1:B:156[B]:LYS:HE2	2.14	0.48
8:A:2390:HOH:O	1:B:44[A]:ASN:OD1	2.20	0.48
1:A:404:HIS:HE1	8:A:2427:HOH:O	1.97	0.47
1:B:243[A]:ARG:CZ	8:B:2291:HOH:O	2.62	0.47
1:B:218:VAL:HG21	1:B:242:TYR:HB2	1.95	0.47
1:C:118:SER:HB3	1:C:289:TRP:CZ2	2.49	0.47
1:C:328:SER:HA	8:C:2329:HOH:O	2.14	0.47
1:C:214:ARG:HG2	1:C:353:ILE:HD13	1.96	0.47
1:B:284[A]:GLU:HG3	1:B:285:GLU:N	2.30	0.47
1:A:218[B]:VAL:HG23	1:A:219:LYS:N	2.30	0.47
1:B:289:TRP:CZ2	5:B:1415:DMS:H23	2.50	0.47
1:B:237:ARG:NH2	8:B:2285:HOH:O	2.48	0.46
1:A:249:ASN:ND2	8:A:2303:HOH:O	2.48	0.46
1:C:131:TYR:CE2	1:C:133:ALA:HB3	2.51	0.46
1:A:303:GLU:HA	1:A:307:LYS:O	2.15	0.46
1:A:151[A]:HIS:CE1	8:A:2206:HOH:O	2.69	0.46
1:A:58:GLU:O	1:A:58:GLU:HG3	2.16	0.46
1:A:43:PHE:CZ	1:A:396:LYS:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:VAL:HB	1:B:239[B]:ILE:HD13	1.98	0.45
1:A:45:GLU:O	1:A:151[A]:HIS:CE1	2.70	0.45
1:A:151[B]:HIS:CD2	1:A:397:CYS:HB2	2.53	0.44
1:A:218[B]:VAL:HG23	1:A:219:LYS:H	1.82	0.44
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.82	0.44
1:B:56:LYS:HB3	1:B:58:GLU:HG2	1.98	0.44
1:B:218:VAL:O	1:B:222[A]:ILE:HG12	2.18	0.44
1:C:266:LYS:HE2	1:C:266:LYS:HB2	1.65	0.43
1:B:325:ASP:OD1	1:B:325:ASP:N	2.50	0.43
1:B:118:SER:HB3	1:B:289:TRP:CZ2	2.53	0.43
1:A:304:GLU:O	1:A:307:LYS:HB2	2.18	0.43
1:B:66:LYS:HE3	8:B:2082:HOH:O	2.19	0.43
1:B:243[A]:ARG:HB3	1:B:243[A]:ARG:HE	1.34	0.43
1:B:44[B]:ASN:HD22	1:B:46:SER:H	1.67	0.43
1:C:33[A]:THR:HG23	1:C:34:GLN:OE1	2.18	0.43
1:C:359:ASN:O	1:C:360[A]:ASN:HB2	2.19	0.43
1:A:271:TYR:HE1	1:A:371:GLN:NE2	2.17	0.42
1:A:121[A]:TYR:C	1:A:121[A]:TYR:CD1	2.92	0.42
1:A:274:GLN:HB3	8:A:2328:HOH:O	2.20	0.42
1:A:270[A]:SER:OG	1:A:273[A]:GLU:OE2	2.33	0.42
1:C:284[A]:GLU:CD	1:C:284[A]:GLU:H	2.23	0.42
1:A:136:LYS:HA	1:A:136:LYS:HD2	1.70	0.42
1:B:151[B]:HIS:HE1	1:B:398:ALA:O	2.03	0.42
1:A:276[A]:ASN:ND2	1:A:400:PHE:CE1	2.85	0.42
1:A:304:GLU:HB2	1:A:309:LYS:HG3	2.02	0.41
1:A:49:GLU:OE2	1:A:396:LYS:NZ	2.53	0.41
1:B:85:SER:HB2	8:B:2111:HOH:O	2.20	0.41
1:C:172:LYS:HE3	8:C:2203:HOH:O	2.19	0.41
1:A:240[A]:LYS:HG3	1:A:243[A]:ARG:NH2	2.35	0.41
1:A:28:TYR:HB3	1:A:31:TRP:HB2	2.02	0.41
1:B:39:ILE:HD11	1:B:201:TYR:CE2	2.56	0.41
1:A:254[B]:ARG:NH2	1:A:303:GLU:OE1	2.49	0.40
1:A:396:LYS:HB2	1:A:396:LYS:HE3	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	407/384 (106%)	395 (97%)	12 (3%)	0	100	100
1	B	400/384 (104%)	392 (98%)	8 (2%)	0	100	100
1	C	380/384 (99%)	367 (97%)	13 (3%)	0	100	100
All	All	1187/1152 (103%)	1154 (97%)	33 (3%)	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	375/350 (107%)	362 (96%)	13 (4%)	43	9
1	B	368/350 (105%)	360 (98%)	8 (2%)	60	22
1	C	351/350 (100%)	342 (97%)	9 (3%)	54	17
All	All	1094/1050 (104%)	1064 (97%)	30 (3%)	58	15

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44[A]	ASN
1	A	44[B]	ASN
1	A	58	GLU
1	A	99	ASP
1	A	110[A]	GLU

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Mol	Chain	Res	Type
1	A	110[B]	GLU
1	A	218[A]	VAL
1	A	218[B]	VAL
1	A	228	SER
1	A	253[A]	MET
1	A	253[B]	MET
1	A	307	LYS
1	A	400	PHE
1	B	39	ILE
1	B	81	GLU
1	B	99	ASP
1	B	122	LEU
1	B	156[A]	LYS
1	B	156[B]	LYS
1	B	232	ARG
1	B	385	ASP
1	C	81	GLU
1	C	211	TYR
1	C	244	VAL
1	C	266	LYS
1	C	294	GLU
1	C	320	GLN
1	C	360[A]	ASN
1	C	360[B]	ASN
1	C	380	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	40	ASN
1	A	106	ASN
1	A	249	ASN
1	A	295	ASN
1	A	331	ASN
1	A	350	GLN
1	A	371	GLN
1	B	34	GLN
1	B	295	ASN
1	B	331	ASN
1	B	350	GLN
1	B	360	ASN

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Mol	Chain	Res	Type
1	C	55	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	3F3	A	1414	-	25,34,34	1.50	3 (12%)	22,47,47	1.81	6 (27%)
5	DMS	A	1415	-	3,3,3	0.31	0	3,3,3	1.07	0
6	NHW	A	1422	2	56,66,66	1.20	4 (7%)	68,92,92	1.83	12 (17%)
7	SO4	B	1411	-	4,4,4	0.39	0	6,6,6	0.42	0
4	3F3	B	1414	-	25,34,34	2.02	4 (16%)	22,47,47	1.49	3 (13%)
5	DMS	B	1415	-	3,3,3	0.27	0	3,3,3	2.12	1 (33%)
6	NHW	B	1422	2	56,66,66	1.31	6 (10%)	68,92,92	1.63	11 (16%)
4	3F3	C	1413	-	25,34,34	2.08	3 (12%)	22,47,47	1.42	3 (13%)
5	DMS	C	1414	-	3,3,3	0.33	0	3,3,3	1.22	0
6	NHW	C	1422	2	56,66,66	1.23	6 (10%)	68,92,92	1.99	7 (10%)

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	3F3	A	1414	-	-	0/6/22/22	0/4/5/5
5	DMS	A	1415	-	-	0/0/0/0	0/0/0/0
6	NHW	A	1422	2	-	0/61/81/81	0/3/3/3
7	SO4	B	1411	-	-	0/0/0/0	0/0/0/0
4	3F3	B	1414	-	-	0/6/22/22	0/4/5/5
5	DMS	B	1415	-	-	0/0/0/0	0/0/0/0
6	NHW	B	1422	2	-	0/61/81/81	0/3/3/3
4	3F3	C	1413	-	-	0/6/22/22	0/4/5/5
5	DMS	C	1414	-	-	0/0/0/0	0/0/0/0
6	NHW	C	1422	2	-	0/61/81/81	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1414	3F3	C18-C19	-3.63	1.36	1.40
4	C	1413	3F3	C18-C19	-3.28	1.36	1.40
6	A	1422	NHW	P3X-O7A	-2.89	1.44	1.54
6	B	1422	NHW	P1A-O2A	-2.62	1.43	1.54
6	C	1422	NHW	P3X-O7A	-2.62	1.45	1.54
6	B	1422	NHW	P2A-O4A	-2.49	1.44	1.54
6	C	1422	NHW	O4X-C1X	-2.34	1.38	1.41
6	C	1422	NHW	P2A-O4A	-2.12	1.45	1.54
6	B	1422	NHW	P3X-O7A	-2.06	1.47	1.54
6	A	1422	NHW	P3X-O8A	2.05	1.62	1.54
4	C	1413	3F3	C16-C15	2.27	1.41	1.36
4	A	1414	3F3	C2-C3	2.29	1.43	1.39
6	C	1422	NHW	C7-N8	2.39	1.51	1.46
6	A	1422	NHW	C7-C6	2.39	1.59	1.51
4	B	1414	3F3	C16-C17	2.45	1.44	1.38
4	B	1414	3F3	C17-C18	2.47	1.42	1.36
6	A	1422	NHW	O4X-C1X	2.81	1.44	1.41
4	B	1414	3F3	N-N1	2.94	1.43	1.37
6	B	1422	NHW	P3X-O8A	3.19	1.66	1.54
6	C	1422	NHW	O10-C10	3.61	1.49	1.42
4	A	1414	3F3	C8-C14	3.81	1.45	1.40
6	C	1422	NHW	O4X-C4X	3.85	1.53	1.45
6	B	1422	NHW	CP-S1	3.87	1.89	1.81
6	B	1422	NHW	C6-C5	4.44	1.60	1.51
4	C	1413	3F3	C8-C14	8.24	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1414	3F3	C8-C14	8.53	1.51	1.40

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1422	NHW	N3A-C2A-N1A	-10.39	120.94	128.89
6	B	1422	NHW	N3A-C2A-N1A	-8.58	122.32	128.89
6	A	1422	NHW	N3A-C2A-N1A	-6.61	123.83	128.89
6	C	1422	NHW	C2X-C1X-N9A	-5.47	105.94	114.29
6	A	1422	NHW	C4X-O4X-C1X	-5.32	103.87	109.72
6	C	1422	NHW	C4X-O4X-C1X	-4.82	104.42	109.72
6	A	1422	NHW	C2X-C1X-N9A	-4.66	107.18	114.29
4	A	1414	3F3	C16-C15-C14	-4.56	114.43	120.88
6	A	1422	NHW	C13-C11-C12	-4.50	102.67	108.50
6	C	1422	NHW	C1X-N9A-C4A	-3.99	120.93	126.94
6	C	1422	NHW	O1M-C1M-CP	-3.85	116.64	122.14
6	A	1422	NHW	O1M-C1M-CP	-3.76	116.76	122.14
6	C	1422	NHW	O6A-C12-C11	-3.67	104.65	110.55
6	B	1422	NHW	O1M-C1M-CP	-3.17	117.61	122.14
6	B	1422	NHW	C6-C7-N8	-2.90	105.52	111.88
6	B	1422	NHW	P3X-O3X-C3X	-2.81	114.81	121.56
4	B	1414	3F3	C1-C2-C3	-2.75	116.79	119.69
6	A	1422	NHW	C2-C3-N4	-2.68	107.00	112.36
4	B	1414	3F3	C16-C17-C18	-2.63	116.63	120.45
6	A	1422	NHW	C5X-C4X-C3X	-2.56	105.10	114.31
6	B	1422	NHW	C2X-C1X-N9A	-2.51	110.45	114.29
6	B	1422	NHW	P2A-O3A-P1A	-2.44	125.87	132.73
4	C	1413	3F3	C13-C12-N2	-2.21	106.70	110.46
6	A	1422	NHW	C4A-C5A-N7A	-2.20	107.46	109.48
4	A	1414	3F3	C21-C20-C3	-2.19	117.16	120.65
6	A	1422	NHW	C2-S1-CP	-2.14	98.33	101.89
4	C	1413	3F3	C17-C16-C15	-2.13	117.36	120.45
6	B	1422	NHW	C4A-C5A-N7A	-2.08	107.57	109.48
6	B	1422	NHW	O6A-C12-C11	-2.01	107.31	110.55
4	A	1414	3F3	C21-C22-C1	2.20	122.72	118.92
6	B	1422	NHW	O7A-P3X-O9A	2.23	117.75	110.58
4	C	1413	3F3	C11-N2-C12	2.35	118.14	110.33
6	C	1422	NHW	C14-C11-C10	2.43	113.78	109.34
6	B	1422	NHW	C13-C11-C10	2.58	114.06	109.34
4	A	1414	3F3	C17-C16-C15	2.63	124.28	120.45
4	A	1414	3F3	C-O-C1	2.66	123.75	117.51
4	B	1414	3F3	C17-C18-C19	2.74	123.02	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1415	DMS	C2-S-C1	2.74	112.62	98.46
4	A	1414	3F3	C10-C11-N2	2.85	115.29	110.46
6	B	1422	NHW	C2A-N1A-C6A	2.89	123.94	118.77
6	A	1422	NHW	C2A-N1A-C6A	3.00	124.12	118.77
6	A	1422	NHW	C13-C11-C10	3.37	115.50	109.34
6	A	1422	NHW	CP-C1M-C2M	3.49	123.08	115.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1414	3F3	1	0
6	A	1422	NHW	1	0
5	B	1415	DMS	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	384/384 (100%)	0.16	9 (2%) 64 65	10, 16, 30, 60	5 (1%)
1	B	384/384 (100%)	-0.05	10 (2%) 59 60	7, 12, 26, 53	10 (2%)
1	C	367/384 (95%)	0.02	11 (2%) 54 54	7, 14, 27, 45	10 (2%)
All	All	1135/1152 (98%)	0.04	30 (2%) 59 60	7, 14, 28, 60	25 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	ARG	5.8
1	A	232	ARG	5.7
1	A	231	SER	4.5
1	B	231	SER	4.5
1	C	27	ASP	4.3
1	C	305	ASN	4.1
1	A	54	ASP	3.8
1	B	323	GLY	3.2
1	B	305	ASN	3.1
1	B	325	ASP	2.9
1	C	222	ILE	2.9
1	A	323	GLY	2.8
1	A	226	PHE	2.7
1	C	100	ASP	2.5
1	B	135	ASN	2.5
1	A	305	ASN	2.4
1	A	27	ASP	2.3
1	C	323	GLY	2.3
1	C	385	ASP	2.2
1	C	102	ILE	2.2
1	B	27	ASP	2.2
1	C	226	PHE	2.2
1	C	54	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	32	TYR	2.1
1	B	40	ASN	2.1
1	C	40	ASN	2.1
1	C	325	ASP	2.1
1	A	39	ILE	2.1
1	B	39	ILE	2.1
1	B	230	ASN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	DMS	B	1415	4/4	0.92	0.17	6.06	25,26,27,36	0
5	DMS	C	1414	4/4	0.93	0.16	3.99	22,25,27,28	0
7	SO4	B	1411	5/5	0.95	0.15	3.36	36,38,41,44	0
5	DMS	A	1415	4/4	0.93	0.13	1.79	27,28,30,31	0
4	3F3	B	1414	30/30	0.96	0.09	0.35	10,12,14,19	0
4	3F3	C	1413	30/30	0.94	0.09	0.25	14,17,21,21	0
4	3F3	A	1414	30/30	0.95	0.09	-0.08	12,16,18,21	0
6	NHW	C	1422	64/64	0.96	0.08	-0.21	8,11,15,17	0
2	MG	C	1411	1/1	0.98	0.07	-0.47	20,20,20,20	0
6	NHW	B	1422	64/64	0.97	0.07	-0.56	7,10,13,14	0
6	NHW	A	1422	64/64	0.96	0.08	-0.83	10,13,16,18	0
3	CL	B	1413	1/1	0.99	0.06	-0.85	13,13,13,13	0
2	MG	B	1412	1/1	0.98	0.07	-0.93	21,21,21,21	0
2	MG	A	1411	1/1	0.99	0.05	-2.13	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	A	1413	1/1	0.99	0.05	-2.42	15,15,15,15	0
3	CL	C	1412	1/1	0.99	0.03	-3.58	12,12,12,12	0
3	CL	A	1412	1/1	0.98	0.06	-	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.