



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 12:56 PM EST

PDB ID : 5G1Z  
Title : Plasmodium vivax N-myristoyltransferase in complex with a quinoline inhibitor (compound 1)  
Authors : Goncalves, V.; Brannigan, J.A.; Laporte, A.; Bell, A.S.; Roberts, S.M.; Wilkinson, A.J.; Leatherbarrow, R.J.; Tate, E.W.  
Deposited on : 2016-04-06  
Resolution : 1.50 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

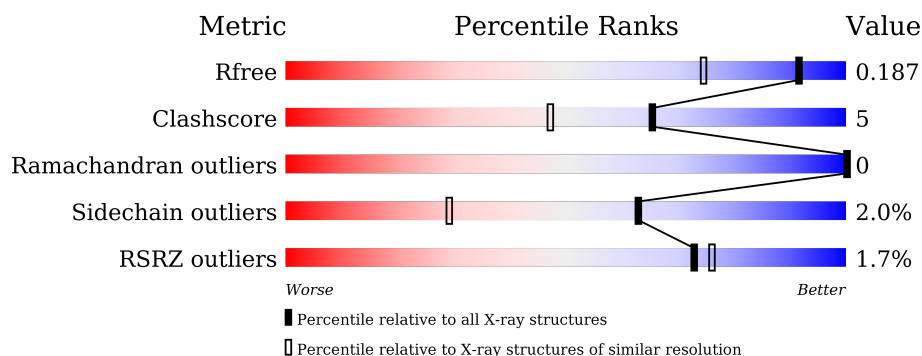
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	385	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	B	385	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	385	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>.</div> <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
3	U53	A	1001	-	-	-	X
3	U53	B	1001	-	-	-	X
3	U53	C	1001	-	-	X	X
4	DMS	A	1411	-	-	-	X
4	DMS	B	1411	-	-	-	X
4	DMS	C	1411[A]	-	-	-	X
4	DMS	C	1411[B]	-	-	-	X
4	DMS	C	1412	-	-	-	X
6	SO4	A	1413	-	-	-	X
6	SO4	A	1414	-	-	-	X

## 2 Entry composition [i](#)

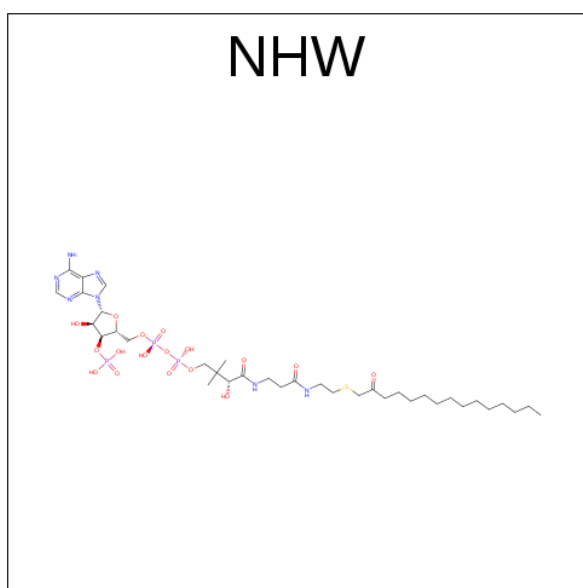
There are 8 unique types of molecules in this entry. The entry contains 11889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

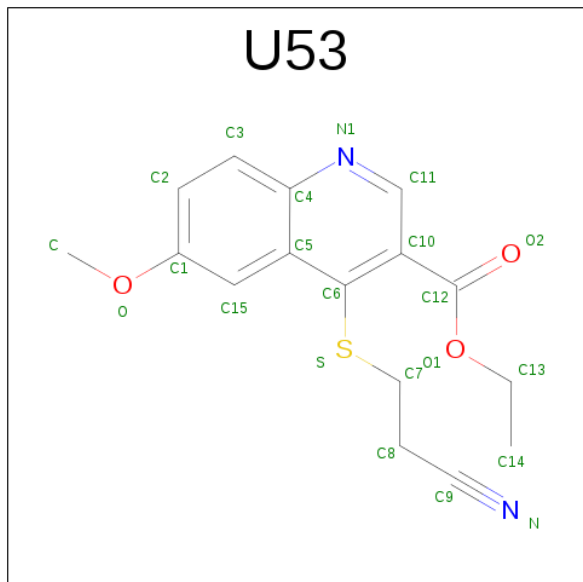
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	34	0
			3398	2225	547	614	12			
1	B	385	Total	C	N	O	S	0	24	0
			3325	2177	538	598	12			
1	C	370	Total	C	N	O	S	0	29	0
			3240	2124	513	592	11			

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



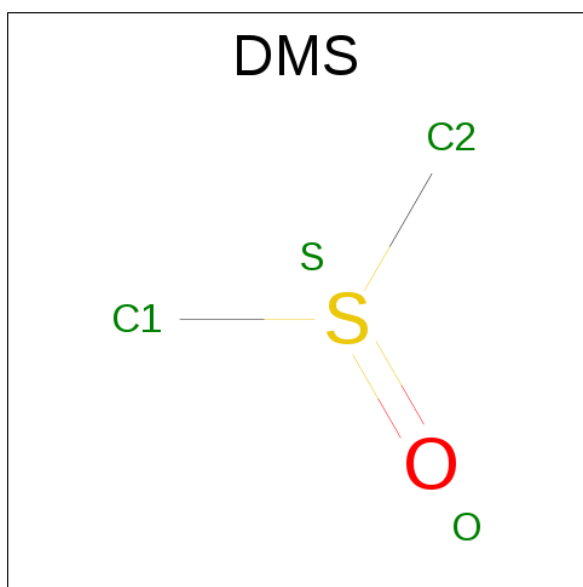
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		
2	C	1	Total	C	N	O	P S	0	0
			64	36	7	17	3 1		

- Molecule 3 is ETHYL 4-(2-CYANOETHYLSULFANYL)-6-METHOXY-QUINOLINE-3-CARBOXYLATE (three-letter code: U53) (formula:  $C_{16}H_{16}N_2O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	16	2	3	1		
3	B	1	Total	C	N	O	S	0	0
			22	16	2	3	1		
3	C	1	Total	C	N	O	S	0	0
			22	16	2	3	1		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).

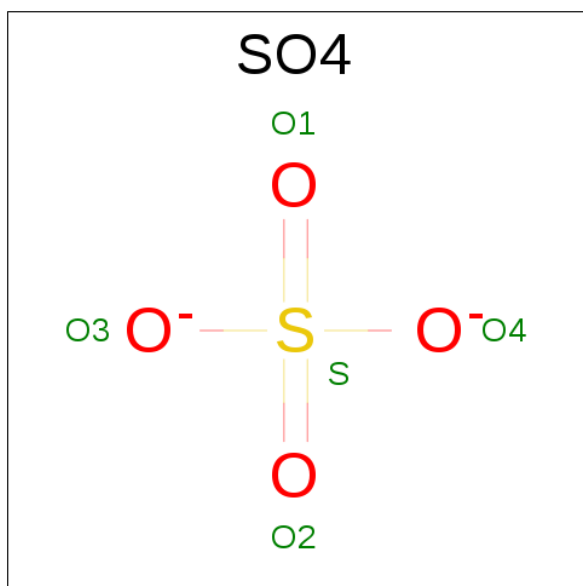


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 8 4 2 2	0	1
4	C	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	615	Total 616	O 616	0	1
8	B	505	Total 505	O 505	0	0
8	C	511	Total 511	O 511	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.40Å 118.90Å 175.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.45 – 1.50 59.45 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (59.45-1.50) 99.4 (59.45-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.149 , 0.187 0.149 , 0.187	Depositor DCC
$R_{free}$ test set	9591 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.6	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, U53, 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	1.22	3/3567 (0.1%)	1.25	11/4824 (0.2%)
1	B	1.24	6/3471 (0.2%)	1.26	15/4695 (0.3%)
1	C	1.29	6/3399 (0.2%)	1.30	23/4600 (0.5%)
All	All	1.25	15/10437 (0.1%)	1.27	49/14119 (0.3%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	TYR	CG-CD1	9.99	1.52	1.39
1	C	245	GLU	CD-OE1	7.48	1.33	1.25
1	A	159	GLU	CD-OE1	7.43	1.33	1.25
1	B	58	GLU	CD-OE2	7.10	1.33	1.25
1	B	114	TRP	CZ3-CH2	6.45	1.50	1.40
1	B	192	TRP	CE2-CZ2	6.39	1.50	1.39
1	B	58	GLU	CD-OE1	6.10	1.32	1.25
1	A	192	TRP	CE3-CZ3	5.79	1.48	1.38
1	C	391	TYR	CG-CD1	5.65	1.46	1.39
1	A	314	PHE	CG-CD1	5.30	1.46	1.38
1	C	284[A]	GLU	CD-OE1	5.28	1.31	1.25
1	C	284[B]	GLU	CD-OE1	5.28	1.31	1.25
1	C	245	GLU	CD-OE2	5.25	1.31	1.25
1	B	212	TYR	CZ-OH	5.22	1.46	1.37
1	C	211	TYR	CG-CD2	5.03	1.45	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH2	-14.14	113.23	120.30
1	C	104	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	104	ARG	NE-CZ-NH1	12.74	126.67	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	ARG	NE-CZ-NH2	-11.89	114.35	120.30
1	B	184	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	B	104	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	B	104	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	C	137	LEU	CB-CG-CD1	10.86	129.47	111.00
1	B	185	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	C	358	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	185	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	C	214[A]	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	C	214[B]	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	254	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	C	77	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	314	PHE	CB-CG-CD2	-6.92	115.96	120.80
1	B	345	PHE	CB-CG-CD1	-6.87	115.99	120.80
1	C	345	PHE	CB-CG-CD1	-6.71	116.11	120.80
1	C	358	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	364	PHE	CB-CG-CD2	-6.42	116.30	120.80
1	B	385	ASP	C-N-CA	-6.40	108.86	122.30
1	A	185	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	C	28	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	284	GLU	CG-CD-OE1	6.23	130.77	118.30
1	B	147	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	208	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	244	VAL	CG1-CB-CG2	5.96	120.44	110.90
1	C	59	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	C	246	ASP	CB-CG-OD2	5.82	123.53	118.30
1	A	253[A]	MET	CA-CB-CG	5.66	122.92	113.30
1	A	253[B]	MET	CA-CB-CG	5.66	122.92	113.30
1	B	212	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	C	254	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	218	VAL	CG1-CB-CG2	-5.60	101.95	110.90
1	C	28	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
1	C	170	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	61	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	105	PHE	CB-CG-CD2	-5.50	116.95	120.80
1	C	185	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	284	GLU	CA-CB-CG	5.31	125.08	113.40
1	C	244	VAL	CA-CB-CG2	5.25	118.78	110.90
1	C	253[A]	MET	CG-SD-CE	5.15	108.44	100.20
1	C	253[B]	MET	CG-SD-CE	5.15	108.44	100.20
1	B	212	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	A	38	LYS	CD-CE-NZ	5.09	123.40	111.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	A	140	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	B	358	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	174	LEU	CB-CG-CD2	-5.00	102.49	111.00

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	3398	0	3462	30	1
1	B	3325	0	3385	23	0
1	C	3240	0	3279	45	0
2	A	64	0	60	0	0
2	B	64	0	60	0	0
2	C	64	0	60	0	0
3	A	22	0	0	3	0
3	B	22	0	0	5	0
3	C	22	0	0	9	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	12	0	18	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	10	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	616	0	0	15	0
8	B	505	0	0	5	0
8	C	511	0	0	10	0
All	All	11889	0	10336	102	1

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 (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156[A]:LYS:HD2	8:A:2304:HOH:O	1.28	1.28
1:B:243[B]:ARG:NH1	8:B:2346:HOH:O	1.63	1.25
4:C:1411[A]:DMS:H13	8:C:2309:HOH:O	1.41	1.20
1:B:243[B]:ARG:NH2	8:B:2346:HOH:O	1.68	1.19
1:A:147[B]:ASP:OD1	1:A:156[B]:LYS:HD3	1.60	1.01
1:A:243[B]:ARG:HD2	8:A:2427:HOH:O	1.61	1.00
1:C:88:TYR:O	1:C:92[B]:THR:HG23	1.62	0.98
1:A:222[A]:ILE:HD13	1:A:227:SER:HB2	1.46	0.97
1:A:156[A]:LYS:CD	8:A:2304:HOH:O	1.93	0.97
1:C:213[B]:HIS:CE1	3:C:1001:U53:N	2.33	0.96
1:C:294[B]:GLU:CD	1:C:294[B]:GLU:H	1.63	0.92
4:C:1411[B]:DMS:O	8:C:2309:HOH:O	1.88	0.92
1:A:156[A]:LYS:CG	8:A:2304:HOH:O	2.13	0.91
1:A:156[A]:LYS:HG3	8:A:2304:HOH:O	1.71	0.91
1:C:304[A]:GLU:OE2	8:C:2420:HOH:O	1.91	0.89
1:B:243[B]:ARG:CZ	8:B:2346:HOH:O	1.84	0.86
1:A:231[B]:SER:HB2	8:A:2417:HOH:O	1.76	0.85
1:C:32[B]:TYR:HE2	8:C:2012:HOH:O	1.60	0.84
3:C:1001:U53:C13	3:C:1001:U53:C11	2.57	0.81
1:C:213[B]:HIS:HE1	3:C:1001:U53:N	1.77	0.80
1:C:243:ARG:HH11	1:C:243:ARG:HG3	1.46	0.79
1:C:33[C]:THR:CA	1:C:34:GLN:N	2.47	0.77
1:C:32[B]:TYR:CE2	8:C:2012:HOH:O	2.39	0.73
1:B:39:ILE:HD11	1:B:201:TYR:HE2	1.53	0.73
1:C:33[A]:THR:HG22	1:C:33[A]:THR:O	1.88	0.73
1:B:32[A]:TYR:CD1	8:B:2006:HOH:O	2.42	0.73
1:B:103:PHE:CZ	1:B:226[B]:PHE:HD2	2.07	0.72
1:C:102:ILE:HD13	1:C:103:PHE:CE1	2.26	0.70
1:A:304:GLU:OE2	1:A:309:LYS:NZ	2.23	0.69
1:C:294[B]:GLU:CD	1:C:294[B]:GLU:N	2.43	0.69
1:C:102:ILE:CD1	1:C:103:PHE:CE1	2.76	0.68
1:C:206[B]:VAL:HG12	1:C:400:PHE:CE1	2.28	0.68
1:C:105:PHE:CE2	3:C:1001:U53:C2	2.76	0.67
1:C:102:ILE:CD1	1:C:103:PHE:CZ	2.77	0.67
1:C:102:ILE:HD13	1:C:103:PHE:CD1	2.29	0.67
1:C:88:TYR:CZ	1:C:92[B]:THR:HG21	2.31	0.66
1:B:226[A]:PHE:CE2	3:B:1001:U53:C14	2.79	0.66
1:A:32[B]:TYR:CD1	8:A:2008:HOH:O	2.48	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASN:OD1	1:B:232:ARG:HG2	1.99	0.63
1:B:346[B]:LYS:HE3	1:B:378:ASP:HB3	1.81	0.63
1:A:96:VAL:HG12	3:A:1001:U53:O	2.00	0.62
1:C:105:PHE:CE2	3:C:1001:U53:C1	2.84	0.61
1:A:147[B]:ASP:OD1	1:A:156[B]:LYS:CD	2.43	0.61
1:C:243:ARG:NH1	1:C:243:ARG:HG3	2.16	0.59
1:A:222[A]:ILE:HD13	1:A:227:SER:CB	2.29	0.58
1:C:146:THR:HG22	1:C:159[B]:GLU:HG3	1.84	0.58
1:A:218[A]:VAL:HG13	8:A:2400:HOH:O	2.03	0.57
1:B:218:VAL:HG13	8:B:2318:HOH:O	2.04	0.57
1:C:32[B]:TYR:CD1	8:C:2008:HOH:O	2.53	0.56
1:C:146:THR:CG2	1:C:159[B]:GLU:HG3	2.36	0.55
1:C:33[A]:THR:O	1:C:33[A]:THR:CG2	2.54	0.55
1:C:332:ALA:HB2	3:C:1001:U53:C14	2.36	0.55
1:C:354[B]:LEU:HD21	1:C:358:ARG:NE	2.22	0.55
1:B:226[A]:PHE:CZ	3:B:1001:U53:C14	2.90	0.54
1:C:92[B]:THR:HG22	8:C:2165:HOH:O	2.06	0.54
1:C:213[B]:HIS:ND1	3:C:1001:U53:N	2.56	0.53
1:B:96:VAL:HG12	3:B:1001:U53:O	2.09	0.53
1:B:218:VAL:HG11	1:B:242:TYR:HB2	1.92	0.52
1:C:226:PHE:HE1	3:C:1001:U53:C12	2.23	0.51
1:C:332:ALA:CB	3:C:1001:U53:C14	2.88	0.51
1:A:156[A]:LYS:HD2	8:A:2303:HOH:O	2.09	0.51
1:C:159[B]:GLU:OE2	4:C:1412:DMS:O	2.28	0.51
1:B:39:ILE:HD11	1:B:201:TYR:CE2	2.40	0.50
1:B:103:PHE:HZ	1:B:226[B]:PHE:HD2	1.55	0.50
1:B:340:THR:HB	1:B:348:LEU:HD22	1.93	0.50
1:C:266[B]:LYS:HG3	8:C:2364:HOH:O	2.10	0.50
1:A:32[A]:TYR:CE1	1:A:38:LYS:HE3	2.46	0.50
1:A:211[A]:TYR:CD1	3:A:1001:U53:C9	2.95	0.49
1:A:86[B]:GLU:HG3	8:A:2181:HOH:O	2.12	0.49
1:A:257:LYS:HE2	8:A:2462:HOH:O	2.13	0.49
1:C:88:TYR:CE2	1:C:92[B]:THR:HG21	2.47	0.49
1:A:45:GLU:HG3	8:A:2042:HOH:O	2.12	0.49
1:C:262[A]:GLU:HG2	1:C:283:LYS:HE3	1.95	0.48
4:C:1411[A]:DMS:H22	8:C:2508:HOH:O	2.14	0.47
1:C:346:LYS:HE2	1:C:378:ASP:HB3	1.97	0.46
1:B:230:ASN:OD1	1:B:232:ARG:CG	2.64	0.46
1:A:32[B]:TYR:CE1	8:A:2008:HOH:O	2.69	0.45
1:C:262[A]:GLU:CG	1:C:283:LYS:HE3	2.47	0.45
1:A:240:LYS:HD3	8:A:2424:HOH:O	2.17	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:VAL:CG1	3:B:1001:U53:O	2.66	0.44
1:C:324:ASN:OD1	1:C:326:LYS:HG2	2.17	0.44
1:B:206[B]:VAL:HG12	1:B:400:PHE:CE1	2.53	0.43
1:A:340:THR:HB	1:A:348:LEU:HD22	2.00	0.42
1:A:39:ILE:HD12	1:A:201:TYR:HE2	1.84	0.42
1:A:96:VAL:CG1	3:A:1001:U53:O	2.65	0.42
1:A:127:ILE:HD11	1:A:185:ARG:HD2	2.01	0.42
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.79	0.42
1:C:39:ILE:HA	1:C:39:ILE:HD12	1.96	0.41
1:C:206[B]:VAL:CG1	1:C:400:PHE:CE1	3.03	0.41
1:B:243[B]:ARG:HB3	1:B:243[B]:ARG:HE	1.77	0.41
1:A:147[A]:ASP:OD1	1:A:156[A]:LYS:NZ	2.51	0.41
1:A:49:GLU:OE2	1:A:396:LYS:HE3	2.21	0.41
1:C:138:ILE:C	1:C:138:ILE:HD12	2.42	0.41
1:C:49:GLU:OE2	1:C:396[B]:LYS:HE2	2.21	0.41
1:C:49:GLU:OE2	1:C:396[B]:LYS:CE	2.69	0.41
1:C:360:ASN:ND2	8:C:2316:HOH:O	2.52	0.41
1:B:211[B]:TYR:CD1	3:B:1001:U53:C9	3.03	0.40
1:B:156:LYS:HZ3	1:B:156:LYS:HG3	1.55	0.40
1:A:156[A]:LYS:HE3	8:A:2143:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	1:A:258:LYS:NZ[4_556]	2.14	0.06

## 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	418/385 (109%)	410 (98%)	8 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	407/385 (106%)	397 (98%)	10 (2%)	0	100	100
1	C	396/385 (103%)	387 (98%)	9 (2%)	0	100	100
All	All	1221/1155 (106%)	1194 (98%)	27 (2%)	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	386/351 (110%)	377 (98%)	9 (2%)	58	24
1	B	374/351 (107%)	367 (98%)	7 (2%)	65	31
1	C	367/351 (105%)	356 (97%)	11 (3%)	48	15
All	All	1127/1053 (107%)	1100 (98%)	27 (2%)	63	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ILE
1	A	136	LYS
1	A	147[A]	ASP
1	A	147[B]	ASP
1	A	232[A]	ARG
1	A	232[B]	ARG
1	A	253[A]	MET
1	A	253[B]	MET
1	A	325	ASP
1	B	156	LYS
1	B	231	SER
1	B	232	ARG
1	B	253[A]	MET
1	B	253[B]	MET
1	B	396[A]	LYS
1	B	396[B]	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	27	ASP
1	C	58	GLU
1	C	99	ASP
1	C	102	ILE
1	C	137	LEU
1	C	243	ARG
1	C	244	VAL
1	C	257	LYS
1	C	326	LYS
1	C	377[A]	GLU
1	C	377[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	106	ASN
1	B	34	GLN
1	B	106	ASN
1	B	249	ASN
1	C	331	ASN
1	C	360	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 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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$
2	NHW	A	1000	5	57,66,66	1.53	7 (12%)	67,92,92	1.56	12 (17%)
3	U53	A	1001	-	23,23,23	1.89	6 (26%)	24,30,30	2.78	10 (41%)
4	DMS	A	1411	-	3,3,3	0.44	0	3,3,3	1.43	1 (33%)
6	SO4	A	1413	-	4,4,4	0.69	0	6,6,6	1.89	2 (33%)
6	SO4	A	1414	-	4,4,4	2.15	1 (25%)	6,6,6	0.82	0
2	NHW	B	1000	5	57,66,66	1.55	10 (17%)	67,92,92	1.74	9 (13%)
3	U53	B	1001	-	23,23,23	2.27	6 (26%)	24,30,30	2.88	10 (41%)
4	DMS	B	1411	-	3,3,3	0.47	0	3,3,3	1.07	0
2	NHW	C	1000	5	57,66,66	1.56	10 (17%)	67,92,92	1.75	10 (14%)
3	U53	C	1001	-	23,23,23	2.26	7 (30%)	24,30,30	2.48	9 (37%)
4	DMS	C	1411[A]	-	3,3,3	0.42	0	3,3,3	0.82	0
4	DMS	C	1411[B]	-	3,3,3	0.44	0	3,3,3	0.68	0
4	DMS	C	1412	-	3,3,3	0.66	0	3,3,3	1.09	0

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	NHW	A	1000	5	-	0/61/81/81	0/3/3/3
3	U53	A	1001	-	-	0/14/14/14	0/2/2/2
4	DMS	A	1411	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1413	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1414	-	-	0/0/0/0	0/0/0/0
2	NHW	B	1000	5	-	0/61/81/81	0/3/3/3
3	U53	B	1001	-	-	0/14/14/14	0/2/2/2
4	DMS	B	1411	-	-	0/0/0/0	0/0/0/0
2	NHW	C	1000	5	-	0/61/81/81	0/3/3/3
3	U53	C	1001	-	-	0/14/14/14	0/2/2/2
4	DMS	C	1411[A]	-	-	0/0/0/0	0/0/0/0
4	DMS	C	1411[B]	-	-	0/0/0/0	0/0/0/0
4	DMS	C	1412	-	-	0/0/0/0	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	U53	C6-S	-6.11	1.69	1.77
3	A	1001	U53	C6-S	-4.90	1.71	1.77
2	C	1000	NHW	P3X-O7A	-4.10	1.40	1.54
2	C	1000	NHW	C2X-C1X	-3.31	1.48	1.53
2	A	1000	NHW	P1A-O1A	-3.27	1.39	1.51
2	B	1000	NHW	C4A-N3A	-2.95	1.31	1.35
3	B	1001	U53	C6-S	-2.66	1.74	1.77
2	A	1000	NHW	P2A-O4A	-2.56	1.44	1.55
3	A	1001	U53	C15-C5	-2.51	1.37	1.42
2	C	1000	NHW	P1A-O2A	-2.25	1.45	1.55
2	B	1000	NHW	P1A-O1A	-2.16	1.43	1.51
2	B	1000	NHW	P3X-O8A	-2.14	1.47	1.54
2	B	1000	NHW	P2A-O4A	-2.06	1.46	1.55
3	C	1001	U53	C6-C5	2.10	1.46	1.43
2	A	1000	NHW	C13-C11	2.29	1.59	1.53
3	C	1001	U53	C3-C2	2.31	1.41	1.36
3	A	1001	U53	C10-C6	2.31	1.45	1.41
3	A	1001	U53	C6-C5	2.32	1.46	1.43
2	C	1000	NHW	C9-N8	2.37	1.38	1.33
2	C	1000	NHW	C2-S1	2.44	1.91	1.81
2	A	1000	NHW	C3-N4	2.45	1.51	1.46
2	B	1000	NHW	C13-C11	2.50	1.59	1.53
2	B	1000	NHW	C9-N8	2.52	1.38	1.33
2	B	1000	NHW	O4X-C1X	2.59	1.44	1.41
3	C	1001	U53	C2-C1	2.66	1.44	1.38
2	C	1000	NHW	O5-C5	2.82	1.29	1.23
3	A	1001	U53	C5-C4	2.84	1.46	1.42
2	B	1000	NHW	O10-C10	2.89	1.48	1.42
2	B	1000	NHW	O2X-C2X	2.91	1.49	1.43
2	C	1000	NHW	C2A-N3A	3.00	1.37	1.32
2	A	1000	NHW	O4X-C4X	3.07	1.52	1.45
3	C	1001	U53	C10-C6	3.11	1.46	1.41
2	C	1000	NHW	CP-S1	3.47	1.89	1.81
2	C	1000	NHW	O10-C10	3.57	1.49	1.42
6	A	1414	SO4	O2-S	3.70	1.60	1.47
3	B	1001	U53	C5-C4	3.73	1.48	1.42
3	C	1001	U53	C5-C4	3.92	1.48	1.42
3	B	1001	U53	C11-N1	3.93	1.38	1.31
2	A	1000	NHW	O4X-C1X	4.12	1.47	1.41
3	C	1001	U53	O1-C12	4.19	1.43	1.33
2	C	1000	NHW	CP-C1M	4.19	1.58	1.51
3	B	1001	U53	O1-C12	4.52	1.43	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	U53	O1-C12	4.56	1.43	1.33
3	B	1001	U53	C10-C6	4.80	1.49	1.41
3	B	1001	U53	C6-C5	5.08	1.50	1.43
2	B	1000	NHW	CP-S1	6.03	1.94	1.81
2	A	1000	NHW	CP-S1	6.34	1.95	1.81

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	NHW	N3A-C2A-N1A	-8.77	121.98	128.87
2	C	1000	NHW	N3A-C2A-N1A	-7.57	122.93	128.87
2	A	1000	NHW	C4X-O4X-C1X	-5.53	103.78	109.64
3	A	1001	U53	C2-C3-C4	-5.01	115.33	120.86
3	B	1001	U53	O1-C12-O2	-4.62	114.62	123.65
3	C	1001	U53	C10-C11-N1	-4.12	120.91	125.52
2	C	1000	NHW	C1X-N9A-C4A	-3.85	122.51	126.81
2	C	1000	NHW	C2-C3-N4	-3.80	104.80	112.43
3	C	1001	U53	C13-O1-C12	-3.78	108.20	116.46
3	A	1001	U53	O1-C12-O2	-3.70	116.42	123.65
3	C	1001	U53	C2-C3-C4	-3.62	116.86	120.86
2	A	1000	NHW	C13-C11-C12	-3.60	103.84	108.50
2	B	1000	NHW	C2-C3-N4	-3.54	105.31	112.43
2	A	1000	NHW	N3A-C2A-N1A	-3.52	126.11	128.87
3	B	1001	U53	C2-C3-C4	-3.43	117.07	120.86
2	B	1000	NHW	C13-C11-C12	-3.43	104.05	108.50
3	A	1001	U53	O-C1-C15	-3.37	116.32	124.57
2	A	1000	NHW	P3X-O3X-C3X	-3.31	113.08	121.56
2	A	1000	NHW	C2-C3-N4	-3.17	106.06	112.43
3	A	1001	U53	C5-C4-N1	-3.08	119.49	122.83
3	C	1001	U53	C1-C15-C5	-3.02	115.41	120.01
3	C	1001	U53	C5-C4-N1	-2.90	119.68	122.83
3	C	1001	U53	O-C1-C15	-2.67	118.03	124.57
3	B	1001	U53	C8-C7-S	-2.66	105.37	113.22
2	B	1000	NHW	C7-N8-C9	-2.60	117.42	122.62
3	B	1001	U53	O2-C12-C10	-2.59	112.94	121.57
2	B	1000	NHW	C4M-C3M-C2M	-2.57	103.78	113.30
2	C	1000	NHW	C6-C5-N4	-2.57	111.99	116.46
3	B	1001	U53	O-C1-C15	-2.56	118.29	124.57
2	C	1000	NHW	P3X-O3X-C3X	-2.54	115.06	121.56
3	A	1001	U53	C8-C7-S	-2.51	105.79	113.22
2	A	1000	NHW	C2X-C1X-N9A	-2.45	106.91	113.47
2	A	1000	NHW	C1X-N9A-C4A	-2.42	124.10	126.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	NHW	C6-C5-N4	-2.41	112.26	116.46
2	C	1000	NHW	O4X-C4X-C5X	-2.35	100.89	109.29
2	C	1000	NHW	C13-C11-C12	-2.32	105.49	108.50
2	A	1000	NHW	O1M-C1M-CP	-2.28	118.95	122.14
2	C	1000	NHW	C2X-C3X-C4X	-2.20	99.03	103.25
4	A	1411	DMS	O-S-C2	2.06	118.09	106.64
2	B	1000	NHW	N6A-C6A-N1A	2.07	121.98	118.52
3	B	1001	U53	C13-O1-C12	2.13	121.11	116.46
2	A	1000	NHW	O5-C5-C6	2.17	125.74	121.97
3	B	1001	U53	C6-C5-C4	2.20	120.31	117.55
2	A	1000	NHW	O8A-P3X-O7A	2.31	115.92	107.44
2	A	1000	NHW	C13-C11-C10	2.32	113.40	109.17
2	B	1000	NHW	C14-C11-C12	2.35	111.54	108.50
3	A	1001	U53	C15-C5-C4	2.38	121.99	118.93
3	B	1001	U53	C-O-C1	2.42	123.12	117.51
6	A	1413	SO4	O4-S-O3	2.55	119.36	109.09
2	B	1000	NHW	C13-C11-C10	2.59	113.90	109.17
3	A	1001	U53	C7-S-C6	2.62	111.39	102.44
3	B	1001	U53	C11-N1-C4	2.84	120.66	116.96
2	B	1000	NHW	C2A-N1A-C6A	2.87	123.89	118.77
3	A	1001	U53	C3-C2-C1	3.12	124.38	120.19
3	C	1001	U53	C15-C5-C4	3.25	123.12	118.93
2	C	1000	NHW	C3X-C2X-C1X	3.33	107.31	100.06
6	A	1413	SO4	O2-S-O1	3.46	121.16	109.59
3	A	1001	U53	C11-N1-C4	3.59	121.64	116.96
2	C	1000	NHW	C13-C11-C10	4.28	116.99	109.17
3	C	1001	U53	C-O-C1	4.89	128.82	117.51
3	C	1001	U53	C11-N1-C4	5.41	124.01	116.96
3	A	1001	U53	O1-C12-C10	8.16	127.22	112.17
3	B	1001	U53	O1-C12-C10	10.12	130.82	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	U53	3	0
3	B	1001	U53	5	0
3	C	1001	U53	9	0
4	C	1411[A]	DMS	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1411[B]	DMS	1	0
4	C	1412	DMS	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

### 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	385/385 (100%)	-0.47	7 (1%) 71 75	10, 15, 32, 60	16 (4%)
1	B	385/385 (100%)	-0.50	6 (1%) 74 78	10, 16, 33, 53	20 (5%)
1	C	370/385 (96%)	-0.47	6 (1%) 74 78	10, 15, 35, 60	12 (3%)
All	All	1140/1155 (98%)	-0.48	19 (1%) 73 76	10, 15, 33, 60	48 (4%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231[A]	SER	4.6
1	C	226	PHE	4.2
1	A	232[A]	ARG	4.1
1	C	325[A]	ASP	4.0
1	C	323	GLY	3.7
1	A	26	ILE	3.2
1	B	26	ILE	3.1
1	C	242	TYR	3.0
1	B	226[A]	PHE	2.9
1	A	386	GLY	2.8
1	A	226	PHE	2.8
1	A	32[A]	TYR	2.8
1	A	325	ASP	2.7
1	C	32[A]	TYR	2.7
1	B	102	ILE	2.7
1	B	103	PHE	2.5
1	B	27	ASP	2.5
1	C	99	ASP	2.2
1	B	232	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
6	SO4	A	1414	5/5	0.68	0.26	17.55	33,42,69,79	0
4	DMS	C	1411[B]	4/4	0.71	0.24	9.80	37,44,49,59	4
4	DMS	C	1411[A]	4/4	0.71	0.24	9.27	37,46,53,57	4
4	DMS	C	1412	4/4	0.93	0.21	6.78	27,29,30,31	0
6	SO4	A	1413	5/5	0.95	0.15	6.50	44,46,50,56	0
3	U53	C	1001	22/22	0.64	0.39	6.17	15,27,31,33	22
4	DMS	B	1411	4/4	0.95	0.14	4.17	28,28,31,32	0
3	U53	A	1001	22/22	0.67	0.24	3.68	17,22,27,31	22
3	U53	B	1001	22/22	0.77	0.20	2.40	17,22,25,29	22
4	DMS	A	1411	4/4	0.95	0.11	2.28	22,26,29,30	0
5	MG	B	1412	1/1	0.99	0.06	0.31	22,22,22,22	0
2	NHW	B	1000	64/64	0.98	0.06	-0.29	9,14,17,19	0
2	NHW	A	1000	64/64	0.98	0.06	-0.37	9,13,16,19	0
2	NHW	C	1000	64/64	0.98	0.06	-0.56	9,13,16,21	0
5	MG	C	1413	1/1	1.00	0.04	-1.93	21,21,21,21	0
7	CL	A	1415	1/1	1.00	0.05	-2.21	14,14,14,14	0
5	MG	A	1412	1/1	0.99	0.04	-2.44	23,23,23,23	0
7	CL	B	1413	1/1	1.00	0.05	-3.43	15,15,15,15	0
7	CL	C	1414	1/1	1.00	0.04	-5.05	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.