



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2017 – 04:56 PM EST

PDB ID : 5FUK  
Title : Crystallization of a dimeric heme peroxxygenase from the fungus *Marasmius rotula*  
Authors : Piontek, K.; Strittmatter, E.; Plattner, D.A.  
Deposited on : 2016-01-27  
Resolution : 1.55 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	:	1.7.1 (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

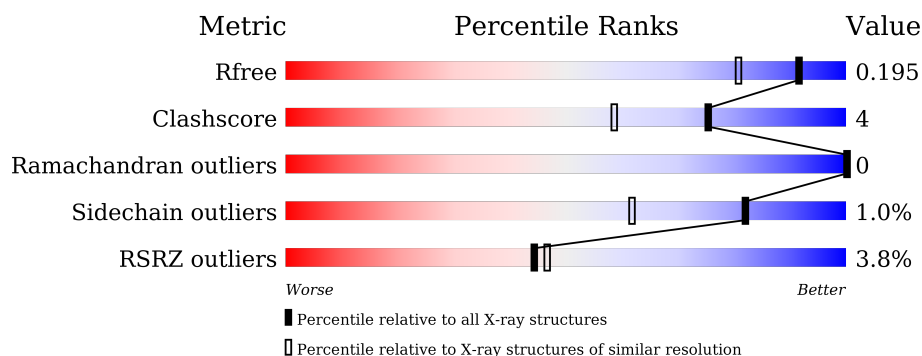
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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	234	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	234	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>6%</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
10	PO4	B	1247	-	-	-	X
3	SNP	A	1236[A]	-	-	-	X
4	PLM	A	1237[B]	-	-	X	X
4	PLM	B	1237[B]	-	-	X	X
5	RNP	A	1238[C]	-	-	-	X
5	RNP	B	1238[C]	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4624 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 MROUPO.

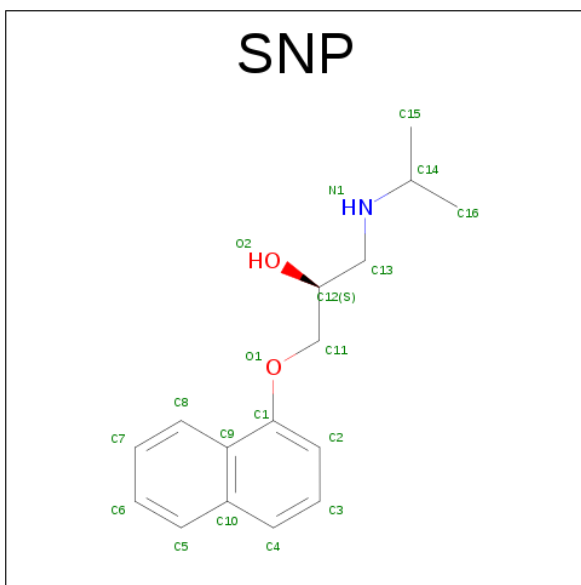
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	2	0
			1798	1130	317	345	6			
1	B	234	Total	C	N	O	S	0	5	0
			1817	1142	322	347	6			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



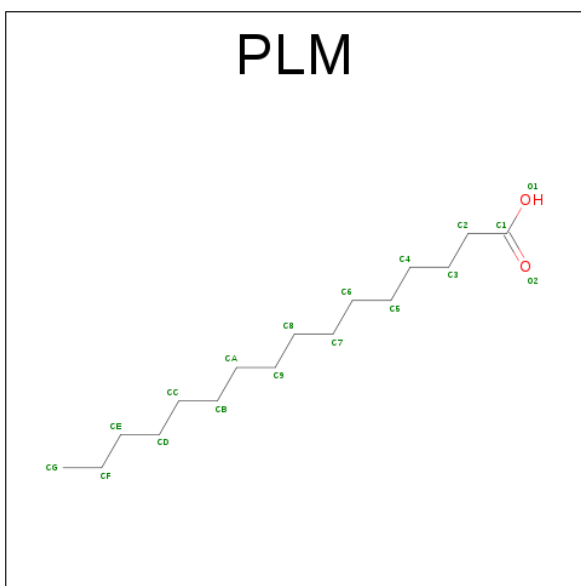
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-(ISOPROPYLAMINO)-3-(1-NAPHTHYLOXY)-2-PROPANOL (three-letter code: SNP) (formula:  $C_{16}H_{21}NO_2$ ).



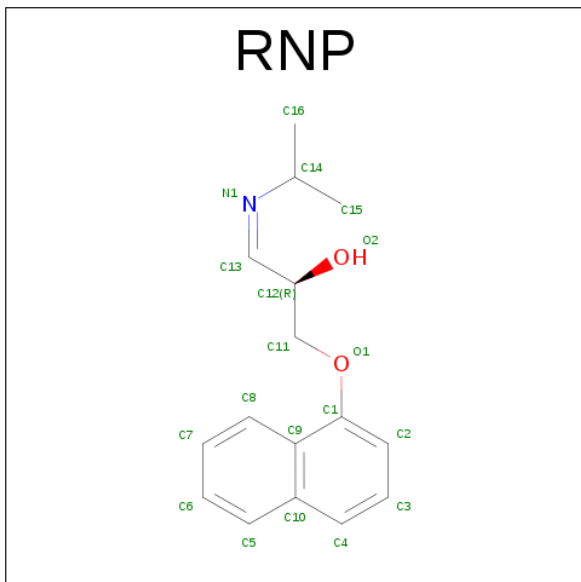
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			19	16	1	2		
3	B	1	Total	C	N	O	0	1
			19	16	1	2		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			18	16	2		
4	B	1	Total	C	O	0	1
			18	16	2		

- Molecule 5 is (1E,2R)-1-(ISOPROPYLIMINO)-3-(1-NAPHTHYLOXY)PROPAN-2-OL (three-letter code: RNP) (formula: C<sub>16</sub>H<sub>19</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			19	16	1	2		
5	B	1	Total	C	N	O	0	1
			19	16	1	2		

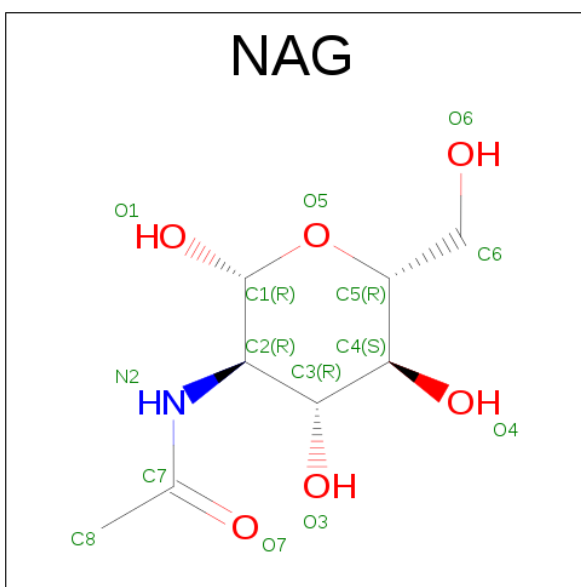
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

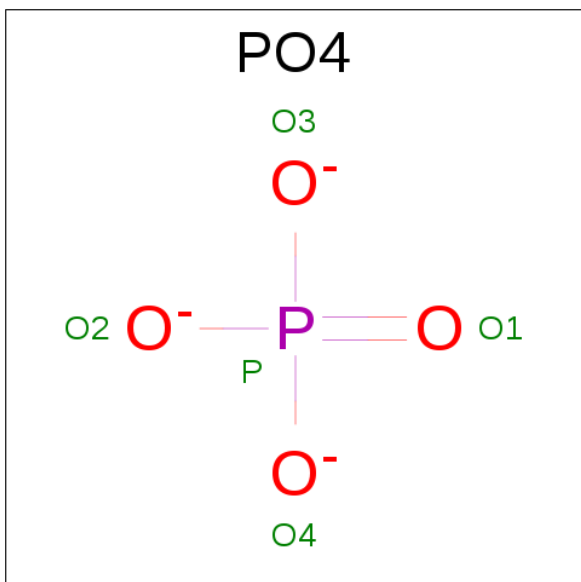


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is water.

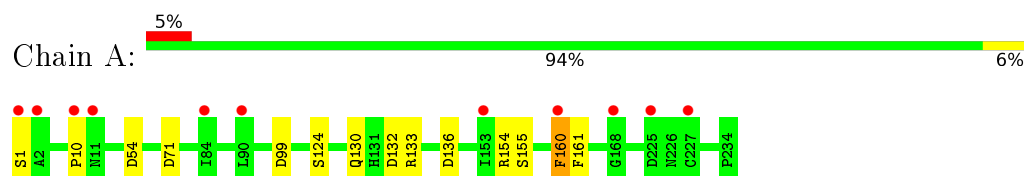
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	333	Total	O	0	0
			333	333		
11	B	310	Total	O	0	0
			310	310		



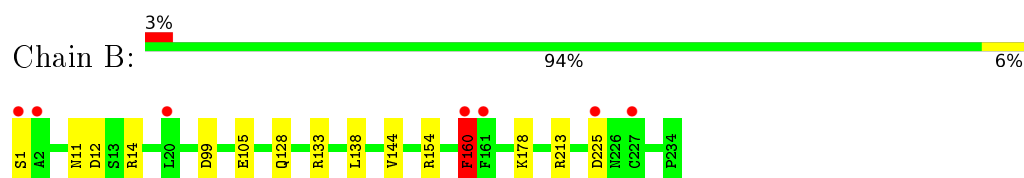
### 3 Residue-property plots [i](#)

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: MROUPO



#### ● Molecule 1: MROUPO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.01Å 76.67Å 120.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.36 – 1.55 29.12 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.36-1.55) 98.3 (29.12-1.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.155 , 0.183 0.168 , 0.195	Depositor DCC
$R_{free}$ test set	3999 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.1	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	4624	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, BMA, NAG, PO4, SNP, HEM, PLM, RNP, MAN

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	0.98	1/1842 (0.1%)	0.97	7/2507 (0.3%)
1	B	1.09	1/1869 (0.1%)	1.05	10/2542 (0.4%)
All	All	1.04	2/3711 (0.1%)	1.01	17/5049 (0.3%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	SER	CB-OG	-5.86	1.34	1.42
1	B	105	GLU	CG-CD	5.18	1.59	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	B	213	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	99	ASP	CB-CG-OD1	7.15	124.73	118.30
1	B	213	ARG	CG-CD-NE	-6.90	97.31	111.80
1	B	133	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	B	99	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	71	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	132	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	154	ARG	NE-CZ-NH2	-5.47	117.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	136	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	54	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	160[A]	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	B	160[B]	PHE	CB-CG-CD2	-5.28	117.10	120.80
1	B	225	ASP	CB-CA-C	-5.08	100.25	110.40
1	B	154	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	133	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	SER	Peptide

## 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	1798	0	1777	6	0
1	B	1817	0	1809	12	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	19	0	21	4	0
3	B	19	0	21	0	0
4	A	18	0	31	9	0
4	B	18	0	31	9	0
5	A	19	0	19	1	0
5	B	19	0	19	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	61	0	52	0	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
9	B	72	0	61	0	0
10	B	5	0	0	0	0
11	A	333	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	310	0	0	5	0
All	All	4624	0	3927	31	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 4.

All (31) 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:160[B]:PHE:CE2	4:B:1237[B]:PLM:H22	1.41	1.52
1:B:160[B]:PHE:HE2	4:B:1237[B]:PLM:C2	1.46	1.28
1:B:160[B]:PHE:CE2	4:B:1237[B]:PLM:C2	2.24	1.16
1:A:160[B]:PHE:HE2	4:A:1237[B]:PLM:H21	1.16	1.08
1:A:160[B]:PHE:CE2	4:A:1237[B]:PLM:H21	1.87	1.08
4:A:1237[B]:PLM:H82	4:A:1237[B]:PLM:HD1	1.34	1.06
3:A:1236[A]:SNP:H161	3:A:1236[A]:SNP:O2	1.71	0.89
5:B:1238[C]:RNP:H161	11:B:2269:HOH:O	1.73	0.88
1:A:160[B]:PHE:HE2	4:A:1237[B]:PLM:C2	1.86	0.88
4:A:1237[B]:PLM:H82	4:A:1237[B]:PLM:CD	2.14	0.75
4:A:1237[B]:PLM:C8	4:A:1237[B]:PLM:HD1	2.18	0.71
1:A:130:GLN:HE22	1:A:155:SER:HA	1.62	0.64
1:B:11:ASN:C	11:B:2014:HOH:O	2.36	0.64
4:A:1237[B]:PLM:C8	4:A:1237[B]:PLM:CD	2.78	0.62
1:B:160[B]:PHE:HE2	4:B:1237[B]:PLM:H22	0.56	0.61
1:B:160[B]:PHE:CE2	4:B:1237[B]:PLM:H21	2.33	0.60
1:B:160[B]:PHE:CZ	4:B:1237[B]:PLM:H22	2.25	0.60
1:A:160[B]:PHE:CZ	4:A:1237[B]:PLM:H21	2.37	0.58
1:B:128[B]:GLN:OE1	11:B:2174:HOH:O	2.18	0.56
1:A:10[A]:PRO:HD2	11:A:2015:HOH:O	2.05	0.56
1:B:178:LYS:HE2	11:B:2236:HOH:O	2.08	0.54
1:B:12:ASP:N	11:B:2014:HOH:O	2.43	0.52
3:A:1236[A]:SNP:C16	3:A:1236[A]:SNP:O2	2.52	0.49
4:A:1237[B]:PLM:H61	4:A:1237[B]:PLM:HE2	1.95	0.48
11:A:2322:HOH:O	4:B:1237[B]:PLM:HA2	2.14	0.47
4:B:1237[B]:PLM:HE2	4:B:1237[B]:PLM:HB2	1.73	0.46
3:A:1236[A]:SNP:H161	3:A:1236[A]:SNP:H2O1	1.79	0.44
1:B:160[B]:PHE:CZ	4:B:1237[B]:PLM:C2	2.95	0.44
1:B:138:LEU:HD23	1:B:144:VAL:HG11	2.00	0.43
5:A:1238[C]:RNP:H13	5:A:1238[C]:RNP:H162	1.73	0.41
3:A:1236[A]:SNP:O2	11:A:2323:HOH:O	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/234 (100%)	229 (98%)	5 (2%)	0	100	100
1	B	237/234 (101%)	233 (98%)	4 (2%)	0	100	100
All	All	471/468 (101%)	462 (98%)	9 (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	A	198/196 (101%)	194 (98%)	4 (2%)	63	31
1	B	201/196 (103%)	199 (99%)	2 (1%)	82	62
All	All	399/392 (102%)	393 (98%)	6 (2%)	82	44

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	160[A]	PHE
1	A	160[B]	PHE
1	A	161	PHE
1	B	160[A]	PHE

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Mol	Chain	Res	Type
1	B	160[B]	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	130	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

11 carbohydrates 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	$\# Z  > 2$
7	NAG	A	1240	1,7	14,14,15	1.74	2 (14%)	15,19,21	1.20	1 (6%)
7	NAG	A	1241	7	14,14,15	0.79	0	15,19,21	1.84	3 (20%)
7	BMA	A	1242	7	11,11,12	0.60	0	15,15,17	1.51	3 (20%)
7	MAN	A	1243	7	11,11,12	0.85	0	15,15,17	1.83	2 (13%)
7	MAN	A	1244	7	11,11,12	0.76	0	15,15,17	1.02	1 (6%)
9	NAG	B	1241	1,9	14,14,15	1.65	3 (21%)	15,19,21	1.76	4 (26%)
9	NAG	B	1242	9	14,14,15	0.68	0	15,19,21	1.63	2 (13%)
9	BMA	B	1243	9	11,11,12	0.74	0	15,15,17	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	B	1244	9	11,11,12	0.86	0	15,15,17	1.02	1 (6%)
9	MAN	B	1245	9	11,11,12	0.94	1 (9%)	15,15,17	1.55	4 (26%)
9	MAN	B	1246	9	11,11,12	0.61	0	15,15,17	1.27	2 (13%)

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
7	NAG	A	1240	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1241	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1242	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1243	7	-	0/2/19/22	0/1/1/1
7	MAN	A	1244	7	-	0/2/19/22	0/1/1/1
9	NAG	B	1241	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	1242	9	-	0/6/23/26	0/1/1/1
9	BMA	B	1243	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1244	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1245	9	-	0/2/19/22	0/1/1/1
9	MAN	B	1246	9	-	0/2/19/22	1/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1240	NAG	O5-C1	-2.67	1.39	1.43
9	B	1241	NAG	O5-C5	-2.07	1.38	1.43
9	B	1245	MAN	C4-C5	2.33	1.58	1.53
9	B	1241	NAG	O5-C1	2.82	1.48	1.43
9	B	1241	NAG	C1-C2	4.39	1.58	1.52
7	A	1240	NAG	C1-C2	5.35	1.60	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1241	NAG	C2-N2-C7	-3.73	118.25	123.11
7	A	1242	BMA	O2-C2-C1	-3.68	101.86	109.23
9	B	1241	NAG	C1-O5-C5	-3.61	106.83	112.14
7	A	1241	NAG	O6-C6-C5	-3.42	99.88	111.30
9	B	1241	NAG	C3-C4-C5	-3.35	104.25	110.23
9	B	1242	NAG	O5-C5-C4	-2.88	105.36	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1243	MAN	O4-C4-C3	-2.87	103.89	110.36
7	A	1240	NAG	C4-C3-C2	-2.81	106.97	111.34
9	B	1241	NAG	C6-C5-C4	-2.72	106.18	112.99
7	A	1242	BMA	O3-C3-C4	-2.62	104.44	110.36
9	B	1242	NAG	O3-C3-C2	-2.61	103.78	109.37
7	A	1242	BMA	O5-C5-C4	-2.60	105.82	110.13
9	B	1241	NAG	O4-C4-C3	-2.56	104.58	110.36
9	B	1246	MAN	C2-C3-C4	-2.49	106.71	111.05
9	B	1243	BMA	O3-C3-C4	-2.06	105.71	110.36
9	B	1244	MAN	C1-O5-C5	2.08	115.20	112.14
9	B	1246	MAN	O5-C5-C6	2.12	111.89	107.34
9	B	1245	MAN	C1-C2-C3	2.32	112.37	109.55
9	B	1245	MAN	C1-O5-C5	2.36	115.61	112.14
9	B	1245	MAN	C6-C5-C4	2.48	119.21	112.99
7	A	1244	MAN	C1-O5-C5	2.58	115.93	112.14
7	A	1241	NAG	O5-C5-C4	2.79	114.75	110.13
9	B	1245	MAN	O3-C3-C4	2.81	116.69	110.36
7	A	1243	MAN	C1-O5-C5	4.61	118.92	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1246	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 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
2	HEM	A	1235	1,6	24,50,50	1.32	3 (12%)	16,82,82	1.68	3 (18%)
3	SNP	A	1236[A]	-	20,20,20	1.10	1 (5%)	24,26,26	0.82	0
4	PLM	A	1237[B]	-	14,17,17	0.26	0	14,17,17	0.86	0
5	RNP	A	1238[C]	-	17,20,20	1.29	2 (11%)	22,26,26	1.32	2 (9%)
8	NAG	A	1245	1	14,14,15	0.54	0	15,19,21	2.09	3 (20%)
2	HEM	B	1235	1,6	24,50,50	1.03	1 (4%)	16,82,82	1.58	4 (25%)
3	SNP	B	1236[A]	-	20,20,20	1.22	2 (10%)	24,26,26	0.81	1 (4%)
4	PLM	B	1237[B]	-	14,17,17	0.36	0	14,17,17	0.55	0
5	RNP	B	1238[C]	-	17,20,20	1.29	2 (11%)	22,26,26	1.83	6 (27%)
8	NAG	B	1240	1	14,14,15	0.93	0	15,19,21	1.33	2 (13%)
10	PO4	B	1247	-	4,4,4	0.82	0	6,6,6	0.27	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	HEM	A	1235	1,6	-	0/6/54/54	0/0/8/8
3	SNP	A	1236[A]	-	-	0/10/10/10	0/2/2/2
4	PLM	A	1237[B]	-	-	0/13/15/15	0/0/0/0
5	RNP	A	1238[C]	-	-	0/8/10/10	0/2/2/2
8	NAG	A	1245	1	-	0/6/23/26	0/1/1/1
2	HEM	B	1235	1,6	-	0/6/54/54	0/0/8/8
3	SNP	B	1236[A]	-	-	0/10/10/10	0/2/2/2
4	PLM	B	1237[B]	-	-	0/13/15/15	0/0/0/0
5	RNP	B	1238[C]	-	-	0/8/10/10	0/2/2/2
8	NAG	B	1240	1	-	0/6/23/26	0/1/1/1
10	PO4	B	1247	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1235	HEM	C3B-C2B	-3.48	1.35	1.40
2	A	1235	HEM	C3C-C2C	-3.26	1.36	1.40
2	B	1235	HEM	C3C-C2C	-2.81	1.36	1.40
2	A	1235	HEM	CMB-C2B	2.00	1.56	1.51
5	A	1238[C]	RNP	C1-C9	2.11	1.48	1.42
3	B	1236[A]	SNP	C1-C9	2.23	1.48	1.42
5	B	1238[C]	RNP	C1-C9	2.50	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1236[A]	SNP	C9-C10	2.57	1.47	1.43
5	A	1238[C]	RNP	C9-C10	2.67	1.47	1.43
5	B	1238[C]	RNP	C9-C10	2.76	1.48	1.43
3	B	1236[A]	SNP	C9-C10	3.06	1.48	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1235	HEM	C3B-CAB-CBB	-3.93	118.50	126.40
5	B	1238[C]	RNP	C16-C14-N1	-3.72	105.02	109.12
8	A	1245	NAG	C2-N2-C7	-2.74	119.53	123.11
2	B	1235	HEM	C3C-CAC-CBC	-2.66	121.05	126.40
2	A	1235	HEM	CMA-C3A-C4A	-2.66	123.80	128.31
2	A	1235	HEM	C3B-CAB-CBB	-2.59	121.19	126.40
2	B	1235	HEM	CAD-CBD-CGD	-2.41	108.10	112.78
5	B	1238[C]	RNP	C16-C14-C15	2.04	115.54	111.15
3	B	1236[A]	SNP	O1-C1-C9	2.10	120.73	114.94
5	A	1238[C]	RNP	C14-N1-C13	2.12	119.88	117.89
5	B	1238[C]	RNP	C11-O1-C1	2.14	125.41	118.25
5	B	1238[C]	RNP	O1-C1-C9	2.24	121.12	114.94
2	B	1235	HEM	CMB-C2B-C3B	2.49	129.96	125.09
8	B	1240	NAG	C4-C3-C2	2.61	115.39	111.34
8	B	1240	NAG	C8-C7-N2	2.91	121.67	116.10
8	A	1245	NAG	O5-C5-C4	3.07	115.22	110.13
5	B	1238[C]	RNP	C15-C14-N1	3.10	112.54	109.12
2	A	1235	HEM	CMC-C2C-C3C	3.11	131.18	125.09
5	A	1238[C]	RNP	C15-C14-N1	3.50	112.97	109.12
5	B	1238[C]	RNP	C14-N1-C13	4.85	122.45	117.89
8	A	1245	NAG	C1-O5-C5	6.03	121.01	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1236[A]	SNP	4	0
4	A	1237[B]	PLM	9	0
5	A	1238[C]	RNP	1	0
4	B	1237[B]	PLM	9	0
5	B	1238[C]	RNP	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	234/234 (100%)	0.09	11 (4%) 35 36	15, 20, 36, 70	0
1	B	234/234 (100%)	0.09	7 (2%) 54 58	14, 19, 33, 67	0
All	All	468/468 (100%)	0.09	18 (3%) 44 47	14, 19, 35, 70	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	6.1
1	B	1	SER	5.4
1	B	160[A]	PHE	4.7
1	B	225	ASP	4.5
1	A	225	ASP	4.1
1	A	160[A]	PHE	3.9
1	B	227	CYS	3.6
1	A	10[A]	PRO	3.3
1	A	227	CYS	3.2
1	B	2	ALA	3.1
1	B	20	LEU	3.1
1	A	2	ALA	3.0
1	A	168	GLY	2.9
1	B	161	PHE	2.4
1	A	11	ASN	2.4
1	A	84	ILE	2.2
1	A	90	LEU	2.2
1	A	153	ILE	2.1

### 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 ⓘ

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
9	NAG	B	1241	14/15	0.92	0.08	-0.64	16,19,23,25	0
7	NAG	A	1240	14/15	0.95	0.07	-0.77	19,22,25,27	0
7	NAG	A	1241	14/15	0.91	0.17	-	27,32,47,49	0
9	MAN	B	1244	11/12	0.85	0.28	-	42,47,53,57	0
9	BMA	B	1243	11/12	0.94	0.17	-	33,37,45,49	0
9	NAG	B	1242	14/15	0.93	0.18	-	25,30,35,43	0
9	MAN	B	1245	11/12	0.76	0.31	-	42,51,56,71	0
7	MAN	A	1243	11/12	0.71	0.25	-	37,41,46,56	0
7	MAN	A	1244	11/12	0.56	0.35	-	62,66,68,68	0
9	MAN	B	1246	11/12	0.55	0.45	-	83,94,100,101	0
7	BMA	A	1242	11/12	0.90	0.20	-	31,34,43,46	0

### 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
4	PLM	A	1237[B]	18/18	0.57	0.38	6.01	9,29,36,36	18
4	PLM	B	1237[B]	18/18	0.51	0.37	4.91	8,24,29,30	18
5	RNP	B	1238[C]	19/19	0.83	0.30	4.49	27,30,35,35	19
5	RNP	A	1238[C]	19/19	0.85	0.25	3.86	29,35,41,43	19
10	PO4	B	1247	5/5	0.92	0.21	2.86	35,35,43,44	0
3	SNP	A	1236[A]	19/19	0.87	0.20	2.21	33,36,44,45	19
3	SNP	B	1236[A]	19/19	0.88	0.20	1.48	50,52,56,56	19
2	HEM	A	1235	43/43	0.99	0.14	0.83	13,14,17,22	0
6	MG	A	1239	1/1	1.00	0.10	0.73	14,14,14,14	0
2	HEM	B	1235	43/43	0.99	0.13	0.33	11,13,15,20	0
6	MG	B	1239	1/1	0.99	0.08	-0.19	15,15,15,15	0
8	NAG	B	1240	14/15	0.64	0.35	-	55,68,75,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	A	1245	14/15	0.76	0.42	-	57,67,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.