



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:55 PM GMT

PDB ID : 4DL1  
Title : Crystal Structure of human Myeloperoxidase with covalent thioxanthine analog  
Authors : Vajdos, F.; Varghese, A.  
Deposited on : 2012-02-05  
Resolution : 2.00 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](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

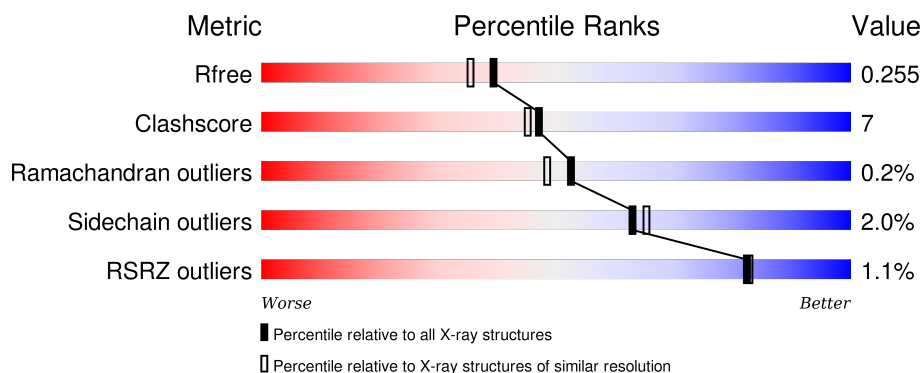
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	104	<div> <div>91%</div> <div>9%</div> </div>
1	B	104	<div> <div>83%</div> <div>17%</div> </div>
1	E	104	<div> <div>81%</div> <div>19%</div> </div>
1	F	104	<div> <div>78%</div> <div>21%</div> </div>
1	I	104	<div> <div>83%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	104	
1	M	104	
1	N	104	
2	C	466	
2	D	466	
2	G	466	
2	H	466	
2	K	466	
2	L	466	
2	O	466	
2	P	466	

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
4	0KY	A	1602	-	-	-	X
4	0KY	B	203	-	-	-	X
4	0KY	G	610	-	-	-	X
4	0KY	H	610	-	-	-	X
4	0KY	I	1603	-	-	-	X
4	0KY	J	203	-	-	-	X
4	0KY	O	610	-	-	-	X
4	0KY	P	614	-	-	-	X
7	NAG	C	609	-	-	-	X
7	NAG	K	608	-	-	-	X
7	NAG	O	608	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 40392 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 Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	E	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	F	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	I	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	J	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	M	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	N	104	Total	C	N	O	S	0	1	0
			841	531	148	157	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	465	Total	C	N	O	S	0	1	0
			3726	2348	686	665	27			
2	D	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	G	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			
2	H	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	K	465	Total	C	N	O	S	0	0	0
			3727	2348	686	666	27			
2	L	466	Total	C	N	O	S	0	0	0
			3730	2350	686	667	27			

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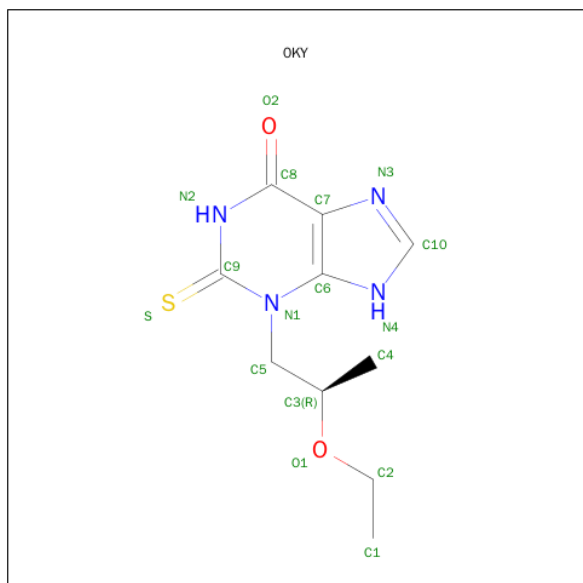
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	466	Total	C	N	O	S	0	0	0
			3729	2349	687	666	27			
2	P	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

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

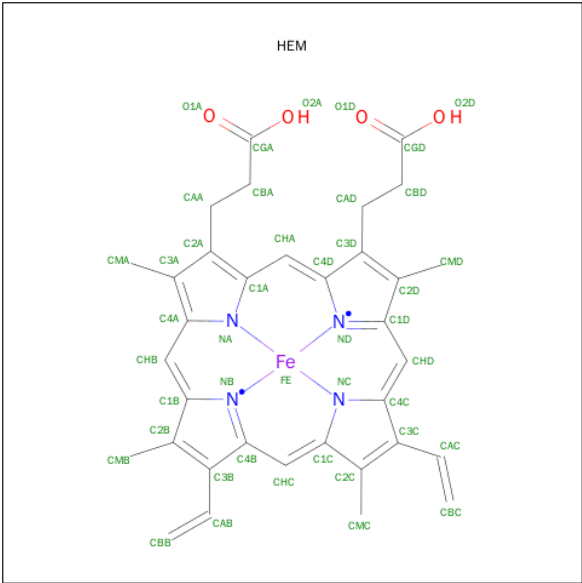
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	N	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	M	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 3-[(2R)-2-ETHOXYPROPYL]-2-THIOXO-1,2,3,9-TETRAHYDRO-6H-PURIN-6-ONE (three-letter code: OKY) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	B	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	G	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	H	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	I	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	J	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	O	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
4	P	1	Total	C	N	O	S	0	0
			17	10	4	2	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

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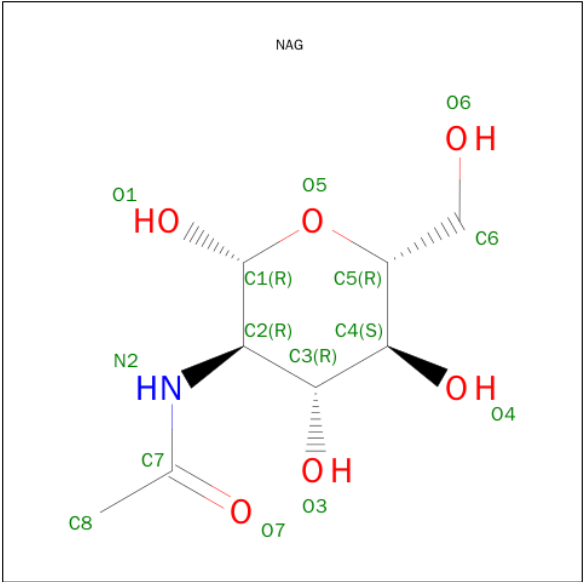
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	J	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	M	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	6	Total 71	C 40	N 2	O 29	0	0
6	D	6	Total 71	C 40	N 2	O 29	0	0
6	G	6	Total 71	C 40	N 2	O 29	0	0
6	H	6	Total 71	C 40	N 2	O 29	0	0
6	K	6	Total 71	C 40	N 2	O 29	0	0
6	L	6	Total 71	C 40	N 2	O 29	0	0
6	O	6	Total 71	C 40	N 2	O 29	0	0
6	P	6	Total 71	C 40	N 2	O 29	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	K	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		
7	O	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	P	1	Total	Ca	0	0
			1	1		
8	G	1	Total	Ca	0	0
			1	1		
8	D	1	Total	Ca	0	0
			1	1		
8	K	1	Total	Ca	0	0
			1	1		
8	H	1	Total	Ca	0	0
			1	1		
8	C	1	Total	Ca	0	0
			1	1		
8	O	1	Total	Ca	0	0
			1	1		
8	L	1	Total	Ca	0	0
			1	1		

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	85	Total	O	0	0
			85	85		
10	C	337	Total	O	0	0
			337	337		
10	B	76	Total	O	0	0
			76	76		
10	D	268	Total	O	0	0
			268	268		
10	E	63	Total	O	0	0
			63	63		

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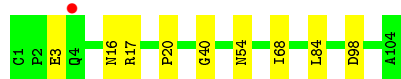
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	245	Total 245	O 245	0	0
10	F	73	Total 73	O 73	0	0
10	H	196	Total 196	O 196	0	0
10	I	75	Total 75	O 75	0	0
10	K	212	Total 212	O 212	0	0
10	J	69	Total 69	O 69	0	0
10	L	250	Total 250	O 250	0	0
10	M	68	Total 68	O 68	0	0
10	O	225	Total 225	O 225	0	0
10	N	61	Total 61	O 61	0	0
10	P	217	Total 217	O 217	0	0

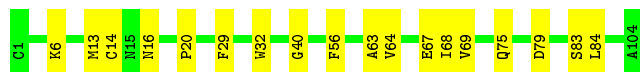
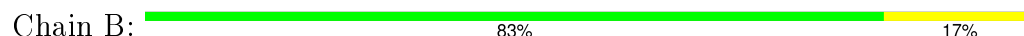
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

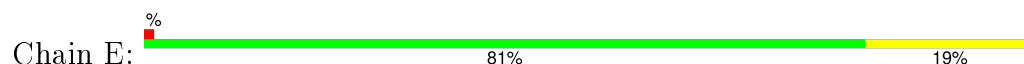
- Molecule 1: Myeloperoxidase light chain



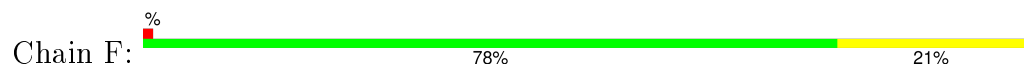
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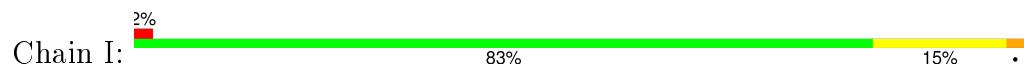
- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain

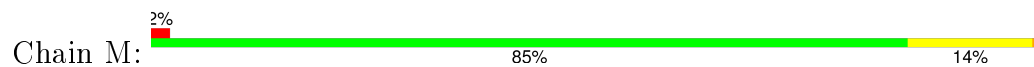


- Molecule 1: Myeloperoxidase light chain

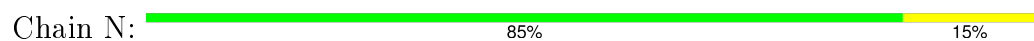




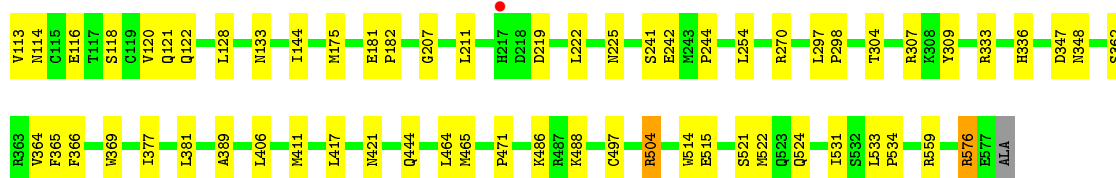
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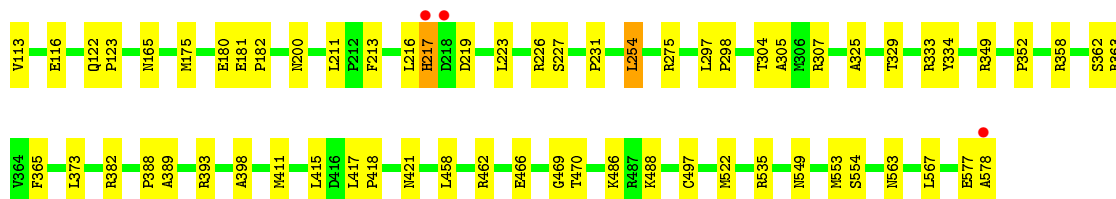
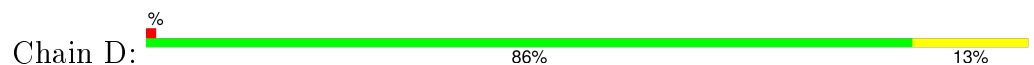
- Molecule 1: Myeloperoxidase light chain



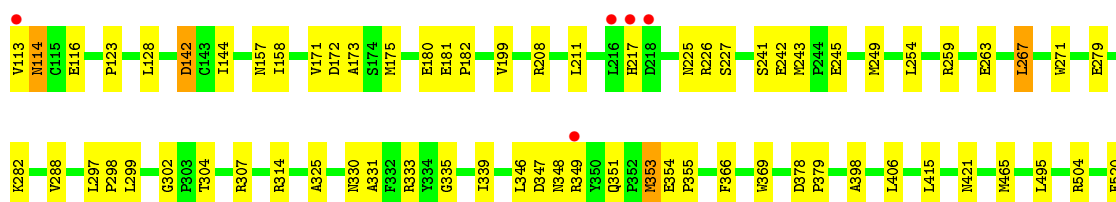
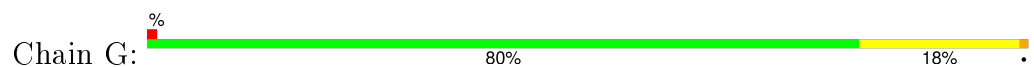
- Molecule 2: Myeloperoxidase heavy chain

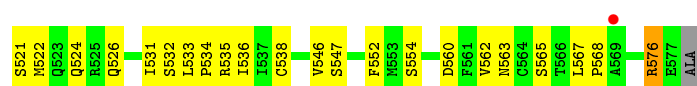


- Molecule 2: Myeloperoxidase heavy chain

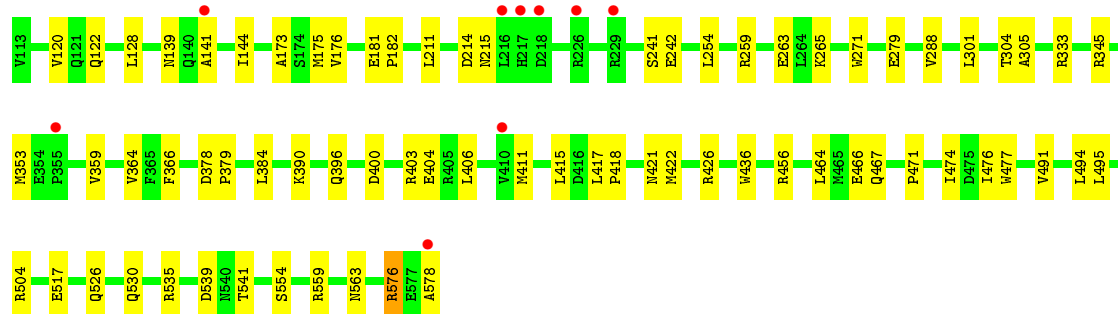
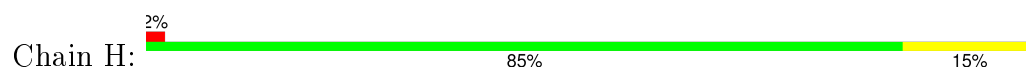


- Molecule 2: Myeloperoxidase heavy chain

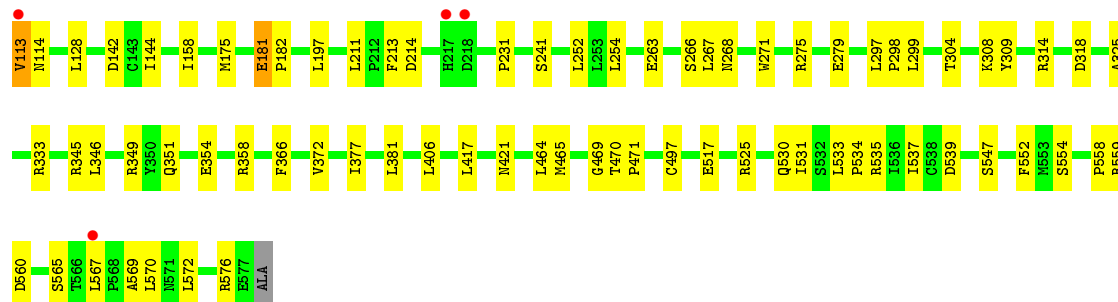
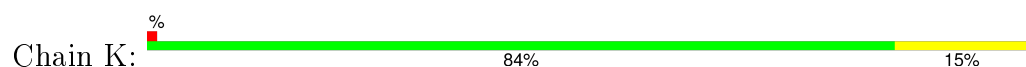




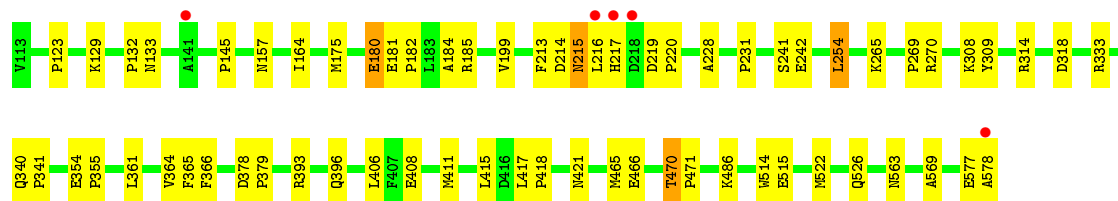
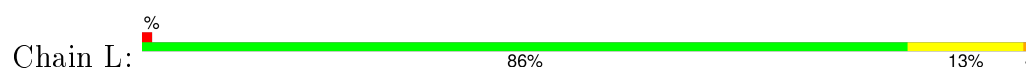
• Molecule 2: Myeloperoxidase heavy chain



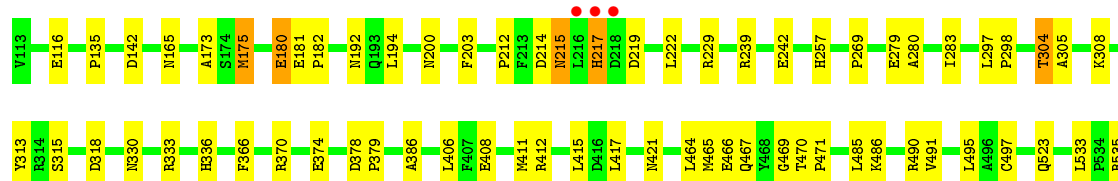
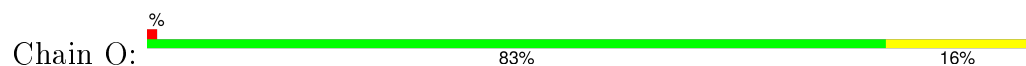
• Molecule 2: Myeloperoxidase heavy chain



• Molecule 2: Myeloperoxidase heavy chain

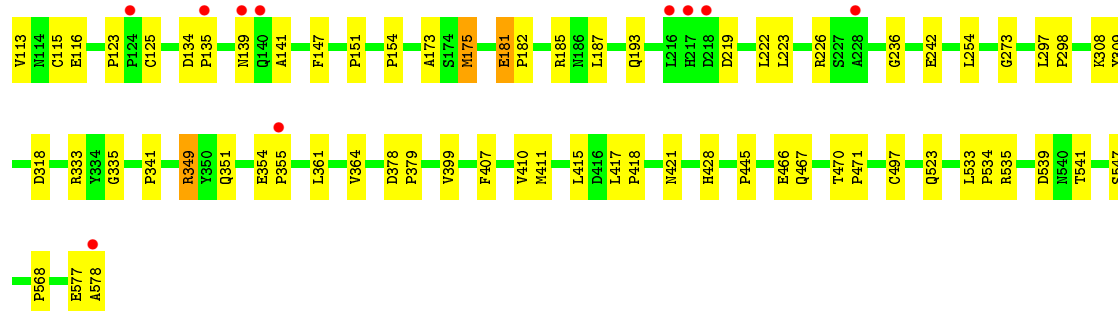
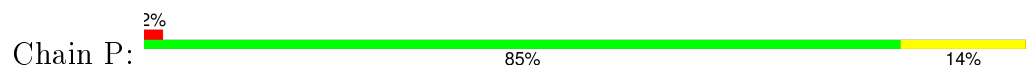


• Molecule 2: Myeloperoxidase heavy chain





● Molecule 2: Myeloperoxidase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.83Å 242.64Å 151.50Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	128.49 – 2.00 128.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (128.49-2.00) 97.6 (128.49-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.190 , 0.246 0.205 , 0.255	Depositor DCC
$R_{free}$ test set	15173 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 25.6	EDS
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 301498 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	40392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.87 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.5328e-03.*

<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: CSO, BMA, NAG, CL, CA, OKY, FUC, HEM, 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	0.58	0/863	0.69	0/1174
1	B	0.53	0/863	0.61	0/1174
1	E	0.58	0/863	0.63	0/1174
1	F	0.47	0/863	0.59	0/1174
1	I	0.52	0/863	0.61	0/1174
1	J	0.49	0/863	0.59	0/1174
1	M	0.47	0/863	0.58	0/1174
1	N	0.47	0/869	0.57	0/1183
2	C	0.58	0/3807	0.61	0/5164
2	D	0.51	0/3807	0.57	0/5163
2	G	0.51	0/3805	0.58	0/5161
2	H	0.44	0/3807	0.53	0/5163
2	K	0.48	0/3805	0.55	0/5161
2	L	0.48	0/3808	0.56	1/5164 (0.0%)
2	O	0.45	0/3807	0.54	0/5163
2	P	0.45	0/3811	0.52	0/5168
All	All	0.50	0/37367	0.57	1/50708 (0.0%)

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	I	0	1
2	D	0	1
2	G	0	2
2	K	0	1
2	L	0	1
2	O	0	3
All	All	0	9



There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	318	ASP	CB-CG-OD1	5.26	123.03	118.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	180	GLU	Peptide
2	G	180	GLU	Peptide
2	G	302	GLY	Peptide
1	I	2	PRO	Peptide
2	K	547	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	838	0	798	9	0
1	B	838	0	798	18	0
1	E	838	0	798	16	0
1	F	838	0	798	27	0
1	I	838	0	798	18	0
1	J	838	0	798	5	0
1	M	838	0	798	11	0
1	N	841	0	803	11	0
2	C	3726	0	3721	63	0
2	D	3729	0	3721	45	0
2	G	3727	0	3720	67	2
2	H	3729	0	3721	70	0
2	K	3727	0	3720	48	0
2	L	3730	0	3721	47	0
2	O	3729	0	3721	63	0
2	P	3733	0	3725	56	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	17	0	14	3	0
4	B	17	0	14	4	0
4	G	17	0	14	1	0
4	H	17	0	14	5	0
4	I	17	0	14	2	0
4	J	17	0	14	1	0
4	O	17	0	14	5	0
4	P	17	0	14	4	0
5	B	43	0	30	5	0
5	C	43	0	30	6	0
5	E	43	0	30	6	0
5	F	43	0	30	5	0
5	I	43	0	30	1	0
5	J	43	0	30	5	0
5	M	43	0	30	5	0
5	N	43	0	30	7	0
6	C	71	0	61	1	0
6	D	71	0	61	0	0
6	G	71	0	61	0	0
6	H	71	0	61	1	0
6	K	71	0	61	0	0
6	L	71	0	61	0	0
6	O	71	0	61	1	0
6	P	71	0	61	2	0
7	C	28	0	26	0	0
7	D	28	0	26	1	0
7	G	28	0	26	2	0
7	H	28	0	26	0	0
7	K	28	0	26	0	0
7	L	28	0	26	0	0
7	O	28	0	26	0	0
7	P	14	0	13	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	P	61	0	52	0	0
10	A	85	0	0	1	0
10	B	76	0	0	0	0
10	C	337	0	0	17	0
10	D	268	0	0	10	0
10	E	63	0	0	4	0
10	F	73	0	0	1	0
10	G	245	0	0	13	0
10	H	196	0	0	12	0
10	I	75	0	0	1	0
10	J	69	0	0	1	0
10	K	212	0	0	9	1
10	L	250	0	0	11	2
10	M	68	0	0	2	0
10	N	61	0	0	1	1
10	O	225	0	0	16	0
10	P	217	0	0	12	0
All	All	40392	0	37246	563	3

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 7.

The worst 5 of 563 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)
2:C:465:MET:CE	2:C:471:PRO:HG3	1.79	1.12
1:N:63:ALA:O	1:N:67:GLU:HG2	1.50	1.09
1:F:84:LEU:HD22	2:H:384:LEU:HD23	1.35	1.09
2:C:465:MET:HE3	2:C:471:PRO:HD3	1.34	1.05
2:P:116:GLU:OE2	2:P:411:MET:HE3	1.57	1.05

All (3) 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)
10:K:879:HOH:O	10:N:346:HOH:O[1_455]	2.12	0.08
2:G:208:ARG:NH2	10:L:946:HOH:O[1_456]	2.13	0.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:522:MET:SD	10:L:904:HOH:O[1_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	102/104 (98%)	101 (99%)	1 (1%)	0	100	100
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	E	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
1	F	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
1	I	102/104 (98%)	97 (95%)	4 (4%)	1 (1%)	19	11
1	J	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
1	M	102/104 (98%)	98 (96%)	2 (2%)	2 (2%)	9	3
1	N	103/104 (99%)	100 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
2	D	463/466 (99%)	443 (96%)	19 (4%)	1 (0%)	52	48
2	G	462/466 (99%)	440 (95%)	19 (4%)	3 (1%)	30	22
2	H	463/466 (99%)	442 (96%)	21 (4%)	0	100	100
2	K	462/466 (99%)	438 (95%)	23 (5%)	1 (0%)	52	48
2	L	463/466 (99%)	447 (96%)	16 (4%)	0	100	100
2	O	463/466 (99%)	442 (96%)	19 (4%)	2 (0%)	39	33
2	P	463/466 (99%)	447 (96%)	16 (4%)	0	100	100
All	All	4519/4560 (99%)	4337 (96%)	172 (4%)	10 (0%)	52	48

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	114	ASN

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Mol	Chain	Res	Type
2	G	142	ASP
1	I	3	GLU
2	K	114	ASN
1	M	3	GLU

### 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	90/90 (100%)	90 (100%)	0	100	100
1	B	90/90 (100%)	89 (99%)	1 (1%)	80	83
1	E	90/90 (100%)	89 (99%)	1 (1%)	80	83
1	F	90/90 (100%)	87 (97%)	3 (3%)	45	43
1	I	90/90 (100%)	88 (98%)	2 (2%)	60	62
1	J	90/90 (100%)	89 (99%)	1 (1%)	80	83
1	M	90/90 (100%)	89 (99%)	1 (1%)	80	83
1	N	91/90 (101%)	88 (97%)	3 (3%)	45	43
2	C	410/410 (100%)	405 (99%)	5 (1%)	78	81
2	D	409/410 (100%)	395 (97%)	14 (3%)	44	41
2	G	410/410 (100%)	398 (97%)	12 (3%)	50	49
2	H	409/410 (100%)	405 (99%)	4 (1%)	82	85
2	K	410/410 (100%)	401 (98%)	9 (2%)	60	62
2	L	409/410 (100%)	402 (98%)	7 (2%)	68	71
2	O	409/410 (100%)	399 (98%)	10 (2%)	57	58
2	P	410/410 (100%)	403 (98%)	7 (2%)	68	71
All	All	3997/4000 (100%)	3917 (98%)	80 (2%)	63	65

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	265	LYS

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Mol	Chain	Res	Type
2	K	181	GLU
2	P	175	MET
2	H	466	GLU
1	I	5	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	16	ASN
2	K	549	ASN
2	P	217	HIS
2	K	201	GLN
2	L	121	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CSO	C	150	2	3,6,7	0.67	0	1,6,8	1.92	0
2	CSO	D	150	2	3,6,7	0.53	0	1,6,8	1.97	0
2	CSO	G	150	2	3,6,7	0.68	0	1,6,8	1.88	0
2	CSO	H	150	2	3,6,7	0.51	0	1,6,8	2.06	1 (100%)
2	CSO	K	150	2	3,6,7	0.52	0	1,6,8	2.18	1 (100%)
2	CSO	L	150	2	3,6,7	0.50	0	1,6,8	2.04	1 (100%)
2	CSO	O	150	2	3,6,7	0.41	0	1,6,8	2.04	1 (100%)
2	CSO	P	150	2	3,6,7	0.61	0	1,6,8	1.64	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	CSO	C	150	2	-	0/1/5/7	0/0/0/0
2	CSO	D	150	2	-	0/1/5/7	0/0/0/0
2	CSO	G	150	2	-	0/1/5/7	0/0/0/0
2	CSO	H	150	2	-	0/1/5/7	0/0/0/0
2	CSO	K	150	2	-	0/1/5/7	0/0/0/0
2	CSO	L	150	2	-	0/1/5/7	0/0/0/0
2	CSO	O	150	2	-	0/1/5/7	0/0/0/0
2	CSO	P	150	2	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	150	CSO	O-C-CA	-2.18	119.80	125.49
2	H	150	CSO	O-C-CA	-2.06	120.12	125.49
2	O	150	CSO	O-C-CA	-2.04	120.17	125.49
2	L	150	CSO	O-C-CA	-2.04	120.19	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

53 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
6	NAG	C	602	2,6	14,14,15	0.47	0	15,19,21	1.31	1 (6%)
6	NAG	C	603	6	14,14,15	0.66	0	15,19,21	0.93	0
6	BMA	C	604	6	11,11,12	0.46	0	14,15,17	1.06	1 (7%)
6	MAN	C	605	6	11,11,12	0.65	0	14,15,17	0.98	0
6	MAN	C	606	6	11,11,12	0.73	0	14,15,17	0.86	0
6	FUC	C	607	6	10,10,11	0.84	0	14,14,16	1.53	1 (7%)
6	NAG	D	601	2,6	14,14,15	0.63	0	15,19,21	1.25	1 (6%)
6	NAG	D	602	6	14,14,15	0.72	0	15,19,21	1.02	1 (6%)
6	BMA	D	603	6	11,11,12	0.53	0	14,15,17	1.56	3 (21%)
6	MAN	D	604	6	11,11,12	0.59	0	14,15,17	0.92	0
6	MAN	D	605	6	11,11,12	0.53	0	14,15,17	1.18	2 (14%)
6	FUC	D	606	6	10,10,11	0.70	0	14,14,16	1.40	1 (7%)
6	NAG	G	601	2,6	14,14,15	0.54	0	15,19,21	1.70	4 (26%)
6	NAG	G	602	6	14,14,15	0.53	0	15,19,21	1.05	1 (6%)
6	BMA	G	603	6	11,11,12	0.38	0	14,15,17	1.30	1 (7%)
6	MAN	G	604	6	11,11,12	0.60	0	14,15,17	0.91	0
6	MAN	G	605	6	11,11,12	0.43	0	14,15,17	1.01	0
6	FUC	G	606	6	10,10,11	0.80	1 (10%)	14,14,16	1.60	2 (14%)
6	NAG	H	601	2,6	14,14,15	0.48	0	15,19,21	1.01	0
6	NAG	H	602	6	14,14,15	0.58	0	15,19,21	0.88	0
6	BMA	H	603	6	11,11,12	0.38	0	14,15,17	0.82	1 (7%)
6	MAN	H	604	6	11,11,12	0.63	0	14,15,17	1.00	1 (7%)
6	MAN	H	605	6	11,11,12	0.68	0	14,15,17	1.09	1 (7%)
6	FUC	H	606	6	10,10,11	0.98	1 (10%)	14,14,16	1.40	2 (14%)
6	NAG	K	601	2,6	14,14,15	0.56	0	15,19,21	0.79	0
6	NAG	K	602	6	14,14,15	0.85	1 (7%)	15,19,21	1.08	0
6	BMA	K	603	6	11,11,12	0.55	0	14,15,17	1.27	2 (14%)
6	MAN	K	604	6	11,11,12	0.50	0	14,15,17	0.70	0
6	MAN	K	605	6	11,11,12	0.60	0	14,15,17	1.10	0
6	FUC	K	606	6	10,10,11	0.65	0	14,14,16	1.43	1 (7%)
6	NAG	L	601	2,6	14,14,15	0.47	0	15,19,21	1.36	2 (13%)
6	NAG	L	602	6	14,14,15	0.73	0	15,19,21	1.11	0
6	BMA	L	603	6	11,11,12	0.49	0	14,15,17	1.15	1 (7%)
6	MAN	L	604	6	11,11,12	0.62	0	14,15,17	1.27	2 (14%)
6	MAN	L	605	6	11,11,12	0.44	0	14,15,17	1.12	1 (7%)
6	FUC	L	606	6	10,10,11	0.77	0	14,14,16	1.13	1 (7%)
6	NAG	O	601	2,6	14,14,15	0.60	0	15,19,21	1.88	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	O	602	6	14,14,15	0.73	1 (7%)	15,19,21	1.28	2 (13%)
6	BMA	O	603	6	11,11,12	0.49	0	14,15,17	1.20	1 (7%)
6	MAN	O	604	6	11,11,12	0.69	0	14,15,17	0.73	0
6	MAN	O	605	6	11,11,12	0.61	0	14,15,17	0.75	0
6	FUC	O	606	6	10,10,11	0.74	0	14,14,16	1.52	1 (7%)
6	NAG	P	602	2,6	14,14,15	0.51	0	15,19,21	1.30	2 (13%)
6	NAG	P	603	6	14,14,15	0.57	0	15,19,21	0.93	1 (6%)
6	BMA	P	604	6	11,11,12	0.37	0	14,15,17	1.38	1 (7%)
6	MAN	P	605	6	11,11,12	0.54	0	14,15,17	1.31	3 (21%)
6	MAN	P	606	6	11,11,12	0.59	0	14,15,17	1.06	1 (7%)
6	FUC	P	607	6	10,10,11	1.02	1 (10%)	14,14,16	1.04	0
9	NAG	P	609	9,2	14,14,15	0.68	0	15,19,21	0.68	0
9	NAG	P	610	9	14,14,15	0.71	0	15,19,21	0.79	0
9	BMA	P	611	9	11,11,12	0.28	0	14,15,17	0.97	1 (7%)
9	MAN	P	612	9	11,11,12	0.46	0	14,15,17	1.06	1 (7%)
9	MAN	P	613	9	11,11,12	0.60	0	14,15,17	0.91	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	602	2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	603	6	-	0/6/23/26	0/1/1/1
6	BMA	C	604	6	-	0/2/19/22	0/1/1/1
6	MAN	C	605	6	-	0/2/19/22	0/1/1/1
6	MAN	C	606	6	-	0/2/19/22	0/1/1/1
6	FUC	C	607	6	-	0/0/17/20	0/1/1/1
6	NAG	D	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	602	6	-	0/6/23/26	0/1/1/1
6	BMA	D	603	6	-	0/2/19/22	0/1/1/1
6	MAN	D	604	6	-	0/2/19/22	0/1/1/1
6	MAN	D	605	6	-	0/2/19/22	0/1/1/1
6	FUC	D	606	6	-	0/0/17/20	0/1/1/1
6	NAG	G	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	602	6	-	0/6/23/26	0/1/1/1
6	BMA	G	603	6	-	0/2/19/22	0/1/1/1
6	MAN	G	604	6	-	0/2/19/22	0/1/1/1
6	MAN	G	605	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FUC	G	606	6	-	0/0/17/20	0/1/1/1
6	NAG	H	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	H	602	6	-	0/6/23/26	0/1/1/1
6	BMA	H	603	6	-	0/2/19/22	0/1/1/1
6	MAN	H	604	6	-	0/2/19/22	0/1/1/1
6	MAN	H	605	6	-	0/2/19/22	0/1/1/1
6	FUC	H	606	6	-	0/0/17/20	0/1/1/1
6	NAG	K	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	K	602	6	-	0/6/23/26	0/1/1/1
6	BMA	K	603	6	-	0/2/19/22	0/1/1/1
6	MAN	K	604	6	-	0/2/19/22	0/1/1/1
6	MAN	K	605	6	-	0/2/19/22	0/1/1/1
6	FUC	K	606	6	-	0/0/17/20	0/1/1/1
6	NAG	L	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	L	602	6	-	0/6/23/26	0/1/1/1
6	BMA	L	603	6	-	0/2/19/22	0/1/1/1
6	MAN	L	604	6	-	0/2/19/22	0/1/1/1
6	MAN	L	605	6	-	0/2/19/22	0/1/1/1
6	FUC	L	606	6	-	0/0/17/20	0/1/1/1
6	NAG	O	601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	O	602	6	-	0/6/23/26	0/1/1/1
6	BMA	O	603	6	-	0/2/19/22	0/1/1/1
6	MAN	O	604	6	-	0/2/19/22	0/1/1/1
6	MAN	O	605	6	-	0/2/19/22	0/1/1/1
6	FUC	O	606	6	-	0/0/17/20	0/1/1/1
6	NAG	P	602	2,6	-	0/6/23/26	0/1/1/1
6	NAG	P	603	6	-	0/6/23/26	0/1/1/1
6	BMA	P	604	6	-	0/2/19/22	0/1/1/1
6	MAN	P	605	6	-	0/2/19/22	0/1/1/1
6	MAN	P	606	6	-	0/2/19/22	0/1/1/1
6	FUC	P	607	6	-	0/0/17/20	0/1/1/1
9	NAG	P	609	9,2	-	0/6/23/26	0/1/1/1
9	NAG	P	610	9	-	0/6/23/26	0/1/1/1
9	BMA	P	611	9	-	0/2/19/22	0/1/1/1
9	MAN	P	612	9	-	0/2/19/22	0/1/1/1
9	MAN	P	613	9	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	607	FUC	O5-C1	-2.56	1.39	1.43
6	H	606	FUC	O5-C1	-2.55	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	602	NAG	O5-C1	-2.16	1.40	1.43
6	G	606	FUC	O5-C1	-2.07	1.40	1.43
6	O	602	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	607	FUC	C1-C2-C3	-4.12	104.66	109.54
6	G	606	FUC	C1-C2-C3	-3.92	104.91	109.54
6	O	606	FUC	C1-C2-C3	-3.80	105.05	109.54
6	D	603	BMA	O3-C3-C2	-3.12	104.36	110.00
6	D	606	FUC	C6-C5-C4	-3.10	106.98	113.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	607	FUC	1	0
6	H	604	MAN	1	0
6	O	604	MAN	1	0
6	P	605	MAN	2	0

## 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 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	0KY	A	1602	5	12,18,18	2.63	5 (41%)	9,25,25	3.21	4 (44%)
5	HEM	B	202	1,10,2,4	30,50,50	2.18	8 (26%)	24,82,82	2.29	9 (37%)
4	0KY	B	203	5	12,18,18	2.54	5 (41%)	9,25,25	3.19	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	C	601	1,2,4	30,50,50	2.29	9 (30%)	24,82,82	2.32	7 (29%)
7	NAG	C	608	2	14,14,15	0.53	0	15,19,21	1.06	1 (6%)
7	NAG	C	609	2	14,14,15	0.58	0	15,19,21	1.02	1 (6%)
7	NAG	D	607	2	14,14,15	0.47	0	15,19,21	0.98	1 (6%)
7	NAG	D	608	2	14,14,15	0.55	0	15,19,21	0.95	0
5	HEM	E	1602	1,2,4	30,50,50	2.40	6 (20%)	24,82,82	2.36	11 (45%)
5	HEM	F	202	1,2,4	30,50,50	2.48	8 (26%)	24,82,82	2.37	9 (37%)
7	NAG	G	607	2	14,14,15	0.58	0	15,19,21	0.88	0
7	NAG	G	608	2	14,14,15	0.60	0	15,19,21	0.59	0
4	OKY	G	610	5	12,18,18	2.57	5 (41%)	9,25,25	3.02	4 (44%)
7	NAG	H	607	2	14,14,15	0.52	0	15,19,21	0.95	0
7	NAG	H	608	2	14,14,15	0.46	0	15,19,21	0.76	0
4	OKY	H	610	5	12,18,18	2.47	5 (41%)	9,25,25	3.07	4 (44%)
5	HEM	I	1602	1,10,2,4	30,50,50	2.09	7 (23%)	24,82,82	2.32	7 (29%)
4	OKY	I	1603	5	12,18,18	2.51	5 (41%)	9,25,25	3.17	4 (44%)
5	HEM	J	202	1,2,4	30,50,50	2.28	9 (30%)	24,82,82	2.51	12 (50%)
4	OKY	J	203	5	12,18,18	2.57	5 (41%)	9,25,25	3.16	4 (44%)
7	NAG	K	607	2	14,14,15	0.60	0	15,19,21	1.05	1 (6%)
7	NAG	K	608	2	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
7	NAG	L	607	2	14,14,15	0.43	0	15,19,21	1.45	2 (13%)
7	NAG	L	608	2	14,14,15	0.68	0	15,19,21	0.88	0
5	HEM	M	1602	1,2,4	30,50,50	2.29	8 (26%)	24,82,82	2.30	9 (37%)
5	HEM	N	202	1,2,4	30,50,50	2.16	9 (30%)	24,82,82	2.30	8 (33%)
7	NAG	O	607	2	14,14,15	0.52	0	15,19,21	0.66	0
7	NAG	O	608	2	14,14,15	0.47	0	15,19,21	0.69	0
4	OKY	O	610	5	12,18,18	2.59	5 (41%)	9,25,25	3.33	4 (44%)
7	NAG	P	608	2	14,14,15	0.47	0	15,19,21	1.06	1 (6%)
4	OKY	P	614	5	12,18,18	2.60	5 (41%)	9,25,25	3.31	4 (44%)

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	OKY	A	1602	5	-	0/7/7/7	0/2/2/2
5	HEM	B	202	1,10,2,4	-	0/10/54/54	0/0/8/8
4	OKY	B	203	5	-	0/7/7/7	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	C	601	1,2,4	-	0/10/54/54	0/0/8/8
7	NAG	C	608	2	-	0/6/23/26	0/1/1/1
7	NAG	C	609	2	-	0/6/23/26	0/1/1/1
7	NAG	D	607	2	-	0/6/23/26	0/1/1/1
7	NAG	D	608	2	-	0/6/23/26	0/1/1/1
5	HEM	E	1602	1,2,4	-	0/10/54/54	0/0/8/8
5	HEM	F	202	1,2,4	-	0/10/54/54	0/0/8/8
7	NAG	G	607	2	-	0/6/23/26	0/1/1/1
7	NAG	G	608	2	-	0/6/23/26	0/1/1/1
4	OKY	G	610	5	-	0/7/7/7	0/2/2/2
7	NAG	H	607	2	-	0/6/23/26	0/1/1/1
7	NAG	H	608	2	-	0/6/23/26	0/1/1/1
4	OKY	H	610	5	-	0/7/7/7	0/2/2/2
5	HEM	I	1602	1,10,2,4	-	0/10/54/54	0/0/8/8
4	OKY	I	1603	5	-	0/7/7/7	0/2/2/2
5	HEM	J	202	1,2,4	-	0/10/54/54	0/0/8/8
4	OKY	J	203	5	-	0/7/7/7	0/2/2/2
7	NAG	K	607	2	-	0/6/23/26	0/1/1/1
7	NAG	K	608	2	-	0/6/23/26	0/1/1/1
7	NAG	L	607	2	-	0/6/23/26	0/1/1/1
7	NAG	L	608	2	-	0/6/23/26	0/1/1/1
5	HEM	M	1602	1,2,4	-	0/10/54/54	0/0/8/8
5	HEM	N	202	1,2,4	-	0/10/54/54	0/0/8/8
7	NAG	O	607	2	-	0/6/23/26	0/1/1/1
7	NAG	O	608	2	-	0/6/23/26	0/1/1/1
4	OKY	O	610	5	-	0/7/7/7	0/2/2/2
7	NAG	P	608	2	-	0/6/23/26	0/1/1/1
4	OKY	P	614	5	-	0/7/7/7	0/2/2/2

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1602	HEM	C3B-C4B	-9.20	1.43	1.51
5	F	202	HEM	C3B-C4B	-8.67	1.44	1.51
5	C	601	HEM	C3B-C4B	-8.03	1.44	1.51
5	M	1602	HEM	C3B-C4B	-7.35	1.45	1.51
5	J	202	HEM	C3B-C4B	-7.13	1.45	1.51

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	203	OKY	C6-C7-N3	-4.76	105.10	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	610	0KY	C7-C8-N2	-4.65	117.23	123.59
4	A	1602	0KY	C7-C8-N2	-4.57	117.34	123.59
4	P	614	0KY	C7-C8-N2	-4.54	117.38	123.59
4	P	614	0KY	C6-C7-N3	-4.53	105.31	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1602	0KY	3	0
5	B	202	HEM	5	0
4	B	203	0KY	4	0
5	C	601	HEM	6	0
7	D	608	NAG	1	0
5	E	1602	HEM	6	0
5	F	202	HEM	5	0
7	G	608	NAG	2	0
4	G	610	0KY	1	0
4	H	610	0KY	5	0
5	I	1602	HEM	1	0
4	I	1603	0KY	2	0
5	J	202	HEM	5	0
4	J	203	0KY	1	0
5	M	1602	HEM	5	0
5	N	202	HEM	7	0
4	O	610	0KY	5	0
4	P	614	0KY	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	104/104 (100%)	-0.35	1 (0%) 84 84	12, 18, 40, 58	0
1	B	104/104 (100%)	-0.35	0 100 100	14, 24, 40, 53	0
1	E	104/104 (100%)	-0.25	1 (0%) 84 84	15, 23, 47, 67	0
1	F	104/104 (100%)	-0.15	1 (0%) 84 84	16, 30, 51, 56	0
1	I	104/104 (100%)	-0.36	2 (1%) 70 70	16, 24, 44, 65	0
1	J	104/104 (100%)	-0.23	0 100 100	16, 26, 45, 52	0
1	M	104/104 (100%)	-0.21	2 (1%) 70 70	16, 26, 49, 67	0
1	N	104/104 (100%)	-0.13	0 100 100	16, 32, 56, 63	0
2	C	464/466 (99%)	-0.43	1 (0%) 95 95	11, 20, 36, 58	0
2	D	465/466 (99%)	-0.28	3 (0%) 90 90	13, 26, 45, 63	0
2	G	464/466 (99%)	-0.22	6 (1%) 79 80	12, 29, 52, 67	0
2	H	465/466 (99%)	-0.09	9 (1%) 70 70	17, 33, 54, 72	0
2	K	464/466 (99%)	-0.23	4 (0%) 85 86	12, 29, 54, 73	0
2	L	465/466 (99%)	-0.25	5 (1%) 82 83	15, 27, 44, 65	0
2	O	465/466 (99%)	-0.25	5 (1%) 82 83	17, 30, 52, 67	0
2	P	465/466 (99%)	-0.17	10 (2%) 65 66	17, 31, 59, 77	0
All	All	4549/4560 (99%)	-0.24	50 (1%) 82 83	11, 28, 51, 77	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	578	ALA	7.8
2	D	217	HIS	5.6
2	H	217	HIS	5.6
2	G	218	ASP	5.0
1	M	4	GLN	4.9

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSO	D	150	7/8	0.97	0.08	-	17,19,23,24	0
2	CSO	G	150	7/8	0.97	0.06	-	15,16,25,26	0
2	CSO	C	150	7/8	0.97	0.08	-	14,15,22,24	0
2	CSO	L	150	7/8	0.95	0.09	-	22,24,25,30	0
2	CSO	O	150	7/8	0.96	0.10	-	19,20,28,28	0
2	CSO	H	150	7/8	0.96	0.09	-	21,24,29,34	0
2	CSO	K	150	7/8	0.95	0.09	-	22,24,26,30	0
2	CSO	P	150	7/8	0.97	0.06	-	26,29,33,36	0

## 6.3 Carbohydrates [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
6	BMA	L	603	11/12	0.93	0.10	1.39	21,26,31,36	0
6	BMA	K	603	11/12	0.94	0.11	1.11	22,25,31,37	0
6	BMA	H	603	11/12	0.95	0.12	0.94	25,27,33,38	0
6	NAG	C	603	14/15	0.97	0.10	0.67	14,22,27,28	0
6	NAG	K	602	14/15	0.95	0.11	0.57	18,23,27,27	0
6	BMA	G	603	11/12	0.89	0.12	0.37	36,42,46,49	0
6	NAG	O	602	14/15	0.95	0.10	0.22	22,30,38,42	0
6	BMA	D	603	11/12	0.97	0.09	0.17	18,22,26,31	0
6	BMA	P	604	11/12	0.95	0.09	-0.02	24,31,36,41	0
6	NAG	H	602	14/15	0.96	0.09	-0.50	21,25,27,27	0
6	BMA	O	603	11/12	0.94	0.08	-0.57	35,37,40,44	0
6	NAG	D	602	14/15	0.98	0.09	-0.60	15,18,22,22	0
6	NAG	L	602	14/15	0.96	0.08	-0.95	15,17,20,22	0
6	BMA	C	604	11/12	0.94	0.07	-1.10	24,28,32,36	0
6	NAG	P	603	14/15	0.96	0.08	-1.27	19,25,28,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	P	609	14/15	0.96	0.07	-1.29	23,27,30,30	0
6	NAG	G	602	14/15	0.97	0.08	-1.44	29,31,35,37	0
9	BMA	P	611	11/12	0.93	0.09	-	28,33,39,46	0
6	MAN	C	605	11/12	0.88	0.13	-	47,52,54,56	0
6	MAN	K	604	11/12	0.83	0.19	-	45,53,54,57	0
6	NAG	P	602	14/15	0.95	0.09	-	25,28,39,40	0
6	MAN	L	604	11/12	0.91	0.15	-	39,46,48,49	0
6	NAG	C	602	14/15	0.96	0.10	-	17,21,28,30	0
6	FUC	O	606	10/11	0.90	0.13	-	36,37,39,40	0
6	NAG	G	601	14/15	0.94	0.11	-	29,34,41,42	0
6	NAG	D	601	14/15	0.95	0.10	-	15,21,28,32	0
6	MAN	L	605	11/12	0.91	0.12	-	26,30,33,33	0
6	FUC	L	606	10/11	0.94	0.11	-	26,29,30,31	0
6	MAN	H	604	11/12	0.87	0.23	-	46,51,53,54	0
6	FUC	D	606	10/11	0.95	0.10	-	18,22,26,27	0
6	NAG	O	601	14/15	0.92	0.10	-	28,33,41,45	0
6	NAG	L	601	14/15	0.96	0.10	-	16,21,28,30	0
6	MAN	D	605	11/12	0.95	0.10	-	23,28,32,33	0
6	FUC	G	606	10/11	0.94	0.11	-	29,36,39,42	0
6	MAN	C	606	11/12	0.97	0.07	-	24,29,31,31	0
9	MAN	P	612	11/12	0.88	0.11	-	43,45,47,51	0
9	NAG	P	610	14/15	0.97	0.11	-	28,30,36,37	0
6	MAN	O	604	11/12	0.91	0.12	-	51,55,64,70	0
6	MAN	G	605	11/12	0.92	0.10	-	34,38,39,39	0
6	FUC	P	607	10/11	0.96	0.09	-	28,30,31,33	0
6	FUC	C	607	10/11	0.95	0.08	-	23,27,29,32	0
6	MAN	D	604	11/12	0.92	0.11	-	44,49,54,54	0
6	FUC	H	606	10/11	0.94	0.10	-	24,27,31,38	0
9	MAN	P	613	11/12	0.87	0.11	-	46,52,57,57	0
6	NAG	H	601	14/15	0.95	0.10	-	19,24,31,34	0
6	FUC	K	606	10/11	0.95	0.08	-	28,31,34,35	0
6	MAN	O	605	11/12	0.93	0.11	-	29,35,37,38	0
6	MAN	P	605	11/12	0.80	0.15	-	44,54,61,62	0
6	MAN	K	605	11/12	0.93	0.11	-	24,30,34,34	0
6	NAG	K	601	14/15	0.96	0.09	-	19,25,32,33	0
6	MAN	P	606	11/12	0.93	0.11	-	28,34,36,37	0
6	MAN	H	605	11/12	0.93	0.10	-	28,33,37,40	0
6	MAN	G	604	11/12	0.94	0.09	-	58,63,67,67	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	0KY	B	203	17/17	0.85	0.29	13.21	50,64,66,67	0
4	0KY	J	203	17/17	0.83	0.27	10.24	50,61,68,68	0
4	0KY	P	614	17/17	0.81	0.36	8.53	68,78,87,88	0
7	NAG	O	608	14/15	0.71	0.26	8.45	71,75,81,84	0
7	NAG	C	609	14/15	0.80	0.17	6.28	54,62,66,66	0
4	0KY	O	610	17/17	0.79	0.26	5.57	53,61,70,70	0
7	NAG	K	608	14/15	0.89	0.15	4.43	49,56,60,61	0
4	0KY	G	610	17/17	0.88	0.19	4.28	38,53,62,62	0
4	0KY	H	610	17/17	0.79	0.28	4.26	52,67,75,75	0
4	0KY	A	1602	17/17	0.85	0.20	4.23	36,43,48,49	0
4	0KY	I	1603	17/17	0.84	0.19	2.16	43,59,63,64	0
7	NAG	H	608	14/15	0.83	0.17	1.83	62,66,70,72	0
5	HEM	E	1602	43/43	0.98	0.11	1.19	13,19,27,28	0
7	NAG	D	608	14/15	0.86	0.16	1.13	46,53,55,57	0
5	HEM	I	1602	43/43	0.97	0.11	1.10	11,20,24,28	0
7	NAG	P	608	14/15	0.86	0.18	0.70	56,61,65,66	0
7	NAG	L	608	14/15	0.93	0.12	0.67	50,56,59,60	0
8	CA	H	609	1/1	1.00	0.11	0.63	19,19,19,19	0
5	HEM	C	601	43/43	0.98	0.10	0.61	11,15,20,27	0
3	CL	F	201	1/1	0.98	0.12	0.55	25,25,25,25	0
5	HEM	F	202	43/43	0.95	0.11	0.29	22,29,33,38	0
7	NAG	L	607	14/15	0.92	0.10	0.23	27,35,38,39	0
7	NAG	G	607	14/15	0.92	0.11	0.09	32,36,41,43	0
5	HEM	N	202	43/43	0.96	0.10	-0.10	21,30,36,43	0
5	HEM	J	202	43/43	0.96	0.10	-0.17	18,24,29,33	0
5	HEM	B	202	43/43	0.98	0.10	-0.24	15,21,27,35	0
7	NAG	H	607	14/15	0.93	0.10	-0.26	31,37,42,45	0
5	HEM	M	1602	43/43	0.98	0.10	-0.34	17,25,28,29	0
8	CA	D	609	1/1	1.00	0.09	-0.37	16,16,16,16	0
3	CL	E	1601	1/1	0.99	0.09	-0.45	18,18,18,18	0
3	CL	I	1601	1/1	1.00	0.09	-0.50	14,14,14,14	0
7	NAG	G	608	14/15	0.90	0.11	-0.54	60,67,69,69	0
7	NAG	D	607	14/15	0.92	0.09	-0.54	24,26,30,36	0
7	NAG	C	608	14/15	0.95	0.09	-0.58	19,25,29,30	0
7	NAG	K	607	14/15	0.88	0.12	-0.64	40,49,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	B	201	1/1	1.00	0.08	-0.84	14,14,14,14	0
7	NAG	O	607	14/15	0.95	0.09	-1.09	26,28,31,34	0
8	CA	L	609	1/1	0.99	0.08	-1.56	20,20,20,20	0
8	CA	K	609	1/1	0.99	0.08	-1.70	24,24,24,24	0
8	CA	G	609	1/1	0.99	0.08	-1.75	22,22,22,22	0
3	CL	A	1601	1/1	1.00	0.07	-1.84	16,16,16,16	0
3	CL	M	1601	1/1	0.99	0.07	-2.13	18,18,18,18	0
8	CA	P	601	1/1	1.00	0.05	-2.68	19,19,19,19	0
8	CA	C	610	1/1	0.99	0.07	-3.08	14,14,14,14	0
8	CA	O	609	1/1	0.99	0.05	-3.68	21,21,21,21	0
3	CL	J	201	1/1	0.99	0.06	-3.75	20,20,20,20	0
3	CL	N	201	1/1	1.00	0.04	-6.00	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.