



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:53 PM GMT

PDB ID : 3F9P  
Title : Crystal structure of myeloperoxidase from human leukocytes  
Authors : Carpena, X.; Fita, I.; Obinger, C.  
Deposited on : 2008-11-14  
Resolution : 2.93 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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

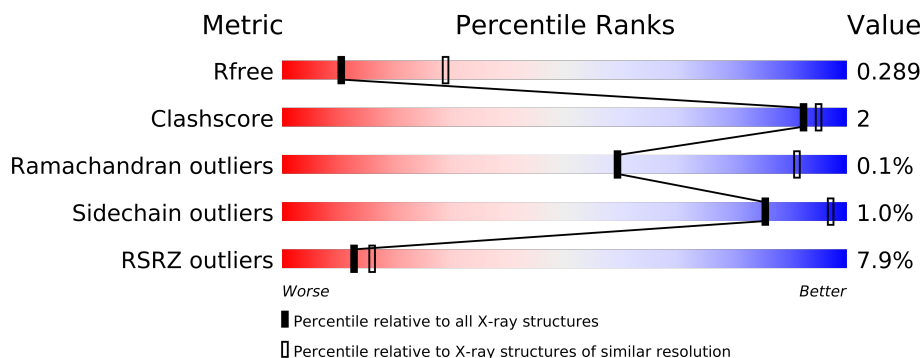
MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683



# 1 Overall quality at a glance

The reported resolution of this entry is 2.93 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))
$R_{free}$	66092	1424 (2.98-2.90)
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RSRZ outliers	66119	1425 (2.98-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	114	
1	B	114	
2	C	467	
2	D	467	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NAG	C	630	-	X
8	ACT	C	703	-	X



## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9483 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			860	542	154	159	5			
1	B	108	Total	C	N	O	S	0	0	1
			861	542	155	159	5			

- Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			
2	D	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

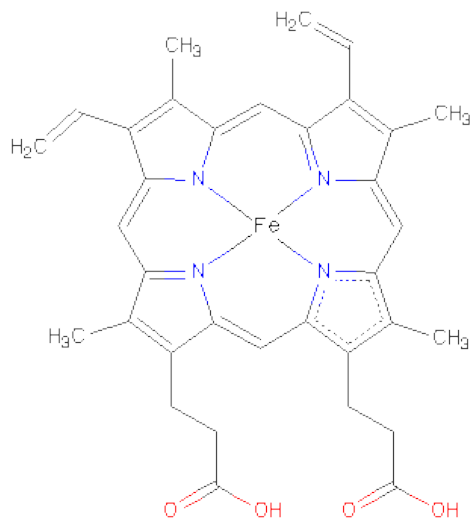
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

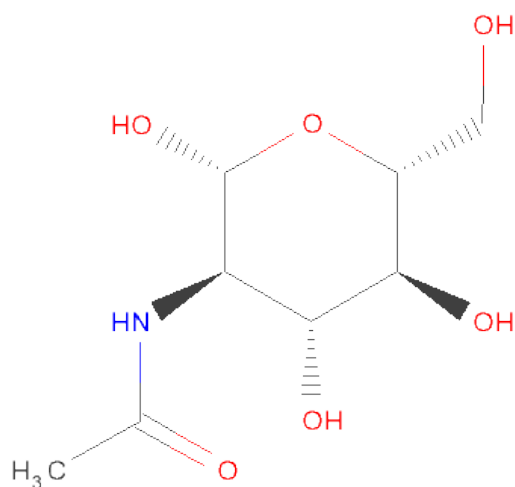
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	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		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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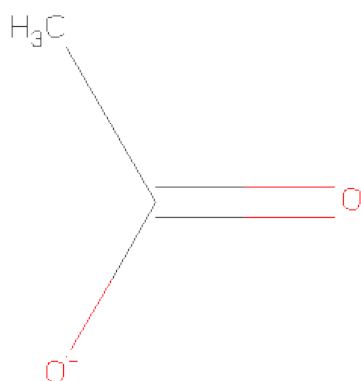
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	6	Total	C	N	O	0	0
			71	40	2	29		
7	D	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

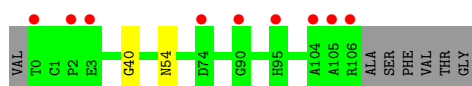


### 3 Residue-property plots

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.

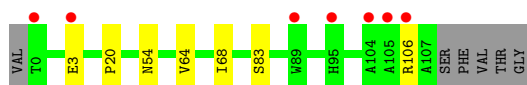
- Molecule 1: Myeloperoxidase

Chain A: 



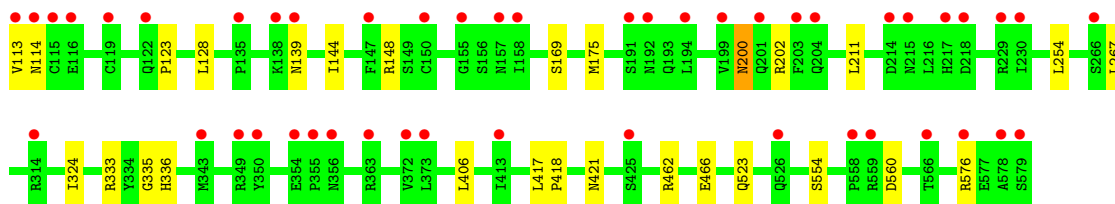
- Molecule 1: Myeloperoxidase

Chain B: 



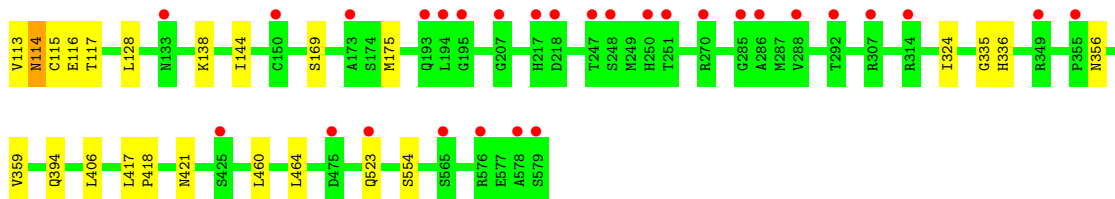
- Molecule 2: Myeloperoxidase

Chain C: 



- Molecule 2: Myeloperoxidase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.74Å 110.74Å 255.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.93 29.92 – 2.93	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.00-2.93) 96.2 (29.92-2.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.236 , 0.257 0.274 , 0.289	Depositor DCC
$R_{free}$ test set	1709 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 7.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 33655 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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, FUC, ACT, HEM

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	0.33	0/885	0.48	0/1205
1	B	0.35	0/886	0.51	0/1207
2	C	0.32	0/3811	0.46	0/5170
2	D	0.32	0/3811	0.47	0/5170
All	All	0.33	0/9393	0.47	0/12752

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	860	0	823	1	0
1	B	861	0	823	6	0
2	C	3733	0	3725	15	0
2	D	3733	0	3725	17	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	43	0	30	2	0
5	B	43	0	30	1	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
7	C	71	0	61	0	0
7	D	71	0	61	0	0
8	C	4	0	3	2	0
8	D	4	0	3	0	0
All	All	9483	0	9336	34	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:113:VAL:HA	2:D:114:ASN:HB2	1.11	1.09
2:D:113:VAL:HA	2:D:114:ASN:CB	1.97	0.95
2:D:113:VAL:CA	2:D:114:ASN:HB2	1.98	0.93
2:C:336:HIS:HD1	2:C:421:ASN:HD21	1.21	0.86
5:A:605:HEM:HBC2	2:C:335:GLY:HA3	1.68	0.74
2:D:336:HIS:HD1	2:D:421:ASN:HD21	1.35	0.74
1:B:106:ARG:H	2:D:113:VAL:HG22	1.63	0.63
2:C:113:VAL:N	2:C:114:ASN:HA	2.14	0.61
2:C:211:LEU:HD23	2:C:254:LEU:HD13	1.87	0.56
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.88	0.54
2:C:148:ARG:HD3	8:C:703:ACT:H1	1.92	0.51
2:C:462:ARG:O	2:C:466:GLU:HG2	2.10	0.51
2:D:169:SER:HB2	2:D:324:ILE:HG12	1.95	0.49
1:A:40:GLY:HA2	1:B:20:PRO:HD2	1.93	0.49
5:A:605:HEM:HAD1	2:C:333:ARG:HH21	1.77	0.49
2:D:116:GLU:HG2	2:D:117:THR:HG23	1.95	0.48
2:C:406:LEU:HD22	2:C:417:LEU:HB2	1.96	0.48
1:B:64:VAL:HG13	1:B:68:ILE:HD12	1.98	0.46
2:C:267:LEU:HD12	2:C:576:ARG:HB2	1.96	0.46
2:C:169:SER:HB2	2:C:324:ILE:HG12	1.97	0.45
2:C:200:ASN:HD22	2:C:202:ARG:H	1.63	0.45
2:D:128:LEU:HB2	2:D:144:ILE:HB	1.99	0.45
2:D:113:VAL:HB	2:D:115:CYS:H	1.82	0.45
2:C:554:SER:HB3	2:C:560:ASP:HB3	1.99	0.44
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.01	0.43
5:B:605:HEM:HBC2	2:D:335:GLY:HA3	2.00	0.43
2:D:356:ASN:HB3	2:D:359:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:394:GLN:HB3	2:D:460:LEU:HD22	2.01	0.42
2:D:406:LEU:HD22	2:D:417:LEU:HB2	2.01	0.42
1:B:83:SER:HB3	2:D:554:SER:O	2.19	0.42
1:B:106:ARG:N	2:D:113:VAL:HG22	2.33	0.41
1:B:68:ILE:HD13	2:D:464:LEU:HD23	2.02	0.41
2:C:123:PRO:HB3	8:C:703:ACT:H3	2.04	0.40
2:D:417:LEU:HB3	2:D:418:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/114 (92%)	102 (97%)	3 (3%)	0	100	100
1	B	106/114 (93%)	102 (96%)	4 (4%)	0	100	100
2	C	464/467 (99%)	452 (97%)	12 (3%)	0	100	100
2	D	464/467 (99%)	450 (97%)	13 (3%)	1 (0%)	56	89
All	All	1139/1162 (98%)	1106 (97%)	32 (3%)	1 (0%)	59	91

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	114	ASN

### 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	92/97 (95%)	91 (99%)	1 (1%)	84	96
1	B	92/97 (95%)	90 (98%)	2 (2%)	64	91
2	C	410/411 (100%)	406 (99%)	4 (1%)	85	97
2	D	410/411 (100%)	407 (99%)	3 (1%)	91	98
All	All	1004/1016 (99%)	994 (99%)	10 (1%)	85	97

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	139	ASN
2	C	175	MET
2	C	200	ASN
2	C	523	GLN
1	B	3	GLU
1	B	54	ASN
2	D	138	LYS
2	D	175	MET
2	D	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	139	ASN
2	C	200	ASN
2	C	421	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	6,6,7	7.63	3 (50%)	3,6,8	0.56	0
2	CSO	D	150	2	6,6,7	7.58	3 (50%)	3,6,8	0.69	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	-	0/2/5/7	0/0/0/0
2	CSO	D	150	2	-	0/2/5/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	150	CSO	O-C	18.03	1.23	1.11
2	D	150	CSO	O-C	17.91	1.23	1.11
2	C	150	CSO	OD-SG	3.82	1.78	1.62
2	D	150	CSO	OD-SG	3.77	1.78	1.62
2	D	150	CSO	CA-C	2.86	1.53	1.48
2	C	150	CSO	CA-C	2.78	1.53	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

12 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	C	640	2,7	12,14,15	0.63	0	15,19,21	0.94	0
7	NAG	C	641	7	12,14,15	0.60	0	15,19,21	0.76	1 (6%)
7	BMA	C	642	7	10,11,12	0.55	0	11,15,17	0.91	0
7	BMA	C	643	7	10,11,12	0.72	0	11,15,17	1.13	1 (9%)
7	BMA	C	644	7	10,11,12	0.76	0	11,15,17	1.48	3 (27%)
7	FUC	C	645	7	9,10,11	0.79	0	10,14,16	0.56	0
7	NAG	D	640	2,7	12,14,15	0.63	0	15,19,21	0.89	0
7	NAG	D	641	7	12,14,15	0.62	0	15,19,21	0.78	1 (6%)
7	BMA	D	642	7	10,11,12	0.59	0	11,15,17	1.03	1 (9%)
7	BMA	D	643	7	10,11,12	0.70	0	11,15,17	0.87	1 (9%)
7	BMA	D	644	7	10,11,12	0.71	0	11,15,17	1.22	2 (18%)
7	FUC	D	645	7	9,10,11	0.76	0	10,14,16	0.59	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
7	NAG	C	640	2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	641	7	-	0/6/23/26	0/1/1/1
7	BMA	C	642	7	-	0/2/19/22	0/1/1/1
7	BMA	C	643	7	-	0/2/19/22	0/1/1/1
7	BMA	C	644	7	-	0/2/19/22	0/1/1/1
7	FUC	C	645	7	-	0/0/17/20	0/1/1/1
7	NAG	D	640	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	641	7	-	0/6/23/26	0/1/1/1
7	BMA	D	642	7	-	0/2/19/22	0/1/1/1
7	BMA	D	643	7	-	0/2/19/22	0/1/1/1
7	BMA	D	644	7	-	0/2/19/22	0/1/1/1
7	FUC	D	645	7	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	644	BMA	O5-C5-C6	3.13	110.27	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	643	BMA	O5-C5-C6	2.94	110.06	106.98
7	D	643	BMA	O5-C5-C6	2.57	109.67	106.98
7	D	644	BMA	C3-C4-C5	2.54	114.73	110.20
7	C	644	BMA	C3-C4-C5	2.53	114.73	110.20
7	C	644	BMA	C4-C3-C2	2.32	113.61	110.50
7	D	641	NAG	O5-C5-C6	2.14	109.22	106.98
7	C	641	NAG	O5-C5-C6	2.06	109.14	106.98
7	D	642	BMA	C3-C4-C5	2.02	113.82	110.20
7	D	644	BMA	O5-C5-C6	2.00	109.08	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z  > 2$
5	HEM	A	605	1,2	49,50,50	2.49	16 (32%)	46,82,82	1.92	7 (15%)
5	HEM	B	605	1,2	49,50,50	2.47	16 (32%)	46,82,82	1.91	8 (17%)
6	NAG	C	620	2	12,14,15	0.60	0	15,19,21	1.00	1 (6%)
6	NAG	C	630	2	12,14,15	0.61	0	15,19,21	0.77	1 (6%)
8	ACT	C	703	-	1,3,3	1.16	0	0,3,3	0.00	-
6	NAG	D	620	2	12,14,15	0.62	0	15,19,21	1.12	1 (6%)
6	NAG	D	630	2	12,14,15	0.63	0	15,19,21	0.85	1 (6%)
8	ACT	D	703	-	1,3,3	1.20	0	0,3,3	0.00	-

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
5	HEM	A	605	1,2	-	0/14/114/114	0/0/8/8
5	HEM	B	605	1,2	-	0/14/114/114	0/0/8/8
6	NAG	C	620	2	-	0/6/23/26	0/1/1/1
6	NAG	C	630	2	-	0/6/23/26	0/1/1/1
8	ACT	C	703	-	-	0/0/0/0	0/0/0/0
6	NAG	D	620	2	-	0/6/23/26	0/1/1/1
6	NAG	D	630	2	-	0/6/23/26	0/1/1/1
8	ACT	D	703	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	HEM	C3D-C2D	5.79	1.53	1.43
5	B	605	HEM	C3D-C2D	5.76	1.53	1.43
5	B	605	HEM	C3B-C2B	-5.55	1.34	1.43
5	A	605	HEM	C3C-C2C	-5.42	1.34	1.43
5	B	605	HEM	FE-NA	5.32	2.15	1.92
5	A	605	HEM	C3B-C2B	-5.30	1.34	1.43
5	A	605	HEM	FE-NA	5.23	2.14	1.92
5	B	605	HEM	C3C-C2C	-5.04	1.34	1.43
5	B	605	HEM	C3C-CAC	4.84	1.55	1.40
5	A	605	HEM	C3C-CAC	4.75	1.55	1.40
5	A	605	HEM	C3B-CAB	4.69	1.55	1.40
5	B	605	HEM	C3B-CAB	4.65	1.55	1.40
5	A	605	HEM	FE-ND	4.48	2.14	1.97
5	B	605	HEM	FE-ND	4.35	2.13	1.97
5	B	605	HEM	C4A-C3A	4.27	1.45	1.40
5	A	605	HEM	C4A-C3A	4.22	1.45	1.40
5	A	605	HEM	FE-NB	4.09	2.12	1.97
5	A	605	HEM	C2B-C1B	3.83	1.45	1.44
5	B	605	HEM	FE-NB	3.58	2.10	1.97
5	B	605	HEM	C3D-C4D	3.37	1.45	1.44
5	B	605	HEM	C2B-C1B	3.22	1.45	1.44
5	B	605	HEM	C2D-C1D	2.82	1.45	1.44
5	A	605	HEM	FE-NC	2.82	2.08	1.97
5	A	605	HEM	C2D-C1D	2.76	1.45	1.44
5	A	605	HEM	CMB-C2B	2.59	1.55	1.47
5	B	605	HEM	FE-NC	2.54	2.07	1.97
5	B	605	HEM	CMB-C2B	2.50	1.55	1.47
5	B	605	HEM	CMD-C2D	2.48	1.55	1.47
5	A	605	HEM	CMD-C2D	2.47	1.55	1.47
5	B	605	HEM	CMC-C2C	2.44	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	HEM	CMC-C2C	2.41	1.54	1.47
5	A	605	HEM	C3D-C4D	2.40	1.45	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	HEM	C3B-C4B-NB	-8.27	108.08	114.00
5	B	605	HEM	C3B-C4B-NB	-8.19	108.14	114.00
5	B	605	HEM	C4D-ND-C1D	6.02	111.32	105.16
5	A	605	HEM	C4D-ND-C1D	6.00	111.30	105.16
5	B	605	HEM	C2D-C1D-ND	-3.42	108.89	112.93
5	A	605	HEM	C2D-C1D-ND	-3.36	108.96	112.93
6	D	620	NAG	O5-C5-C6	3.15	110.29	106.98
6	C	620	NAG	O5-C5-C6	3.04	110.17	106.98
5	A	605	HEM	CBA-CAA-C2A	-2.77	107.82	112.69
5	B	605	HEM	CBD-CAD-C3D	-2.54	108.84	114.37
5	A	605	HEM	C1B-NB-C4B	2.48	107.69	105.16
5	B	605	HEM	C1B-NB-C4B	2.36	107.58	105.16
5	A	605	HEM	C4C-NC-C1C	2.36	107.98	105.53
5	B	605	HEM	C4C-NC-C1C	2.22	107.84	105.53
5	A	605	HEM	CBD-CAD-C3D	-2.07	109.85	114.37
6	D	630	NAG	O5-C5-C6	2.07	109.15	106.98
5	B	605	HEM	CBA-CAA-C2A	-2.02	109.13	112.69
5	B	605	HEM	CMA-C3A-C4A	-2.02	125.51	128.62
6	C	630	NAG	O5-C5-C6	2.02	109.10	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	107/114 (93%)	0.68	9 (8%) 11 14	66, 67, 69, 70	0
1	B	108/114 (94%)	0.56	7 (6%) 18 24	66, 67, 69, 70	0
2	C	467/467 (100%)	0.65	47 (10%) 7 10	66, 67, 68, 69	0
2	D	467/467 (100%)	0.55	29 (6%) 20 25	66, 67, 68, 69	0
All	All	1149/1162 (98%)	0.61	92 (8%) 13 15	66, 67, 68, 70	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	579	SER	10.8
2	D	578	ALA	8.5
1	A	106	ARG	7.2
2	C	217	HIS	5.8
2	C	578	ALA	5.2
1	A	104	ALA	4.9
2	C	355	PRO	4.9
1	B	0	THR	4.5
1	A	3	GLU	4.3
2	C	192	ASN	4.2
2	C	373	LEU	4.2
2	C	194	LEU	4.1
2	D	217	HIS	4.0
2	C	558	PRO	3.9
2	C	579	SER	3.8
2	C	356	ASN	3.7
2	C	157	ASN	3.6
2	D	195	GLY	3.6
2	C	349	ARG	3.5
1	A	0	THR	3.3
2	C	191	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	150	CSO	3.2
1	A	105	ALA	3.2
2	D	523	GLN	3.2
2	C	215	ASN	3.1
2	C	203	PHE	3.1
2	C	122	GLN	3.1
1	B	105	ALA	3.1
2	C	372	VAL	3.0
2	D	576	ARG	3.0
2	C	115	CYS	3.0
2	D	349	ARG	3.0
2	C	218	ASP	3.0
2	D	270	ARG	2.9
2	C	113	VAL	2.9
2	C	138	LYS	2.9
2	C	266	SER	2.8
2	C	425	SER	2.8
2	C	155	GLY	2.8
2	D	247	THR	2.8
2	C	576	ARG	2.8
2	C	199	VAL	2.8
2	D	218	ASP	2.7
2	C	114	ASN	2.7
2	C	350	TYR	2.7
2	C	559	ARG	2.7
2	D	194	LEU	2.6
1	B	106	ARG	2.6
2	D	286	ALA	2.6
2	C	413	ILE	2.6
2	C	150	CSO	2.5
2	C	230	ILE	2.5
2	C	201	GLN	2.5
2	C	147	PHE	2.5
1	B	3	GLU	2.5
2	D	425	SER	2.5
2	D	285	GLY	2.5
2	C	229	ARG	2.4
2	C	314	ARG	2.4
2	C	214	ASP	2.4
2	C	135	PRO	2.4
1	B	104	ALA	2.4
2	D	173	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	193	GLN	2.3
2	C	116	GLU	2.3
2	D	475	ASP	2.3
2	C	526	GLN	2.3
2	D	355	PRO	2.3
2	D	314	ARG	2.3
2	D	288	VAL	2.3
2	C	204	GLN	2.2
2	D	133	ASN	2.2
1	B	95	HIS	2.2
2	D	565	SER	2.2
1	A	2	PRO	2.2
2	C	158	ILE	2.2
2	C	139	ASN	2.2
2	D	307	ARG	2.2
2	C	354	GLU	2.2
1	A	95	HIS	2.2
2	D	251	THR	2.2
2	C	566	THR	2.1
2	D	248	SER	2.1
2	D	250	HIS	2.1
2	D	292	THR	2.1
1	B	89	TRP	2.1
2	C	119	CYS	2.1
1	A	90	GLY	2.1
2	D	207	GLY	2.1
2	C	343	MET	2.1
1	A	74	ASP	2.0
2	C	363	ARG	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSO	D	150	7/8	0.27	0.83	67,67,68,68	0
2	CSO	C	150	7/8	0.24	0.39	67,68,68,68	0



## 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	BMA	D	643	11/12	0.33	5.25	68,68,68,69	0
7	BMA	C	643	11/12	0.35	3.18	69,69,69,70	0
7	BMA	D	644	11/12	0.26	2.83	67,67,68,68	0
7	BMA	C	644	11/12	0.25	1.30	66,67,67,67	0
7	NAG	D	641	14/15	0.23	0.88	63,64,64,65	0
7	NAG	D	640	14/15	0.20	0.76	62,63,64,64	0
7	NAG	C	640	14/15	0.19	-0.13	64,65,65,65	0
7	BMA	D	642	11/12	0.17	-0.82	66,66,67,67	0
7	NAG	C	641	14/15	0.17	-1.07	65,66,66,66	0
7	BMA	C	642	11/12	0.16	-1.11	67,67,68,68	0
7	FUC	C	645	10/11	0.18	-2.06	63,63,64,64	0
7	FUC	D	645	10/11	0.17	-2.11	62,62,62,62	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	ACT	C	703	4/4	0.33	5.63	69,69,69,69	0
6	NAG	D	630	14/15	0.34	1.97	65,65,65,66	0
6	NAG	C	630	14/15	0.50	1.84	65,66,66,66	0
6	NAG	D	620	14/15	0.29	0.18	65,65,65,65	0
6	NAG	C	620	14/15	0.35	-0.03	65,65,66,66	0
5	HEM	B	605	43/43	0.24	-0.19	66,67,67,68	0
5	HEM	A	605	43/43	0.23	-0.31	67,67,68,68	0
3	CA	D	601	1/1	0.16	-2.10	67,67,67,67	0
4	CL	A	602	1/1	0.13	-2.61	48,48,48,48	0
3	CA	C	601	1/1	0.10	-2.78	67,67,67,67	0
8	ACT	D	703	4/4	0.13	-3.82	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	D	602	1/1	0.08	-5.63	53,53,53,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.