



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 12:09 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 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

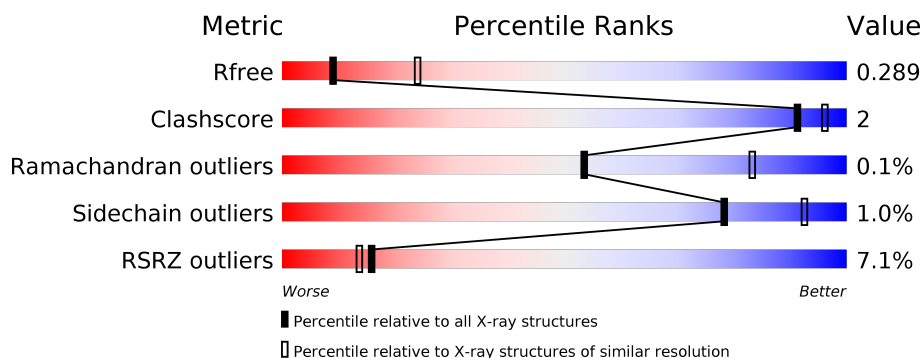
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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))
$R_{free}$	111664	2506 (2.98-2.90)
Clashscore	122126	2745 (2.98-2.90)
Ramachandran outliers	120053	2675 (2.98-2.90)
Sidechain outliers	120020	2677 (2.98-2.90)
RSRZ outliers	108989	2445 (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. 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	114	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	B	114	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
2	C	467	<div> <div>9%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
2	D	467	<div> <div>6%</div> <div> <div></div> <div>95%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	630	-	-	-	X
9	ACT	C	703	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9483 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.

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			

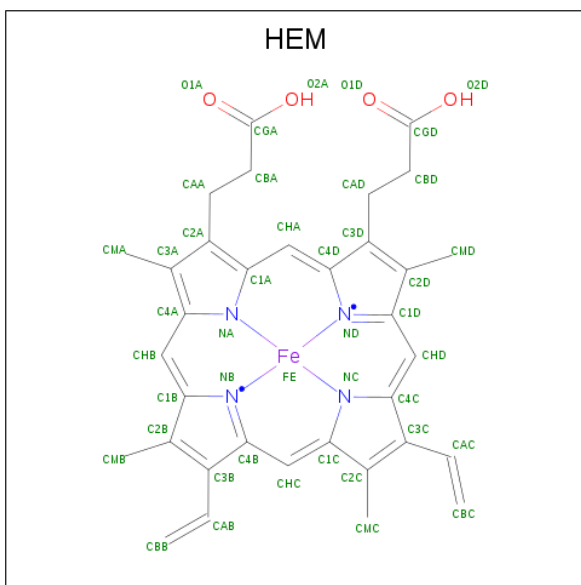
- Molecule 2 is a protein called Myeloperoxidase.

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

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

- Molecule 4 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
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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



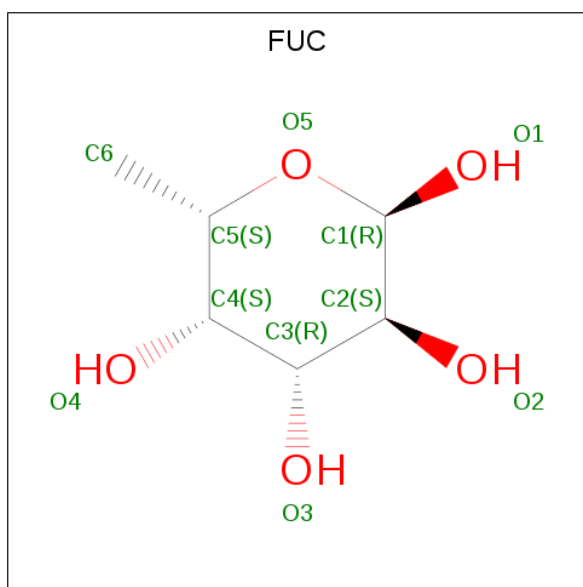
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



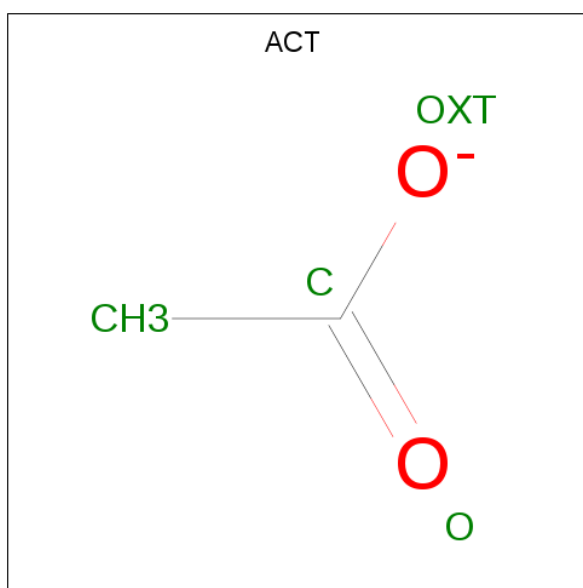
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



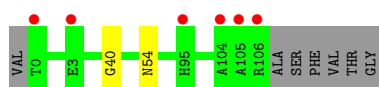
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		



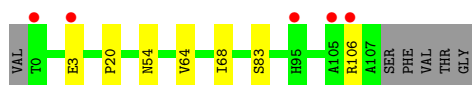
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

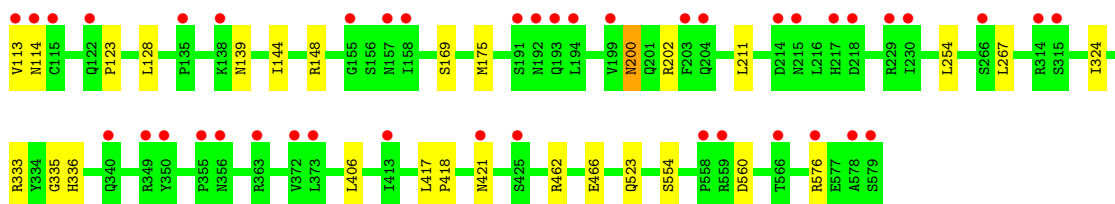
- Molecule 1: Myeloperoxidase



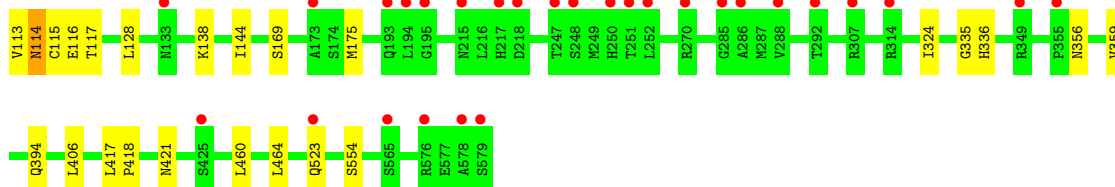
- Molecule 1: Myeloperoxidase



- Molecule 2: Myeloperoxidase



- Molecule 2: Myeloperoxidase



## 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	1710 reflections (5.08%)	wwPDB-VP
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> )	0.30 , 8.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

<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 [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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	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	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	43	0	30	2	0
4	B	43	0	30	1	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	C	56	0	49	0	0
6	D	56	0	49	0	0
7	C	33	0	28	0	0
7	D	33	0	28	0	0
8	C	10	0	10	0	0
8	D	10	0	10	0	0
9	C	4	0	3	2	0
9	D	4	0	3	0	0
All	All	9483	0	9336	34	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 2.

All (34) 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: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
4: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	9: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
4: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:605:HEM:HBC2	2:D:335:GLY:HA3	2.00	0.43
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.01	0.43
2:D:356:ASN:HB3	2:D:359:VAL:HG22	2.00	0.43
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	9: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%)	49	79
All	All	1139/1162 (98%)	1106 (97%)	32 (3%)	1 (0%)	53	83

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%)	76	91
1	B	92/97 (95%)	90 (98%)	2 (2%)	55	82
2	C	410/411 (100%)	406 (99%)	4 (1%)	78	92
2	D	410/411 (100%)	407 (99%)	3 (1%)	85	95
All	All	1004/1016 (99%)	994 (99%)	10 (1%)	78	92

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 molecules 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	4,6,7	1.35	1 (25%)	1,6,8	1.72	0
2	CSO	D	150	2	4,6,7	1.41	1 (25%)	1,6,8	1.78	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	150	CSO	CA-C	2.48	1.53	1.50
2	D	150	CSO	CA-C	2.60	1.53	1.50

There are no bond angle outliers.

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	HEM	A	605	1,2	27,50,50	2.18	5 (18%)	17,82,82	1.37	2 (11%)
4	HEM	B	605	1,2	27,50,50	2.18	5 (18%)	17,82,82	1.32	1 (5%)
6	NAG	C	620	2	14,14,15	0.50	0	17,19,21	0.81	0
6	NAG	C	630	2	14,14,15	0.48	0	17,19,21	0.70	0
6	NAG	C	640	8,2,6	14,14,15	0.53	0	17,19,21	1.13	2 (11%)
6	NAG	C	641	7,6	14,14,15	0.46	0	17,19,21	0.70	0
7	BMA	C	642	7,6	11,11,12	0.48	0	15,15,17	0.88	0
7	BMA	C	643	7	11,11,12	0.58	0	15,15,17	0.73	0
7	BMA	C	644	7	11,11,12	0.61	0	15,15,17	1.28	2 (13%)
8	FUC	C	645	6	9,10,11	0.65	0	13,14,16	0.49	0
9	ACT	C	703	-	1,3,3	1.37	0	0,3,3	0.00	-
6	NAG	D	620	2	14,14,15	0.54	0	17,19,21	0.82	0
6	NAG	D	630	2	14,14,15	0.49	0	17,19,21	0.71	0
6	NAG	D	640	8,2,6	14,14,15	0.52	0	17,19,21	1.07	1 (5%)
6	NAG	D	641	7,6	14,14,15	0.49	0	17,19,21	0.66	0
7	BMA	D	642	7,6	11,11,12	0.48	0	15,15,17	0.94	0
7	BMA	D	643	7	11,11,12	0.54	0	15,15,17	0.61	0
7	BMA	D	644	7	11,11,12	0.55	0	15,15,17	1.05	1 (6%)
8	FUC	D	645	6	9,10,11	0.67	0	13,14,16	0.55	0
9	ACT	D	703	-	1,3,3	1.42	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
4	HEM	A	605	1,2	-	0/6/54/54	0/0/8/8
4	HEM	B	605	1,2	-	0/6/54/54	0/0/8/8
6	NAG	C	620	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	630	2	-	0/6/23/26	0/1/1/1
6	NAG	C	640	8,2,6	-	0/6/23/26	0/1/1/1
6	NAG	C	641	7,6	-	0/6/23/26	0/1/1/1
7	BMA	C	642	7,6	-	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
8	FUC	C	645	6	-	0/0/17/20	0/1/1/1
9	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
6	NAG	D	640	8,2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	641	7,6	-	0/6/23/26	0/1/1/1
7	BMA	D	642	7,6	-	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
8	FUC	D	645	6	-	0/0/17/20	0/1/1/1
9	ACT	D	703	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	HEM	C3B-C2B	-4.56	1.34	1.40
4	A	605	HEM	C3C-C2C	-4.39	1.34	1.40
4	A	605	HEM	C3B-C2B	-4.25	1.34	1.40
4	B	605	HEM	C3C-C2C	-3.92	1.34	1.40
4	B	605	HEM	C3B-CAB	3.61	1.55	1.47
4	A	605	HEM	C3B-CAB	3.68	1.55	1.47
4	A	605	HEM	C3C-CAC	3.84	1.55	1.47
4	B	605	HEM	C3C-CAC	3.99	1.55	1.47
4	B	605	HEM	C3D-C2D	5.46	1.53	1.37
4	A	605	HEM	C3D-C2D	5.47	1.53	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	HEM	CBA-CAA-C2A	-2.44	107.82	112.48
6	C	640	NAG	O5-C1-C2	-2.38	108.24	111.52
4	A	605	HEM	C1D-C2D-C3D	-2.28	105.41	107.00
7	C	644	BMA	C1-O5-C5	-2.25	109.10	112.19
4	B	605	HEM	C1D-C2D-C3D	-2.01	105.59	107.00
6	C	640	NAG	C4-C3-C2	2.13	114.13	111.02
6	D	640	NAG	C1-O5-C5	2.25	115.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	644	BMA	C3-C4-C5	2.51	114.73	110.24
7	D	644	BMA	C3-C4-C5	2.51	114.73	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	HEM	2	0
4	B	605	HEM	1	0
9	C	703	ACT	2	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(Å²)	Q<0.9
1	A	107/114 (93%)	0.58	6 (5%)	24	22	66, 67, 69, 70	0
1	B	108/114 (94%)	0.49	5 (4%)	32	31	66, 67, 69, 70	0
2	C	466/467 (99%)	0.61	42 (9%)	9	8	66, 67, 68, 69	0
2	D	466/467 (99%)	0.49	28 (6%)	22	19	66, 67, 68, 69	0
All	All	1147/1162 (98%)	0.55	81 (7%)	16	14	66, 67, 68, 70	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	579	SER	10.2
2	D	578	ALA	7.6
1	A	106	ARG	6.9
2	C	217	HIS	5.5
2	C	355	PRO	5.2
1	A	104	ALA	4.5
2	C	356	ASN	4.4
1	B	0	THR	4.4
2	C	192	ASN	4.3
2	C	373	LEU	4.2
2	C	578	ALA	4.1
2	C	194	LEU	4.0
2	D	217	HIS	3.9
2	C	558	PRO	3.8
1	A	3	GLU	3.8
1	A	0	THR	3.6
2	C	157	ASN	3.3
2	C	349	ARG	3.2
2	C	579	SER	3.1
2	D	195	GLY	3.1
2	C	113	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	372	VAL	3.0
2	C	114	ASN	2.9
2	C	122	GLN	2.9
2	C	218	ASP	2.9
2	C	191	SER	2.8
2	C	230	ILE	2.8
2	D	247	THR	2.8
1	A	105	ALA	2.8
2	C	215	ASN	2.8
2	C	203	PHE	2.8
2	C	115	CYS	2.7
2	C	199	VAL	2.7
2	D	349	ARG	2.6
2	D	355	PRO	2.6
2	C	559	ARG	2.6
2	D	523	GLN	2.5
2	C	425	SER	2.5
2	C	138	LYS	2.5
2	D	270	ARG	2.5
2	C	229	ARG	2.5
2	C	214	ASP	2.5
2	C	350	TYR	2.5
2	D	576	ARG	2.4
2	D	218	ASP	2.4
2	C	413	ILE	2.4
2	D	194	LEU	2.4
2	C	266	SER	2.4
2	C	576	ARG	2.4
1	B	3	GLU	2.4
2	D	565	SER	2.4
2	D	215	ASN	2.4
2	D	288	VAL	2.3
2	C	135	PRO	2.3
1	B	105	ALA	2.3
2	C	155	GLY	2.3
2	D	252	LEU	2.3
1	A	95	HIS	2.3
2	D	285	GLY	2.3
2	D	193	GLN	2.2
1	B	95	HIS	2.2
2	D	307	ARG	2.2
2	D	173	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	314	ARG	2.2
2	D	314	ARG	2.2
2	D	133	ASN	2.2
2	C	204	GLN	2.2
2	D	425	SER	2.1
2	C	363	ARG	2.1
2	D	286	ALA	2.1
2	C	566	THR	2.1
2	D	251	THR	2.1
2	C	315	SER	2.1
1	B	106	ARG	2.1
2	D	248	SER	2.1
2	C	158	ILE	2.1
2	C	421	ASN	2.1
2	D	292	THR	2.1
2	C	193	GLN	2.0
2	C	340	GLN	2.0
2	D	250	HIS	2.0

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSO	C	150	7/8	0.83	0.22	67,68,68,68	0
2	CSO	D	150	7/8	0.84	0.26	67,67,68,68	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BMA	C	643	11/12	0.68	0.35	69,69,69,70	0
6	NAG	C	630	14/15	0.74	0.50	65,66,66,66	0
7	BMA	D	643	11/12	0.75	0.35	68,68,68,69	0
9	ACT	C	703	4/4	0.80	0.31	69,69,69,69	0
7	BMA	D	644	11/12	0.82	0.26	67,67,68,68	0
6	NAG	D	630	14/15	0.83	0.34	65,65,65,66	0
7	BMA	C	644	11/12	0.84	0.24	66,67,67,67	0
6	NAG	D	620	14/15	0.84	0.30	65,65,65,65	0
5	CA	C	601	1/1	0.86	0.09	67,67,67,67	0
4	HEM	A	605	43/43	0.90	0.24	67,67,68,68	0
6	NAG	C	620	14/15	0.91	0.38	65,65,66,66	0
6	NAG	C	640	14/15	0.92	0.20	64,65,65,65	0
6	NAG	C	641	14/15	0.93	0.17	65,66,66,66	0
7	BMA	D	642	11/12	0.93	0.18	66,66,67,67	0
6	NAG	D	640	14/15	0.93	0.21	62,63,64,64	0
8	FUC	C	645	10/11	0.93	0.21	63,63,64,64	0
9	ACT	D	703	4/4	0.94	0.13	68,68,68,68	0
8	FUC	D	645	10/11	0.94	0.17	62,62,62,62	0
7	BMA	C	642	11/12	0.94	0.16	67,67,68,68	0
4	HEM	B	605	43/43	0.94	0.25	66,67,67,68	0
6	NAG	D	641	14/15	0.94	0.22	63,64,64,65	0
5	CA	D	601	1/1	0.96	0.15	67,67,67,67	0
3	CL	A	602	1/1	0.96	0.12	48,48,48,48	0
3	CL	D	602	1/1	0.97	0.09	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.