



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:35 AM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

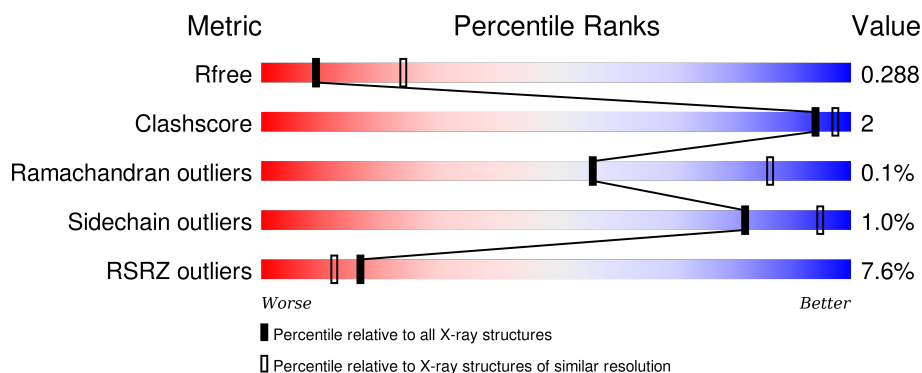
1 Overall quality at a glance i

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}	91344	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (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 ≥ 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>92%</div> <div>6%</div> </div>
1	B	114	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
2	C	467	<div> <div>10%</div> <div>94%</div> <div>6%</div> </div>
2	D	467	<div> <div>6%</div> <div>95%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 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 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: C₃₄H₃₂FeN₄O₄).



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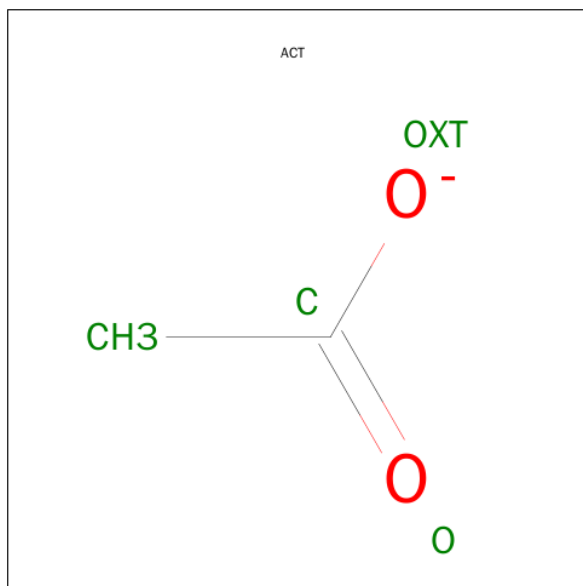
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- 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: $C_2H_3O_2$).

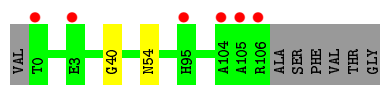


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

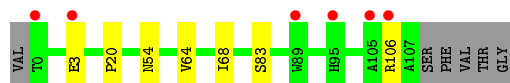
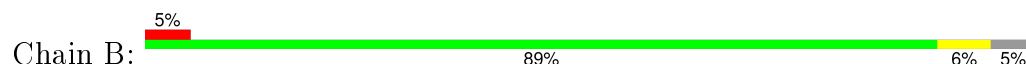
3 Residue-property plots [i](#)

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.

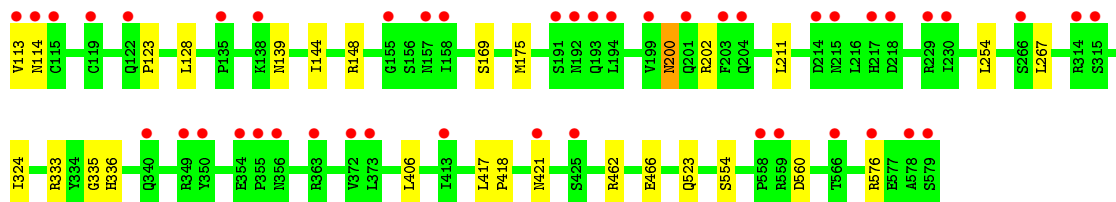
- Molecule 1: Myeloperoxidase



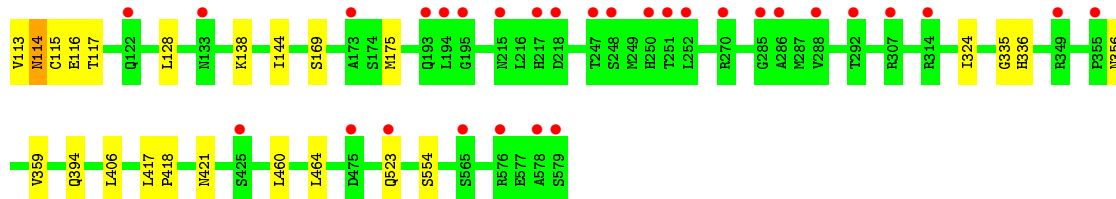
- Molecule 1: Myeloperoxidase



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.257 0.272 , 0.288	Depositor DCC
R_{free} test set	1709 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 8.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	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
5	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	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 [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	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%)	52	83
All	All	1139/1162 (98%)	1106 (97%)	32 (3%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	114	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/97 (95%)	91 (99%)	1 (1%)	80	94
1	B	92/97 (95%)	90 (98%)	2 (2%)	60	86
2	C	410/411 (100%)	406 (99%)	4 (1%)	82	95
2	D	410/411 (100%)	407 (99%)	3 (1%)	88	96
All	All	1004/1016 (99%)	994 (99%)	10 (1%)	82	95

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	3,6,7	0.56	0	1,6,8	2.01	1 (100%)
2	CSO	D	150	2	3,6,7	0.59	0	1,6,8	2.08	1 (100%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	150	CSO	O-C-CA	-2.08	120.06	125.49
2	C	150	CSO	O-C-CA	-2.01	120.25	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

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	14,14,15	0.51	0	15,19,21	1.02	0
7	NAG	C	641	7	14,14,15	0.45	0	15,19,21	0.65	0
7	BMA	C	642	7	11,11,12	0.49	0	14,15,17	0.93	0
7	BMA	C	643	7	11,11,12	0.57	0	14,15,17	0.67	0
7	BMA	C	644	7	11,11,12	0.60	0	14,15,17	1.30	2 (14%)
7	FUC	C	645	7	10,10,11	0.62	0	14,14,16	0.85	1 (7%)
7	NAG	D	640	2,7	14,14,15	0.51	0	15,19,21	1.04	1 (6%)
7	NAG	D	641	7	14,14,15	0.47	0	15,19,21	0.60	0
7	BMA	D	642	7	11,11,12	0.49	0	14,15,17	1.00	1 (7%)
7	BMA	D	643	7	11,11,12	0.54	0	14,15,17	0.57	0
7	BMA	D	644	7	11,11,12	0.54	0	14,15,17	1.05	1 (7%)
7	FUC	D	645	7	10,10,11	0.64	0	14,14,16	0.86	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
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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	644	BMA	C1-O5-C5	-2.48	109.10	112.25
7	D	642	BMA	C3-C4-C5	2.08	113.82	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	640	NAG	C1-O5-C5	2.39	115.29	112.25
7	D	645	FUC	O5-C5-C6	2.44	110.16	106.13
7	C	645	FUC	O5-C5-C6	2.48	110.23	106.13
7	C	644	BMA	C3-C4-C5	2.60	114.73	110.20
7	D	644	BMA	C3-C4-C5	2.60	114.73	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	30,50,50	2.25	11 (36%)	24,82,82	2.32	10 (41%)
5	HEM	B	605	1,2	30,50,50	2.22	9 (30%)	24,82,82	2.30	8 (33%)
6	NAG	C	620	2	14,14,15	0.49	0	15,19,21	0.74	0
6	NAG	C	630	2	14,14,15	0.47	0	15,19,21	0.65	0
8	ACT	C	703	-	1,3,3	1.20	0	0,3,3	0.00	-
6	NAG	D	620	2	14,14,15	0.53	0	15,19,21	0.77	0
6	NAG	D	630	2	14,14,15	0.48	0	15,19,21	0.67	0
8	ACT	D	703	-	1,3,3	1.24	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	-	0/10/54/54	0/0/8/8
5	HEM	B	605	1,2	-	0/10/54/54	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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	HEM	C3B-C4B	-6.93	1.45	1.51
5	A	605	HEM	C3B-C4B	-6.67	1.45	1.51
5	A	605	HEM	C3D-C4D	-5.00	1.45	1.51
5	B	605	HEM	C3D-C4D	-4.81	1.45	1.51
5	A	605	HEM	C2C-C1C	-3.65	1.45	1.52
5	B	605	HEM	C2C-C1C	-3.64	1.45	1.52
5	A	605	HEM	C2D-C1D	-2.02	1.45	1.51
5	B	605	HEM	C2D-C1D	-2.02	1.45	1.51
5	B	605	HEM	C1C-NC	2.04	1.38	1.36
5	A	605	HEM	C3B-CAB	2.06	1.55	1.51
5	A	605	HEM	C4C-NC	2.13	1.38	1.36
5	A	605	HEM	C3C-CAC	2.16	1.55	1.51
5	A	605	HEM	C1C-NC	2.25	1.38	1.36
5	B	605	HEM	C3C-CAC	2.31	1.55	1.51
5	B	605	HEM	FE-NB	2.52	2.10	1.97
5	A	605	HEM	FE-NB	2.87	2.12	1.97
5	B	605	HEM	FE-NC	2.93	2.07	1.95
5	B	605	HEM	FE-ND	3.05	2.13	1.97
5	A	605	HEM	FE-ND	3.14	2.14	1.97
5	A	605	HEM	FE-NC	3.20	2.08	1.95

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	605	HEM	C3B-CAB-CBB	-2.65	120.40	124.46
5	A	605	HEM	CBA-CAA-C2A	-2.63	107.82	112.53
5	A	605	HEM	C3B-CAB-CBB	-2.35	120.86	124.46
5	A	605	HEM	C2C-C1C-CHC	2.08	126.85	123.68
5	B	605	HEM	C2D-C3D-C4D	2.13	105.11	101.50
5	A	605	HEM	C2D-C3D-C4D	2.20	105.24	101.50
5	B	605	HEM	C3B-C4B-CHC	2.39	126.53	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	HEM	C3B-C4B-CHC	2.61	126.83	123.16
5	A	605	HEM	CMD-C2D-C3D	2.89	127.11	114.35
5	B	605	HEM	CMD-C2D-C3D	2.89	127.14	114.35
5	A	605	HEM	CMC-C2C-C3C	3.97	126.43	116.53
5	B	605	HEM	CMB-C2B-C3B	4.07	126.69	116.53
5	A	605	HEM	CMB-C2B-C3B	4.18	126.96	116.53
5	A	605	HEM	CAD-C3D-C4D	4.27	127.54	112.47
5	B	605	HEM	CAD-C3D-C4D	4.35	127.81	112.47
5	B	605	HEM	CMC-C2C-C3C	4.37	127.43	116.53
5	B	605	HEM	CAD-C3D-C2D	4.82	127.09	113.22
5	A	605	HEM	CAD-C3D-C2D	4.87	127.22	113.22

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
5	A	605	HEM	2	0
5	B	605	HEM	1	0
8	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, 95th 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 ²)	Q<0.9
1	A	107/114 (93%)	0.60	6 (5%)	28 23	66, 67, 69, 70	0
1	B	108/114 (94%)	0.51	6 (5%)	28 23	66, 67, 69, 70	0
2	C	466/467 (99%)	0.63	45 (9%)	10 7	66, 67, 68, 69	0
2	D	466/467 (99%)	0.51	30 (6%)	23 18	66, 67, 68, 69	0
All	All	1147/1162 (98%)	0.56	87 (7%)	17 12	66, 67, 68, 70	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	579	SER	10.3
2	D	578	ALA	7.6
1	A	106	ARG	6.6
2	C	217	HIS	5.5
2	C	355	PRO	5.3
2	C	356	ASN	4.5
1	B	0	THR	4.5
1	A	104	ALA	4.5
2	C	192	ASN	4.5
2	C	373	LEU	4.3
2	C	578	ALA	4.1
2	C	194	LEU	4.0
2	C	558	PRO	3.9
2	D	217	HIS	3.9
1	A	3	GLU	3.9
1	A	0	THR	3.7
2	C	157	ASN	3.4
2	C	579	SER	3.2
2	D	195	GLY	3.1
2	C	349	ARG	3.1
2	C	114	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	3.0
2	C	122	GLN	3.0
2	C	372	VAL	3.0
2	C	218	ASP	3.0
2	C	191	SER	2.9
2	C	215	ASN	2.9
2	D	247	THR	2.9
2	C	230	ILE	2.9
2	C	115	CYS	2.8
2	C	203	PHE	2.8
1	A	105	ALA	2.8
2	D	355	PRO	2.7
2	C	199	VAL	2.7
2	D	523	GLN	2.6
2	C	214	ASP	2.6
2	C	425	SER	2.5
2	C	138	LYS	2.5
2	D	218	ASP	2.5
2	C	559	ARG	2.5
2	C	350	TYR	2.5
2	D	349	ARG	2.5
2	C	266	SER	2.5
2	C	413	ILE	2.5
2	D	215	ASN	2.5
1	B	3	GLU	2.5
2	D	194	LEU	2.4
2	D	565	SER	2.4
2	C	135	PRO	2.4
2	C	229	ARG	2.4
2	D	270	ARG	2.4
2	D	288	VAL	2.4
2	D	576	ARG	2.4
2	D	252	LEU	2.4
2	C	155	GLY	2.4
2	D	193	GLN	2.3
2	C	576	ARG	2.3
1	A	95	HIS	2.3
1	B	105	ALA	2.3
2	D	285	GLY	2.3
1	B	95	HIS	2.2
2	C	204	GLN	2.2
2	D	133	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	425	SER	2.2
2	C	566	THR	2.2
2	D	251	THR	2.2
2	D	248	SER	2.2
2	C	315	SER	2.1
2	C	421	ASN	2.1
2	D	173	ALA	2.1
2	C	340	GLN	2.1
2	D	292	THR	2.1
2	C	193	GLN	2.1
2	C	158	ILE	2.1
2	D	286	ALA	2.1
2	D	307	ARG	2.1
2	C	314	ARG	2.1
2	D	475	ASP	2.1
2	D	314	ARG	2.1
2	C	201	GLN	2.1
1	B	89	TRP	2.1
2	D	250	HIS	2.1
2	C	119	CYS	2.0
1	B	106	ARG	2.0
2	C	363	ARG	2.0
2	C	354	GLU	2.0
2	D	122	GLN	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. 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, 95th 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 ²)	Q<0.9
2	CSO	D	150	7/8	0.84	0.26	-	67,67,68,68	0
2	CSO	C	150	7/8	0.83	0.22	-	67,68,68,68	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, 95th 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 ²)	Q<0.9
7	NAG	D	641	14/15	0.94	0.22	0.32	63,64,64,65	0
7	BMA	D	642	11/12	0.93	0.18	-0.85	66,66,67,67	0
7	NAG	C	641	14/15	0.93	0.17	-1.08	65,66,66,66	0
7	BMA	C	642	11/12	0.94	0.16	-1.25	67,67,68,68	0
7	BMA	C	644	11/12	0.84	0.24	-	66,67,67,67	0
7	BMA	D	644	11/12	0.82	0.26	-	67,67,68,68	0
7	NAG	D	640	14/15	0.93	0.21	-	62,63,64,64	0
7	FUC	C	645	10/11	0.93	0.22	-	63,63,64,64	0
7	NAG	C	640	14/15	0.92	0.20	-	64,65,65,65	0
7	FUC	D	645	10/11	0.95	0.17	-	62,62,62,62	0
7	BMA	C	643	11/12	0.68	0.35	-	69,69,69,70	0
7	BMA	D	643	11/12	0.75	0.35	-	68,68,68,69	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, 95th 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 ²)	Q<0.9
6	NAG	D	630	14/15	0.83	0.34	1.98	65,65,65,66	0
6	NAG	C	630	14/15	0.74	0.50	1.61	65,66,66,66	0
6	NAG	C	620	14/15	0.91	0.38	0.15	65,65,66,66	0
6	NAG	D	620	14/15	0.84	0.31	0.09	65,65,65,65	0
5	HEM	B	605	43/43	0.94	0.25	-0.20	66,67,67,68	0
5	HEM	A	605	43/43	0.90	0.24	-0.29	67,67,68,68	0
3	CA	D	601	1/1	0.96	0.15	-2.58	67,67,67,67	0
4	CL	A	602	1/1	0.96	0.12	-2.65	48,48,48,48	0
3	CA	C	601	1/1	0.86	0.09	-3.29	67,67,67,67	0
4	CL	D	602	1/1	0.97	0.09	-5.65	53,53,53,53	0
8	ACT	D	703	4/4	0.94	0.13	-	68,68,68,68	0
8	ACT	C	703	4/4	0.80	0.32	-	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.