Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 11:09 PM GMT

PDB ID	:	5FIW
Title	:	CRYSTAL STRUCTURE OF HUMAN MYELOPEROXIDASE AT 1.7 ANGSTROMS RESOLUTION
Authors	:	Bonnefond, L.; Cavarelli, J.
Deposited on	:	2015-10-02
Resolution	:	1.70 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

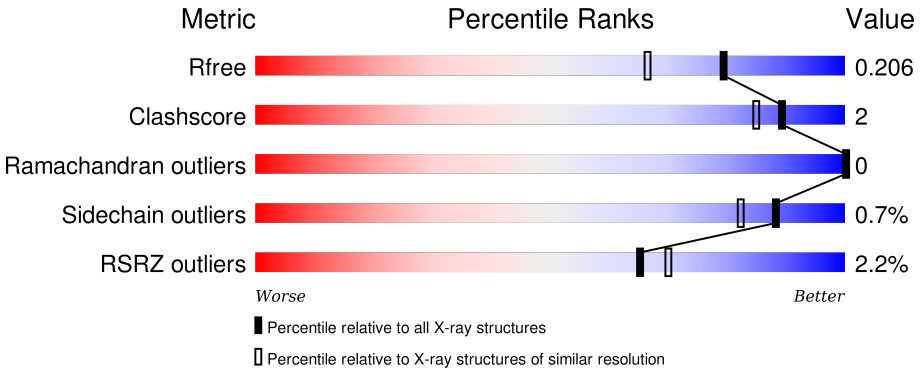
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 <=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	105	4% 97%
1	B	105	5% 94%
2	C	466	2% 94% 5%
2	D	466	2% 94% 5%

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	620	-	-	-	X
6	NAG	C	630	-	-	-	X
6	NAG	D	630	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10331 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	105	Total	C	N	O	S	0	0	0
			842	532	149	156	5			
1	B	103	Total	C	N	O	S	0	0	0
			832	526	147	154	5			

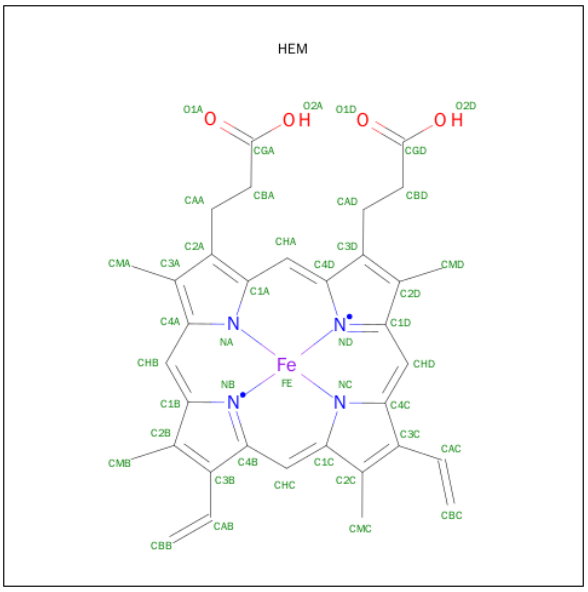
- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	464	Total	C	N	O	S	0	0	0
			3720	2343	685	665	27			
2	D	464	Total	C	N	O	S	0	0	0
			3720	2343	685	665	27			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	2	Total	Cl	0	0
			2	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

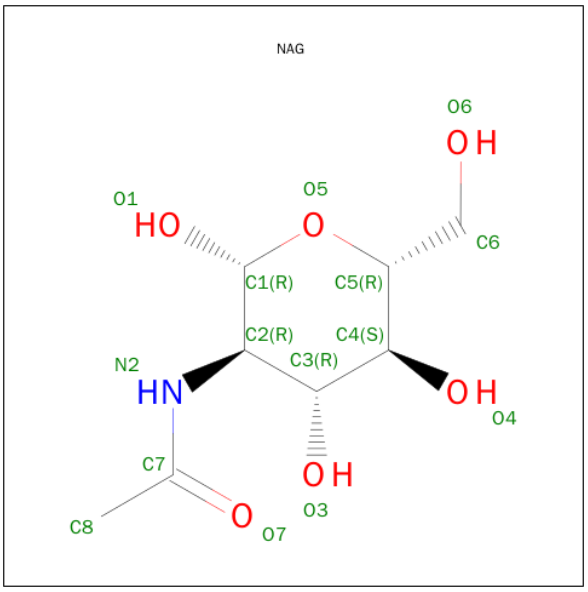


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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

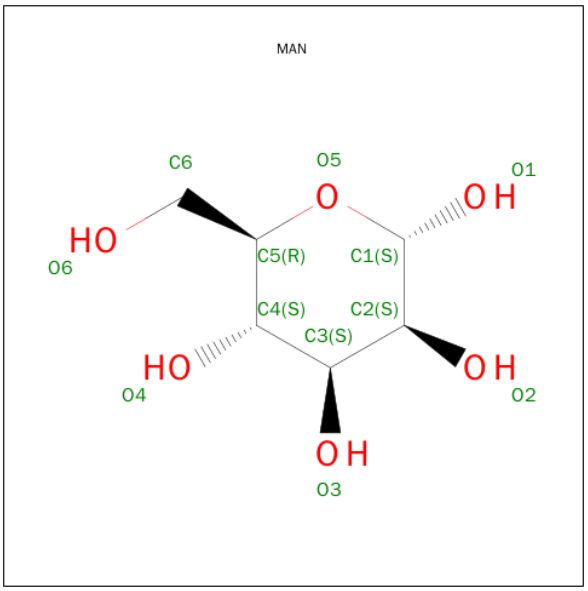


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

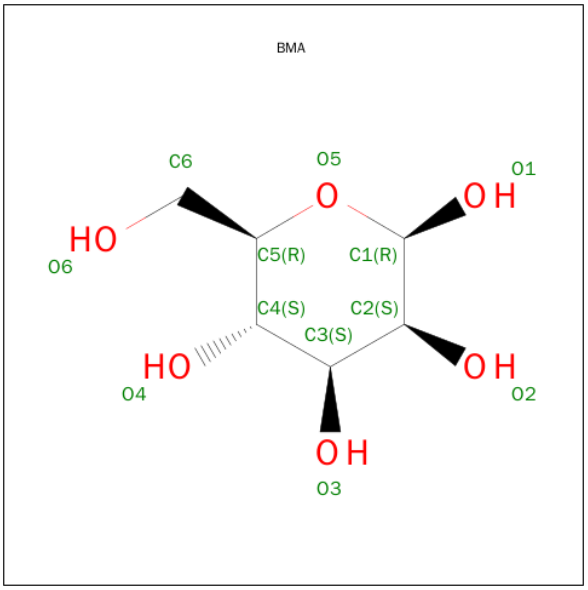
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	4	Total C N O 49 28 2 19	0	0

- Molecule 8 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 9 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

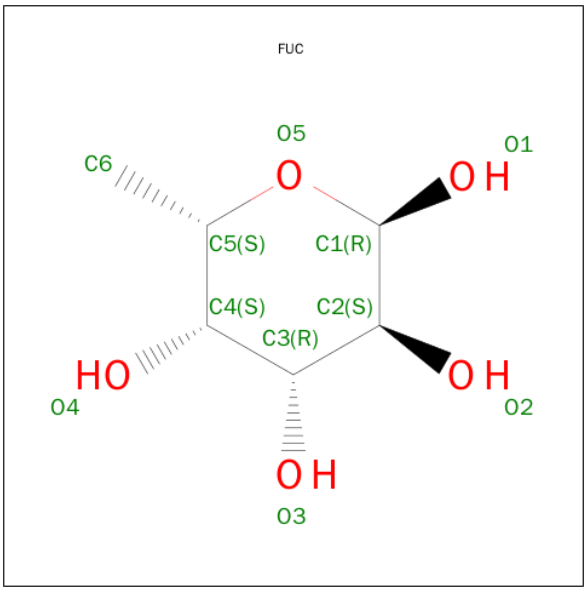


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 11 6 5	0	0
9	D	1	Total C O 11 6 5	0	0

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 12 is water.

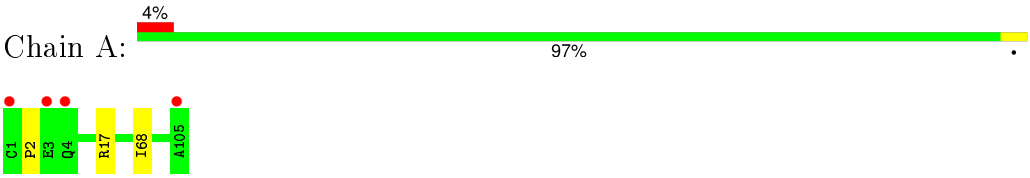
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	129	Total	O	0	0
			129	129		
12	B	118	Total	O	0	0
			118	118		
12	C	334	Total	O	0	0
			334	334		
12	D	345	Total	O	0	0
			345	345		

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.

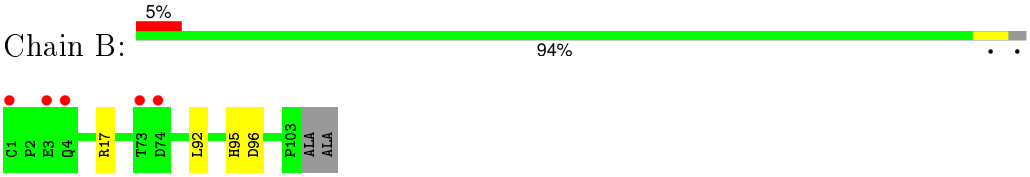
- Molecule 1: MYELOPEROXIDASE

Chain A:



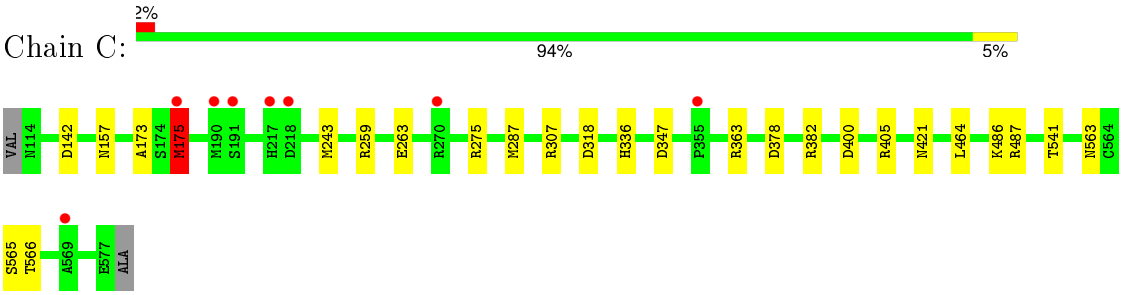
- Molecule 1: MYELOPEROXIDASE

Chain B:



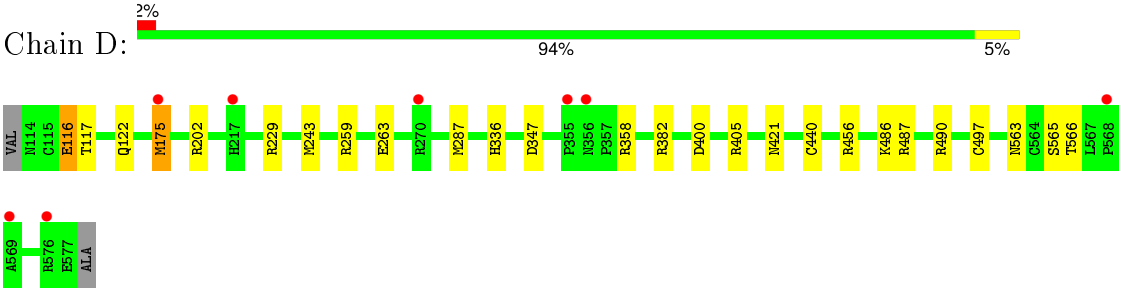
- Molecule 2: MYELOPEROXIDASE

Chain C:



- Molecule 2: MYELOPEROXIDASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.16Å 105.16Å 225.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.31 – 1.70 52.87 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.31-1.70) 99.8 (52.87-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.163 , 0.193 0.178 , 0.206	Depositor DCC
R_{free} test set	6869 reflections (5.22%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	2 of 138420 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10331	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 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	0.76	0/867	0.91	0/1181
1	B	0.75	0/857	0.94	1/1167 (0.1%)
2	C	0.74	0/3798	0.88	12/5151 (0.2%)
2	D	0.78	4/3798 (0.1%)	0.89	14/5151 (0.3%)
All	All	0.76	4/9320 (0.0%)	0.89	27/12650 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	116	GLU	CD-OE2	9.72	1.36	1.25
2	D	116	GLU	CG-CD	6.16	1.61	1.51
2	D	116	GLU	CB-CG	5.60	1.62	1.52
2	D	175	MET	CA-CB	5.04	1.65	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	243	MET	CG-SD-CE	8.77	114.23	100.20
2	C	243	MET	CG-SD-CE	8.11	113.17	100.20
2	C	175	MET	CG-SD-CE	-6.92	89.14	100.20
2	C	382	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	D	358	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	C	347	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	17	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	D	382	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	D	490	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	D	287	MET	CG-SD-CE	-5.90	90.77	100.20
2	D	382	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	D	229	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	D	175	MET	CB-CG-SD	5.56	129.08	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	287	MET	CG-SD-CE	-5.51	91.39	100.20
2	C	405	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	C	487	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	D	400	ASP	CB-CG-OD1	5.40	123.16	118.30
2	D	456	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	D	487	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	C	142	ASP	CB-CG-OD1	5.36	123.13	118.30
2	D	347	ASP	CB-CG-OD1	5.35	123.12	118.30
2	D	486	LYS	CB-CG-CD	5.31	125.40	111.60
2	C	363	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	D	405	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	C	275	ARG	NE-CZ-NH1	5.05	122.82	120.30
2	C	382	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	C	400	ASP	CB-CG-OD1	5.02	122.82	118.30

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	842	0	803	3	0
1	B	832	0	793	8	0
2	C	3720	0	3713	9	0
2	D	3720	0	3713	13	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
7	C	49	0	43	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	11	0	10	2	0
8	D	11	0	10	2	0
9	C	11	0	10	3	0
9	D	11	0	10	3	0
10	D	39	0	33	7	0
11	D	10	0	10	2	0
12	A	129	0	0	0	0
12	B	118	0	0	1	0
12	C	334	0	0	2	0
12	D	345	0	0	5	0
All	All	10331	0	9260	39	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 (39) 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)
7:C:642:BMA:O6	9:C:644:BMA:C1	2.00	1.09
10:D:642:BMA:O6	9:D:644:BMA:C1	2.02	1.08
7:C:642:BMA:C6	9:C:644:BMA:C1	2.36	1.03
7:C:642:BMA:H61	9:C:644:BMA:C1	2.00	0.89
10:D:642:BMA:C6	9:D:644:BMA:C1	2.51	0.88
2:D:202:ARG:NH2	12:D:2099:HOH:O	2.07	0.86
2:D:440:CYS:HG	2:D:497:CYS:HG	1.11	0.82
7:C:642:BMA:C3	8:C:643:MAN:C1	2.60	0.80
2:C:157:ASN:ND2	12:C:2060:HOH:O	2.16	0.77
1:B:96:ASP:HB2	2:D:175:MET:HE3	1.66	0.76
10:D:642:BMA:C3	8:D:643:MAN:C1	2.63	0.76
10:D:640:NAG:C6	11:D:645:FUC:C1	2.64	0.75
2:C:336:HIS:HD1	2:C:421:ASN:HD21	1.38	0.71
2:D:336:HIS:HD1	2:D:421:ASN:HD21	1.38	0.71
7:C:642:BMA:O3	8:C:643:MAN:C2	2.44	0.66
10:D:642:BMA:O3	8:D:643:MAN:C2	2.43	0.65
10:D:642:BMA:H61	9:D:644:BMA:C1	2.27	0.64
1:B:92:LEU:HG	2:D:175:MET:HE2	1.80	0.64
1:B:95:HIS:HD2	12:D:2134:HOH:O	1.85	0.59
1:B:92:LEU:O	2:D:175:MET:CE	2.51	0.58
2:C:259:ARG:NH1	2:C:263:GLU:OE2	2.38	0.56
10:D:640:NAG:O6	11:D:645:FUC:C2	2.49	0.55
2:D:259:ARG:NH1	2:D:263:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:563:ASN:OD1	2:C:566:THR:HG23	2.10	0.52
2:D:563:ASN:OD1	2:D:566:THR:HG23	2.10	0.51
2:D:116:GLU:HG3	2:D:117:THR:HG23	1.93	0.51
2:D:563:ASN:ND2	12:D:2327:HOH:O	2.24	0.50
4:B:605:HEM:HMC1	4:B:605:HEM:HBC2	1.94	0.49
2:C:173:ALA:HA	2:C:175:MET:HE1	1.94	0.49
1:B:92:LEU:HG	2:D:175:MET:CE	2.43	0.48
2:C:563:ASN:ND2	12:C:2313:HOH:O	2.41	0.47
1:B:95:HIS:CD2	12:D:2134:HOH:O	2.65	0.47
1:A:2:PRO:O	1:A:17:ARG:NH1	2.50	0.45
2:D:563:ASN:ND2	12:D:2328:HOH:O	2.48	0.45
1:B:92:LEU:O	2:D:175:MET:HE2	2.16	0.43
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.49	0.42
1:A:68:ILE:HD13	2:C:464:LEU:HD23	2.00	0.42
1:B:95:HIS:HE1	12:B:2107:HOH:O	2.02	0.41
2:C:378:ASP:OD1	2:C:541:THR:HB	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
1	B	101/105 (96%)	100 (99%)	1 (1%)	0	100	100
2	C	461/466 (99%)	452 (98%)	9 (2%)	0	100	100
2	D	461/466 (99%)	454 (98%)	7 (2%)	0	100	100
All	All	1126/1142 (99%)	1107 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	90 (100%)	0	100	100
2	C	409/410 (100%)	404 (99%)	5 (1%)	78	65
2	D	409/410 (100%)	407 (100%)	2 (0%)	92	88
All	All	998/1000 (100%)	991 (99%)	7 (1%)	88	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	175	MET
2	C	307	ARG
2	C	318	ASP
2	C	486	LYS
2	C	565	SER
2	D	122	GLN
2	D	565	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	HIS
2	C	250	HIS
2	C	396	GLN
2	C	523	GLN
2	D	250	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	0.81	0	2,6,8	1.36	0
2	CSO	D	150	2	3,6,7	0.79	0	2,6,8	1.37	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

There are no bond length outliers.

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 (i)

7 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	0.42	0	15,19,21	1.20	2 (13%)
7	NAG	C	641	7	14,14,15	1.11	1 (7%)	15,19,21	1.42	3 (20%)
7	BMA	C	642	8,7	11,11,12	0.93	0	15,15,17	2.43	5 (33%)
7	FUC	C	645	7	10,10,11	0.59	0	13,14,16	1.27	3 (23%)
10	NAG	D	640	11,10,2	14,14,15	0.44	0	15,19,21	2.20	6 (40%)
10	NAG	D	641	10	14,14,15	0.94	1 (7%)	15,19,21	1.22	1 (6%)
10	BMA	D	642	10,8	11,11,12	1.07	0	15,15,17	2.75	6 (40%)

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	8,7	-	0/2/19/22	0/1/1/1
7	FUC	C	645	7	-	0/0/17/20	0/1/1/1
10	NAG	D	640	11,10,2	-	0/6/23/26	0/1/1/1
10	NAG	D	641	10	-	0/6/23/26	0/1/1/1
10	BMA	D	642	10,8	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	641	NAG	O5-C1	-2.28	1.40	1.43
7	C	641	NAG	O5-C1	-2.26	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	642	BMA	C1-C2-C3	-7.84	100.06	109.55
7	C	642	BMA	C1-C2-C3	-4.53	104.06	109.55
7	C	642	BMA	C6-C5-C4	-4.46	101.81	112.99
10	D	640	NAG	O5-C5-C4	-4.07	103.40	110.13
10	D	642	BMA	O3-C3-C2	-3.88	102.90	110.01
10	D	641	NAG	C4-C3-C2	-3.74	105.54	111.34
7	C	642	BMA	O3-C3-C4	-3.70	102.02	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	640	NAG	O4-C4-C5	-3.49	100.04	109.23
10	D	640	NAG	O4-C4-C3	-2.84	103.96	110.36
7	C	642	BMA	O3-C3-C2	-2.82	104.84	110.01
7	C	641	NAG	C1-O5-C5	-2.81	108.00	112.14
10	D	642	BMA	C1-O5-C5	-2.77	108.07	112.14
7	C	645	FUC	O3-C3-C2	-2.71	105.04	110.01
7	C	641	NAG	C4-C3-C2	-2.57	107.35	111.34
10	D	642	BMA	C6-C5-C4	-2.24	107.37	112.99
10	D	640	NAG	C4-C3-C2	-2.22	107.89	111.34
7	C	645	FUC	O4-C4-C3	-2.13	105.56	110.36
7	C	640	NAG	O4-C4-C3	-2.10	105.63	110.36
7	C	640	NAG	C3-C4-C5	2.03	113.84	110.23
7	C	645	FUC	O5-C1-C2	2.09	114.24	110.89
10	D	640	NAG	C1-O5-C5	2.09	115.22	112.14
10	D	642	BMA	C2-C3-C4	2.77	115.87	111.05
10	D	642	BMA	O5-C5-C6	2.93	113.61	107.34
10	D	640	NAG	C3-C4-C5	2.93	115.46	110.23
7	C	641	NAG	O3-C3-C4	3.66	118.60	110.36
7	C	642	BMA	O5-C5-C6	4.45	116.87	107.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	642	BMA	5	0
10	D	640	NAG	2	0
10	D	642	BMA	5	0

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HEM	A	605	1,2	24,50,50	2.16	5 (20%)	16,82,82	2.26	7 (43%)
4	HEM	B	605	1,2	24,50,50	2.08	5 (20%)	16,82,82	1.83	6 (37%)
6	NAG	C	620	2	14,14,15	0.80	0	15,19,21	0.97	1 (6%)
6	NAG	C	630	2	14,14,15	0.59	0	15,19,21	1.36	2 (13%)
8	MAN	C	643	7	11,11,12	0.44	0	15,15,17	1.81	3 (20%)
9	BMA	C	644	-	11,11,12	0.45	0	15,15,17	1.05	1 (6%)
6	NAG	D	620	2	14,14,15	0.84	0	15,19,21	1.01	1 (6%)
6	NAG	D	630	2	14,14,15	0.48	0	15,19,21	0.80	0
8	MAN	D	643	10	11,11,12	0.59	0	15,15,17	1.94	5 (33%)
9	BMA	D	644	-	11,11,12	0.72	0	15,15,17	1.15	2 (13%)
11	FUC	D	645	10	10,10,11	0.88	0	13,14,16	0.95	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
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
6	NAG	C	630	2	-	0/6/23/26	0/1/1/1
8	MAN	C	643	7	-	0/2/19/22	0/1/1/1
9	BMA	C	644	-	-	0/2/19/22	0/1/1/1
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	MAN	D	643	10	-	0/2/19/22	0/1/1/1
9	BMA	D	644	-	-	0/2/19/22	0/1/1/1
11	FUC	D	645	10	-	0/0/17/20	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	HEM	C1C-NC	-4.73	1.30	1.36
4	B	605	HEM	C1B-NB	-4.24	1.31	1.36
4	B	605	HEM	C3B-C2B	-3.94	1.35	1.40
4	B	605	HEM	C4D-ND	-3.61	1.31	1.36
4	A	605	HEM	C1C-NC	-2.80	1.33	1.36
4	A	605	HEM	C3B-CAB	2.85	1.53	1.47
4	A	605	HEM	C1B-NB	4.19	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	C4D-ND	4.68	1.43	1.36
4	B	605	HEM	C4C-NC	4.69	1.43	1.36
4	A	605	HEM	C4C-NC	6.77	1.45	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	605	HEM	CBD-CAD-C3D	-3.61	106.13	112.47
4	B	605	HEM	CBA-CAA-C2A	-3.57	106.22	112.49
4	A	605	HEM	C3C-C4C-NC	-3.22	104.87	110.94
4	B	605	HEM	CBD-CAD-C3D	-3.18	106.89	112.47
4	A	605	HEM	CBA-CAA-C2A	-3.15	106.95	112.49
8	D	643	MAN	O2-C2-C1	-2.80	103.62	109.23
4	B	605	HEM	C3C-C4C-NC	-2.73	105.80	110.94
9	C	644	BMA	O2-C2-C1	-2.50	104.22	109.23
6	C	630	NAG	O6-C6-C5	-2.47	103.04	111.30
9	D	644	BMA	C2-C3-C4	-2.45	106.77	111.05
9	D	644	BMA	O2-C2-C1	-2.33	104.58	109.23
8	C	643	MAN	O2-C2-C1	-2.26	104.71	109.23
8	D	643	MAN	O4-C4-C3	-2.17	105.47	110.36
6	D	620	NAG	O3-C3-C2	-2.12	104.84	109.37
4	B	605	HEM	CMC-C2C-C3C	2.03	129.06	125.09
4	A	605	HEM	CMB-C2B-C3B	2.09	129.18	125.09
11	D	645	FUC	O5-C1-C2	2.10	114.26	110.89
6	C	620	NAG	O4-C4-C3	2.12	115.14	110.36
4	A	605	HEM	C3C-CAC-CBC	2.19	130.80	126.40
4	B	605	HEM	CAD-CBD-CGD	2.23	117.12	112.78
8	C	643	MAN	C1-O5-C5	2.37	115.63	112.14
4	A	605	HEM	C3B-C4B-NB	2.46	112.39	109.21
4	B	605	HEM	CMB-C2B-C3B	2.60	130.17	125.09
6	C	630	NAG	C1-O5-C5	3.01	116.57	112.14
8	D	643	MAN	C1-C2-C3	3.15	113.36	109.55
8	D	643	MAN	C1-O5-C5	3.19	116.83	112.14
8	D	643	MAN	O5-C1-C2	4.05	117.37	110.89
4	A	605	HEM	C3B-CAB-CBB	4.89	136.22	126.40
8	C	643	MAN	O5-C1-C2	5.23	119.26	110.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	605	HEM	1	0
8	C	643	MAN	2	0
9	C	644	BMA	3	0
8	D	643	MAN	2	0
9	D	644	BMA	3	0
11	D	645	FUC	2	0

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^{th} 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	105/105 (100%)	0.26	4 (3%) 44 49	14, 19, 40, 81	0
1	B	103/105 (98%)	0.24	5 (4%) 33 36	14, 19, 41, 74	0
2	C	463/466 (99%)	0.18	8 (1%) 73 77	13, 20, 40, 80	0
2	D	463/466 (99%)	0.18	8 (1%) 73 77	13, 20, 41, 65	0
All	All	1134/1142 (99%)	0.19	25 (2%) 65 70	13, 20, 41, 81	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	355	PRO	4.2
1	A	1	CYS	3.9
1	A	3	GLU	3.8
2	D	569	ALA	3.5
2	C	217	HIS	3.5
2	C	190	MET	3.4
2	C	218	ASP	3.3
2	D	568	PRO	2.9
2	D	217	HIS	2.9
1	B	74	ASP	2.8
1	B	4	GLN	2.8
2	D	576	ARG	2.8
2	C	270	ARG	2.8
2	C	569	ALA	2.6
1	B	1	CYS	2.6
1	A	105	ALA	2.5
1	A	4	GLN	2.5
2	D	356	ASN	2.3
2	D	270	ARG	2.3
2	C	191	SER	2.2
1	B	3	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	175	MET	2.1
2	D	355	PRO	2.1
1	B	73	THR	2.1
2	C	175	MET	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, 95^{th} 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	C	150	7/8	0.96	0.09	-	12,17,26,36	0
2	CSO	D	150	7/8	0.96	0.12	-	14,16,27,40	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^{th} 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	BMA	C	642	11/12	0.85	0.12	0.63	17,20,24,71	0
10	BMA	D	642	11/12	0.94	0.11	0.48	16,21,24,63	0
10	NAG	D	641	14/15	0.96	0.10	-0.29	12,16,19,19	0
7	NAG	C	641	14/15	0.96	0.09	-0.44	14,16,18,19	0
7	NAG	C	640	14/15	0.94	0.09	-1.10	13,17,27,30	0
7	FUC	C	645	10/11	0.94	0.10	-	21,24,26,28	0
10	NAG	D	640	14/15	0.94	0.09	-	14,17,24,26	0

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. 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^{th} 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	C	630	14/15	0.84	0.28	13.60	29,41,53,78	0
6	NAG	D	630	14/15	0.86	0.29	5.09	38,56,77,78	0
6	NAG	C	620	14/15	0.78	0.23	2.67	23,29,41,43	0
5	CA	D	701	1/1	1.00	0.12	1.50	10,10,10,10	1
3	CL	B	201	1/1	1.00	0.13	1.27	14,14,14,14	0
4	HEM	A	605	43/43	0.95	0.11	1.25	12,15,19,60	0
4	HEM	B	605	43/43	0.94	0.12	1.23	11,15,20,37	0
6	NAG	D	620	14/15	0.86	0.12	1.10	23,29,40,43	0
3	CL	A	602	1/1	0.99	0.13	0.66	14,14,14,14	0
3	CL	D	612	1/1	0.98	0.11	0.46	27,27,27,27	0
5	CA	C	601	1/1	1.00	0.10	-0.02	14,14,14,14	0
3	CL	C	611	1/1	0.99	0.09	-0.13	22,22,22,22	0
3	CL	C	612	1/1	0.98	0.09	-0.47	29,29,29,29	0
8	MAN	C	643	11/12	0.83	0.16	-	34,39,44,57	0
9	BMA	D	644	11/12	0.88	0.10	-	22,24,29,33	0
11	FUC	D	645	10/11	0.91	0.10	-	23,25,27,27	0
8	MAN	D	643	11/12	0.74	0.21	-	38,44,51,63	0
9	BMA	C	644	11/12	0.81	0.12	-	24,27,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.