Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:17 PM GMT

PDB ID	:	4C1M
Title	:	Myeloperoxidase in complex with the revesible inhibitor HX1
Authors	:	Forbes, L.V.; Sjogren, T.; Auchere, F.; Jenkins, D.W.; Thong, B.; Laughton, D.; Hemsley, P.; Pairaudeau, G.; Eriksson, H.; Unitt, J.F.; Kettle, A.J.
Deposited on	:	2013-08-13
Resolution	:	2.00 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:

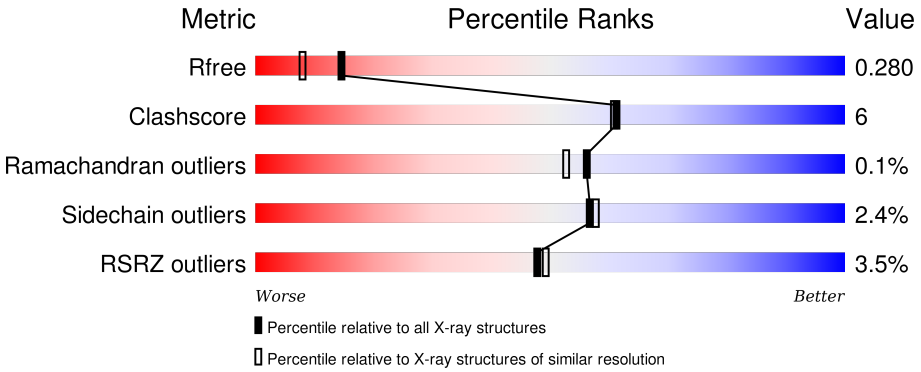
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	108	3%, 82%, 11%, 6%
1	B	108	3%, 84%, 12%
2	C	467	2%, 91%, 9%
2	D	467	6%, 87%, 12%

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
11	BMA	C	1642	-	-	-	X
11	BMA	D	2642	-	-	-	X
4	NIH	A	606	-	-	-	X
4	NIH	B	606	-	-	-	X
9	ACT	D	1581	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10168 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

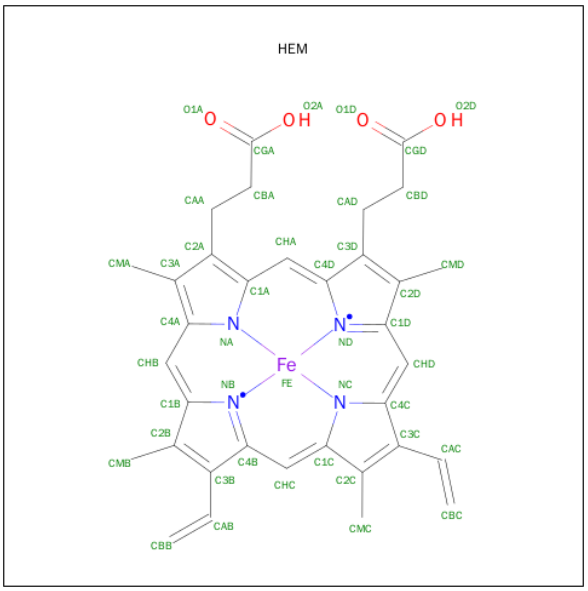
- Molecule 1 is a protein called MYELOPEROXIDASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	1
			816	516	146	150	4			
1	B	105	Total	C	N	O	S	0	0	1
			838	529	149	155	5			

- Molecule 2 is a protein called MYELOPEROXIDASE HEAVY CHAIN.

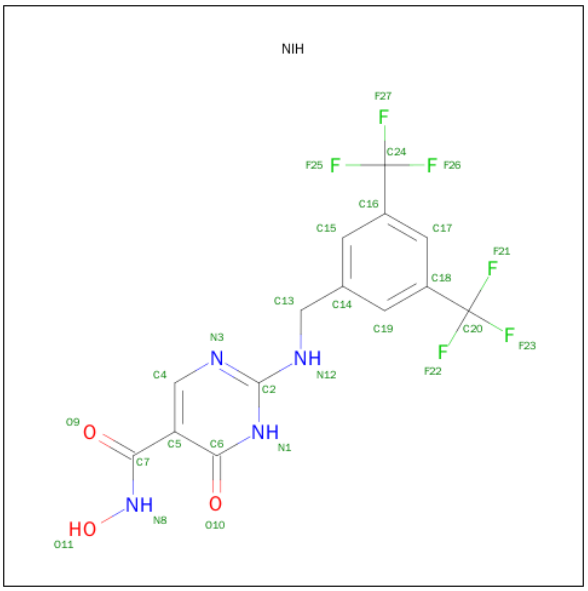
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			
2	D	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



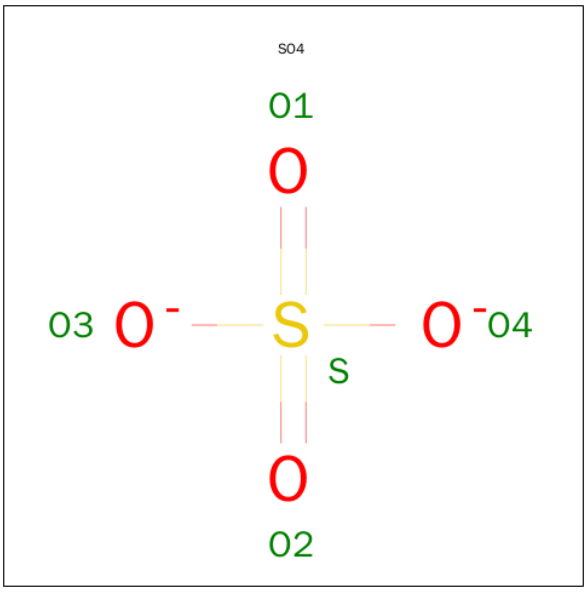
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is 2-{[3,5-BIS(TRIFLUOROMETHYL)BENZYL]AMINO}-N-HYDROXY-6-OXO-1,6-DIHYDROPYRIMIDINE-5-CARBOXAMIDE (three-letter code: NIH) (formula: $C_{14}H_{10}F_6N_4O_3$).



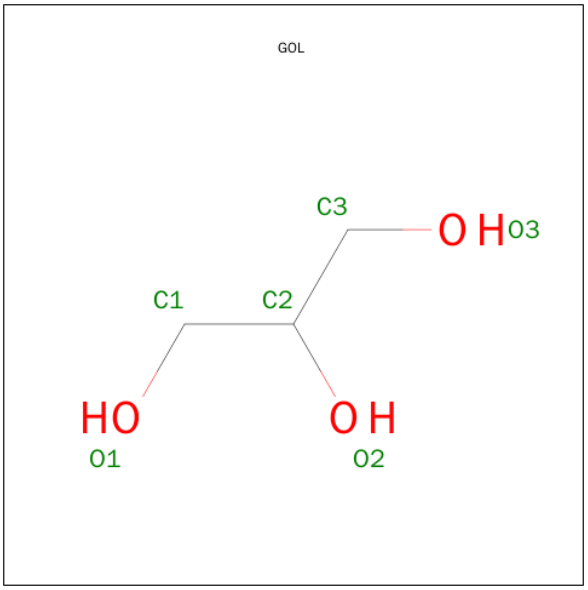
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	14	6	4	3		
4	B	1	Total	C	F	N	O	0	0
			27	14	6	4	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0

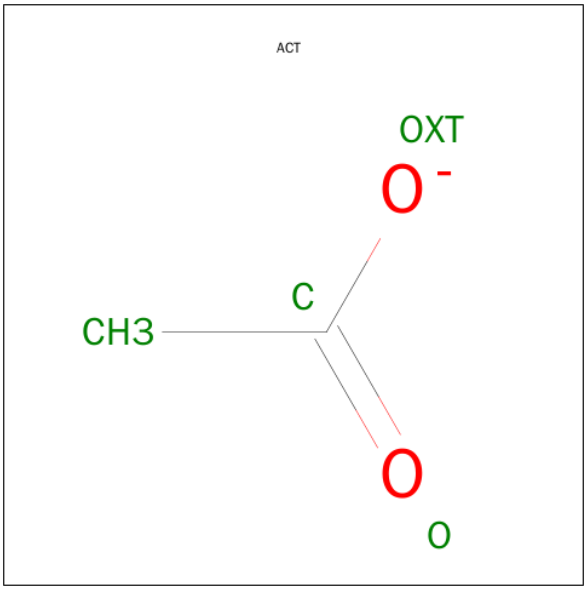
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

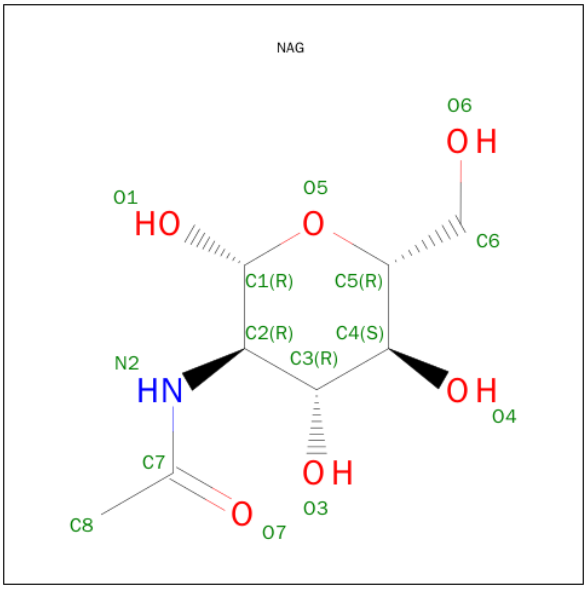
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Cl 1 1	0	0
8	C	1	Total Cl 1 1	0	0

- 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 4 2 2	0	0
9	C	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0
9	D	1	Total C O 4 2 2	0	0

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	103	Total O 103 103	0	0
12	B	108	Total O 108 108	0	0

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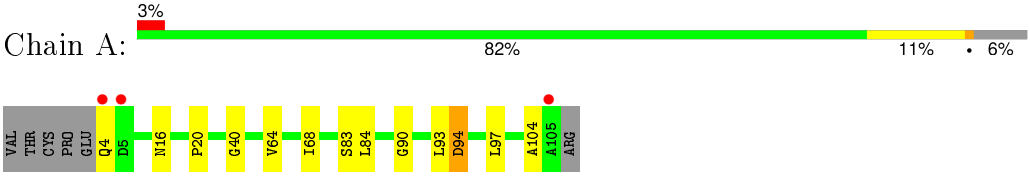
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	254	Total O 254 254	0	0
12	D	199	Total O 199 199	0	0

3 Residue-property plots (i)

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

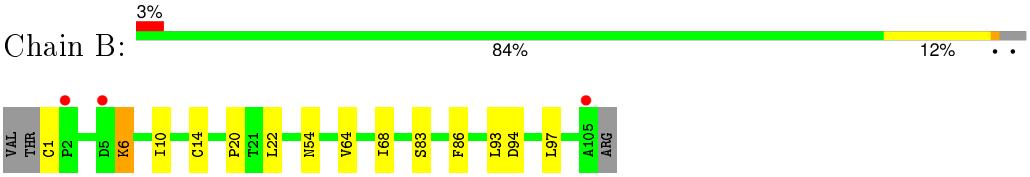
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN

Chain A:



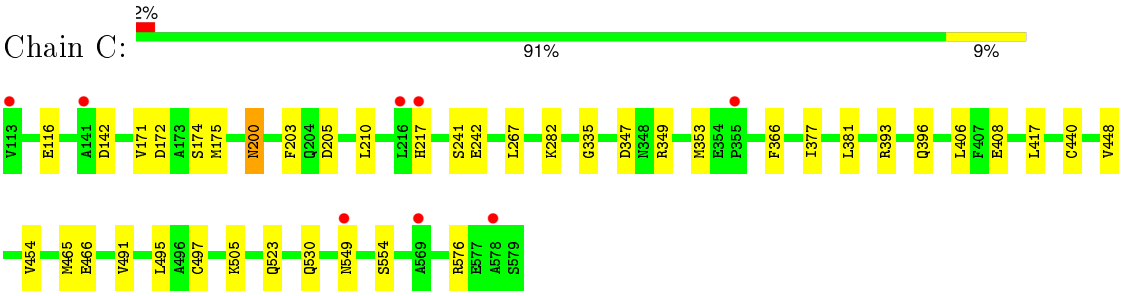
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN

Chain B:



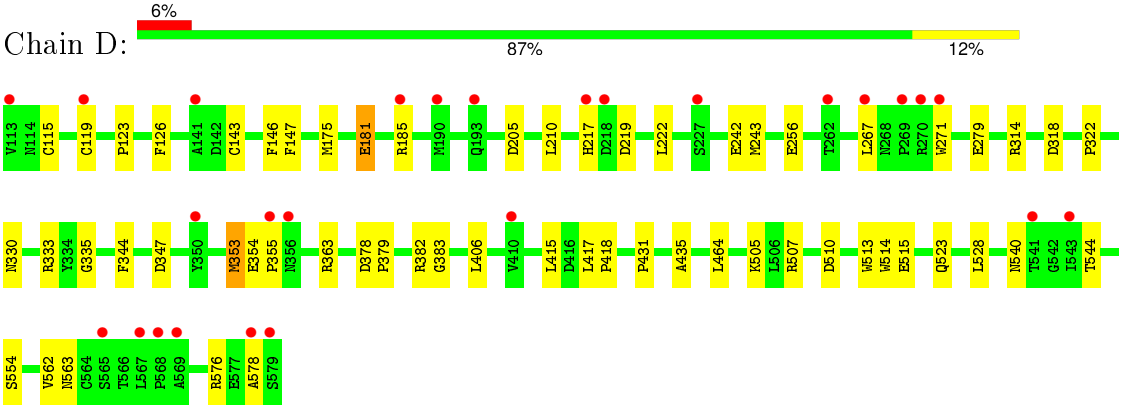
- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN

Chain C:



- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.28Å 63.44Å 92.38Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 55.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.00) 94.0 (55.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.278 0.226 , 0.280	Depositor DCC
R_{free} test set	4064 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.945	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	1 of 81440 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10168	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% 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: GOL, CSO, BMA, NAG, CL, SO4, CA, NIH, FUC, ACT, 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	0.81	1/840 (0.1%)	0.87	1/1144 (0.1%)
1	B	0.73	0/863	0.82	0/1176
2	C	0.76	0/3811	0.79	0/5170
2	D	0.69	0/3811	0.74	1/5170 (0.0%)
All	All	0.73	1/9325 (0.0%)	0.78	2/12660 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ALA	C-N	-5.02	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	510	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	94	ASP	CB-CG-OD2	-5.19	113.63	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	779	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	838	0	800	15	0
2	C	3733	0	3727	31	0
2	D	3733	0	3729	41	0
3	A	43	0	30	10	0
3	B	43	0	30	17	0
4	A	27	0	10	1	0
4	B	27	0	10	1	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	8	0	6	0	0
9	D	12	0	9	0	0
10	C	28	0	26	0	0
10	D	28	0	26	0	0
11	C	71	0	61	6	0
11	D	71	0	61	4	0
12	A	103	0	0	4	0
12	B	108	0	0	2	0
12	C	254	0	0	10	0
12	D	199	0	0	7	0
All	All	10168	0	9320	104	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 6.

All (104) 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)
3:B:605:HEM:HBB1	2:D:243:MET:SD	1.57	1.44
1:A:94:ASP:OD2	3:A:605:HEM:CMD	1.64	1.44
3:A:605:HEM:CMB	2:C:242:GLU:OE2	1.69	1.37
3:B:605:HEM:CBB	2:D:243:MET:SD	2.13	1.35
3:A:605:HEM:HMB1	2:C:242:GLU:OE2	1.17	1.33
1:B:94:ASP:OD2	3:B:605:HEM:CMD	1.78	1.31
3:B:605:HEM:HMB1	2:D:242:GLU:OE2	1.45	1.15
3:B:605:HEM:CMB	2:D:242:GLU:OE2	1.98	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:605:HEM:HBB1	2:D:243:MET:CE	1.81	1.10
1:B:94:ASP:OD2	3:B:605:HEM:HMD1	0.87	1.04
1:A:94:ASP:OD2	3:A:605:HEM:HMD1	0.80	0.97
11:C:1642:BMA:O3	11:C:1644:MAN:H2	1.67	0.93
11:C:1642:BMA:H3	11:C:1643:MAN:H2	1.52	0.91
1:A:90:GLY:HA2	12:A:2093:HOH:O	1.74	0.88
3:A:605:HEM:HMB2	2:C:242:GLU:OE2	1.76	0.83
2:C:448:VAL:HA	12:C:2194:HOH:O	1.81	0.81
3:B:605:HEM:HBB1	2:D:243:MET:HE3	1.69	0.74
2:D:431:PRO:HB2	12:D:2145:HOH:O	1.86	0.74
3:A:605:HEM:C2B	2:C:242:GLU:OE2	2.39	0.74
1:B:94:ASP:CG	3:B:605:HEM:HMD1	1.99	0.73
1:A:93:LEU:HB3	12:A:2093:HOH:O	1.90	0.72
1:A:94:ASP:OD2	3:A:605:HEM:C2D	2.45	0.67
3:B:605:HEM:C2B	2:D:242:GLU:OE2	2.51	0.62
3:A:605:HEM:CBC	2:C:335:GLY:HA3	2.30	0.62
11:D:2642:BMA:H3	11:D:2643:MAN:O5	2.02	0.60
11:D:2642:BMA:O3	11:D:2643:MAN:H3	2.03	0.59
11:D:2642:BMA:C3	11:D:2643:MAN:O5	2.50	0.59
2:D:382:ARG:NH2	12:D:2130:HOH:O	2.34	0.57
3:B:605:HEM:CBB	2:D:243:MET:CE	2.70	0.57
3:A:605:HEM:HBC2	2:C:335:GLY:HA3	1.87	0.57
1:A:94:ASP:CG	3:A:605:HEM:CMD	2.68	0.57
1:A:83:SER:HB3	2:C:554:SER:O	2.05	0.56
3:B:605:HEM:HMB2	2:D:242:GLU:OE2	2.03	0.54
2:C:440:CYS:HG	2:C:497:CYS:HG	1.54	0.54
2:C:347:ASP:HB2	12:C:2159:HOH:O	2.08	0.53
2:C:205:ASP:HB2	2:C:210:LEU:HD21	1.91	0.53
2:C:200:ASN:HD22	2:C:203:PHE:H	1.55	0.53
2:D:205:ASP:HB2	2:D:210:LEU:HD21	1.90	0.53
1:B:64:VAL:HG13	1:B:68:ILE:HD12	1.91	0.52
3:B:605:HEM:CBB	2:D:243:MET:HE3	2.40	0.51
2:C:116:GLU:HG3	12:C:2015:HOH:O	2.10	0.51
2:D:576:ARG:NH2	12:D:2192:HOH:O	2.43	0.51
2:C:530:GLN:NE2	12:C:2222:HOH:O	2.43	0.50
2:C:454:VAL:HA	12:C:2198:HOH:O	2.10	0.50
1:A:64:VAL:HG13	1:A:68:ILE:HD12	1.92	0.50
11:C:1642:BMA:C3	11:C:1643:MAN:H2	2.31	0.50
1:B:10:ILE:HB	12:B:2019:HOH:O	2.10	0.50
2:C:377:ILE:HD12	2:C:381:LEU:HD11	1.93	0.49
4:A:606:NIH:O10	4:A:606:NIH:N8	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:ARG:HB2	2:C:396:GLN:HB2	1.94	0.49
1:B:6:LYS:H	1:B:6:LYS:HE2	1.78	0.49
1:B:94:ASP:OD2	3:B:605:HEM:C2D	2.62	0.49
2:C:200:ASN:ND2	2:C:203:PHE:H	2.10	0.49
2:D:563:ASN:HB3	12:D:2188:HOH:O	2.13	0.49
3:B:605:HEM:CBC	2:D:335:GLY:HA3	2.44	0.48
2:C:505:LYS:HE3	11:D:2644:MAN:O4	2.13	0.48
3:B:605:HEM:HBB2	3:B:605:HEM:HMB2	1.96	0.48
2:D:435:ALA:HB3	12:D:2145:HOH:O	2.14	0.47
2:D:119:CYS:SG	2:D:143:CYS:SG	3.09	0.47
1:B:94:ASP:CG	3:B:605:HEM:CMD	2.71	0.47
1:B:22:LEU:HB3	2:D:322:PRO:HD2	1.96	0.47
1:B:83:SER:HB3	2:D:554:SER:O	2.15	0.47
2:C:142:ASP:HB3	12:C:2038:HOH:O	2.15	0.46
4:B:606:NIH:H4	2:D:242:GLU:HG3	1.98	0.46
2:D:123:PRO:HA	12:D:2016:HOH:O	2.16	0.46
2:C:406:LEU:HD22	2:C:417:LEU:HB2	1.98	0.46
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.51	0.45
2:D:344:PHE:O	2:D:383:GLY:HA3	2.16	0.45
2:D:528:LEU:HD22	12:D:2091:HOH:O	2.16	0.45
2:D:271:TRP:CZ3	2:D:279:GLU:HG3	2.52	0.45
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.99	0.45
1:B:93:LEU:O	1:B:97:LEU:HG	2.16	0.45
2:C:241:SER:O	2:C:366:PHE:HA	2.17	0.45
12:B:2019:HOH:O	2:D:181:GLU:HG3	2.16	0.44
2:D:347:ASP:HB3	2:D:353:MET:HG3	1.99	0.44
1:A:40:GLY:HA3	1:B:20:PRO:HG2	1.99	0.44
2:D:507:ARG:HG3	2:D:513:TRP:CE2	2.51	0.44
1:B:68:ILE:HD13	2:D:464:LEU:HD23	1.99	0.44
2:D:378:ASP:HB2	2:D:379:PRO:HD3	1.99	0.44
1:A:93:LEU:HD23	12:A:2093:HOH:O	2.18	0.44
11:C:1644:MAN:H61	2:D:505:LYS:HE3	2.00	0.43
2:C:465:MET:HG2	12:C:2194:HOH:O	2.18	0.43
2:C:393:ARG:HB3	2:C:393:ARG:HE	1.62	0.43
2:C:172:ASP:OD1	2:C:174:SER:HB3	2.19	0.43
2:D:115:CYS:HB2	2:D:147:PHE:CZ	2.53	0.43
12:A:2004:HOH:O	2:C:282:LYS:HE3	2.19	0.43
2:D:267:LEU:HD12	2:D:576:ARG:HB2	2.01	0.42
2:C:465:MET:CG	12:C:2194:HOH:O	2.67	0.42
2:C:491:VAL:HB	2:C:495:LEU:HB2	2.00	0.42
2:C:440:CYS:SG	2:C:497:CYS:SG	3.11	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:GLU:HB3	2:D:355:PRO:HA	2.00	0.42
1:B:1:CYS:HG	1:B:14:CYS:HG	1.67	0.42
2:D:330:ASN:O	2:D:333:ARG:HB2	2.20	0.42
2:D:126:PHE:HB3	2:D:146:PHE:CD1	2.55	0.42
2:C:549:ASN:HB3	12:C:2232:HOH:O	2.20	0.42
1:A:16:ASN:O	1:A:20:PRO:HA	2.19	0.41
2:D:219:ASP:HB3	2:D:222:LEU:HD12	2.02	0.41
1:B:83:SER:O	1:B:86:PHE:HB3	2.20	0.41
2:D:256:GLU:OE1	2:D:540:ASN:ND2	2.43	0.41
1:A:84:LEU:HA	1:A:84:LEU:HD12	1.88	0.40
2:D:406:LEU:HB3	2:D:415:LEU:HB2	2.03	0.40
11:C:1645:FUC:H5	12:C:2148:HOH:O	2.20	0.40
11:C:1642:BMA:H3	11:C:1643:MAN:C2	2.37	0.40
1:A:97:LEU:HD21	2:C:171:VAL:HG22	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	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
1	B	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
2	C	464/467 (99%)	449 (97%)	15 (3%)	0	100	100
2	D	464/467 (99%)	452 (97%)	11 (2%)	1 (0%)	52	48
All	All	1131/1150 (98%)	1098 (97%)	32 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	578	ALA

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	87/93 (94%)	86 (99%)	1 (1%)	80	83
1	B	90/93 (97%)	88 (98%)	2 (2%)	60	62
2	C	410/411 (100%)	400 (98%)	10 (2%)	57	58
2	D	410/411 (100%)	399 (97%)	11 (3%)	52	52
All	All	997/1008 (99%)	973 (98%)	24 (2%)	57	58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	B	6	LYS
1	B	54	ASN
2	C	175	MET
2	C	200	ASN
2	C	217	HIS
2	C	267	LEU
2	C	349	ARG
2	C	353	MET
2	C	408	GLU
2	C	466	GLU
2	C	523	GLN
2	C	576	ARG
2	D	175	MET
2	D	181	GLU
2	D	185	ARG
2	D	217	HIS
2	D	314	ARG
2	D	318	ASP
2	D	353	MET
2	D	363	ARG
2	D	523	GLN
2	D	544	THR
2	D	562	VAL

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

Mol	Chain	Res	Type
1	A	54	ASN
1	B	80	GLN
2	C	200	ASN
2	C	421	ASN
2	C	530	GLN

5.3.3 RNA (i)

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	0.52	0	1,6,8	1.75	0
2	CSO	D	150	2	3,6,7	0.53	0	1,6,8	1.70	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)

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	$\#\|Z\| > 2$
11	NAG	C	1640	11,2	14,14,15	0.96	1 (7%)	15,19,21	1.96	5 (33%)
11	NAG	C	1641	11	14,14,15	1.26	2 (14%)	15,19,21	2.06	6 (40%)
11	BMA	C	1642	11	11,11,12	0.85	0	14,15,17	2.05	6 (42%)
11	MAN	C	1643	11	11,11,12	0.74	0	14,15,17	1.65	2 (14%)
11	MAN	C	1644	11	11,11,12	0.83	0	14,15,17	1.54	4 (28%)
11	FUC	C	1645	11	10,10,11	0.79	0	14,14,16	1.92	5 (35%)
11	NAG	D	2640	11,2	14,14,15	0.55	0	15,19,21	1.58	2 (13%)
11	NAG	D	2641	11	14,14,15	1.15	2 (14%)	15,19,21	1.76	3 (20%)
11	BMA	D	2642	11	11,11,12	1.34	2 (18%)	14,15,17	2.07	4 (28%)
11	MAN	D	2643	11	11,11,12	1.05	1 (9%)	14,15,17	3.17	4 (28%)
11	MAN	D	2644	11	11,11,12	0.39	0	14,15,17	1.57	5 (35%)
11	FUC	D	2645	11	10,10,11	0.68	0	14,14,16	1.39	2 (14%)

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
11	NAG	C	1640	11,2	-	0/6/23/26	0/1/1/1
11	NAG	C	1641	11	-	0/6/23/26	0/1/1/1
11	BMA	C	1642	11	-	0/2/19/22	1/1/1/1
11	MAN	C	1643	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	C	1644	11	-	0/2/19/22	0/1/1/1
11	FUC	C	1645	11	-	0/0/17/20	0/1/1/1
11	NAG	D	2640	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	2641	11	-	0/6/23/26	0/1/1/1
11	BMA	D	2642	11	-	0/2/19/22	0/1/1/1
11	MAN	D	2643	11	-	0/2/19/22	0/1/1/1
11	MAN	D	2644	11	-	0/2/19/22	0/1/1/1
11	FUC	D	2645	11	-	0/0/17/20	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1641	NAG	C2-N2	-2.93	1.41	1.46
11	D	2641	NAG	O5-C1	-2.57	1.39	1.43
11	D	2642	BMA	C2-C3	-2.51	1.49	1.52
11	C	1640	NAG	C1-C2	-2.37	1.49	1.52
11	C	1641	NAG	O5-C1	-2.33	1.39	1.43
11	D	2641	NAG	C2-N2	-2.29	1.42	1.46
11	D	2643	MAN	C2-C3	2.34	1.55	1.52
11	D	2642	BMA	C4-C5	3.13	1.59	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	2642	BMA	O3-C3-C2	-4.11	102.57	110.00
11	C	1642	BMA	O2-C2-C3	-3.98	102.12	110.12
11	D	2641	NAG	C4-C3-C2	-3.86	105.23	111.23
11	C	1640	NAG	C3-C2-N2	-3.28	102.71	110.56
11	C	1641	NAG	O4-C4-C5	-2.83	101.73	109.24
11	D	2640	NAG	O4-C4-C3	-2.82	104.00	110.34
11	C	1645	FUC	C6-C5-C4	-2.80	107.57	113.08
11	C	1645	FUC	O4-C4-C3	-2.63	104.41	110.34
11	D	2645	FUC	C2-C3-C4	-2.49	106.82	111.04
11	D	2642	BMA	O4-C4-C3	-2.39	104.95	110.34
11	C	1640	NAG	O7-C7-C8	-2.33	117.79	122.06
11	C	1644	MAN	O5-C1-C2	-2.31	107.10	110.86
11	C	1641	NAG	O7-C7-C8	-2.28	117.87	122.06
11	C	1644	MAN	O3-C3-C2	-2.23	105.98	110.00
11	C	1641	NAG	C4-C3-C2	-2.18	107.84	111.23
11	D	2644	MAN	C1-C2-C3	-2.14	107.01	109.54
11	C	1642	BMA	O3-C3-C2	-2.02	106.35	110.00
11	D	2644	MAN	O4-C4-C3	-2.01	105.81	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	2643	MAN	C2-C3-C4	2.03	114.49	111.04
11	C	1642	BMA	O6-C6-C5	2.04	118.06	111.33
11	D	2644	MAN	O3-C3-C4	2.14	115.17	110.34
11	C	1644	MAN	C1-O5-C5	2.27	115.13	112.25
11	C	1645	FUC	O5-C5-C6	2.28	109.90	106.13
11	C	1642	BMA	O2-C2-C1	2.43	114.08	109.21
11	D	2644	MAN	O2-C2-C1	2.50	114.22	109.21
11	C	1642	BMA	C1-C2-C3	2.60	112.61	109.54
11	D	2641	NAG	C2-N2-C7	2.61	126.39	123.04
11	D	2644	MAN	C1-O5-C5	2.66	115.62	112.25
11	C	1641	NAG	O7-C7-N2	2.76	127.48	121.86
11	D	2645	FUC	C3-C4-C5	2.84	114.50	109.72
11	C	1640	NAG	O7-C7-N2	2.91	127.80	121.86
11	D	2641	NAG	O3-C3-C2	2.94	114.94	109.11
11	C	1644	MAN	C1-C2-C3	2.99	113.08	109.54
11	C	1641	NAG	C2-N2-C7	3.06	126.97	123.04
11	C	1645	FUC	C3-C4-C5	3.12	114.99	109.72
11	C	1640	NAG	C2-N2-C7	3.25	127.22	123.04
11	D	2642	BMA	O4-C4-C5	3.40	118.25	109.24
11	C	1642	BMA	C1-O5-C5	3.45	116.63	112.25
11	C	1643	MAN	C1-C2-C3	3.55	113.74	109.54
11	D	2642	BMA	C6-C5-C4	3.61	121.92	113.02
11	D	2640	NAG	C1-O5-C5	3.75	117.01	112.25
11	C	1640	NAG	C1-O5-C5	3.85	117.14	112.25
11	C	1645	FUC	O5-C5-C4	3.92	116.32	109.53
11	C	1643	MAN	C1-O5-C5	4.22	117.60	112.25
11	C	1641	NAG	C1-O5-C5	4.85	118.40	112.25
11	D	2643	MAN	O5-C5-C6	4.88	117.92	107.35
11	D	2643	MAN	C1-C2-C3	4.92	115.36	109.54
11	D	2643	MAN	C1-O5-C5	8.59	123.15	112.25

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	1642	BMA	C1-C2-C3-C4-C5-O5

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1642	BMA	4	0
11	C	1643	MAN	3	0
11	C	1644	MAN	2	0
11	C	1645	FUC	1	0
11	D	2642	BMA	3	0
11	D	2643	MAN	3	0
11	D	2644	MAN	1	0

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	$\#\|Z\| > 2$
3	HEM	A	605	2	30,50,50	2.65	14 (46%)	24,82,82	2.82	9 (37%)
4	NIH	A	606	-	28,28,28	1.38	2 (7%)	34,42,42	1.78	6 (17%)
5	SO4	B	1003	-	4,4,4	0.46	0	6,6,6	0.32	0
3	HEM	B	605	2	30,50,50	2.67	15 (50%)	24,82,82	2.58	11 (45%)
4	NIH	B	606	-	28,28,28	1.27	3 (10%)	34,42,42	1.89	10 (29%)
5	SO4	C	1581	-	4,4,4	0.37	0	6,6,6	0.44	0
9	ACT	C	1582	-	1,3,3	1.72	0	0,3,3	0.00	-
9	ACT	C	1583	-	1,3,3	1.41	0	0,3,3	0.00	-
10	NAG	C	1620	2	14,14,15	0.64	0	15,19,21	1.61	4 (26%)
10	NAG	C	1630	2	14,14,15	0.71	0	15,19,21	2.14	5 (33%)
6	GOL	C	631	-	5,5,5	0.30	0	5,5,5	0.44	0
9	ACT	D	1581	-	1,3,3	1.77	0	0,3,3	0.00	-
9	ACT	D	1582	-	1,3,3	1.01	0	0,3,3	0.00	-
9	ACT	D	1583	-	1,3,3	1.43	0	0,3,3	0.00	-
10	NAG	D	2620	2	14,14,15	0.50	0	15,19,21	1.36	2 (13%)
10	NAG	D	2630	2	14,14,15	0.59	0	15,19,21	1.47	4 (26%)
6	GOL	D	631	-	5,5,5	0.37	0	5,5,5	0.57	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
3	HEM	A	605	2	-	0/10/54/54	0/0/8/8
4	NIH	A	606	-	-	0/23/23/23	0/2/2/2
5	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
3	HEM	B	605	2	-	0/10/54/54	0/0/8/8
4	NIH	B	606	-	-	0/23/23/23	0/2/2/2
5	SO4	C	1581	-	-	0/0/0/0	0/0/0/0
9	ACT	C	1582	-	-	0/0/0/0	0/0/0/0
9	ACT	C	1583	-	-	0/0/0/0	0/0/0/0
10	NAG	C	1620	2	-	0/6/23/26	0/1/1/1
10	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
6	GOL	C	631	-	-	0/4/4/4	0/0/0/0
9	ACT	D	1581	-	-	0/0/0/0	0/0/0/0
9	ACT	D	1582	-	-	0/0/0/0	0/0/0/0
9	ACT	D	1583	-	-	0/0/0/0	0/0/0/0
10	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
10	NAG	D	2630	2	-	0/6/23/26	0/1/1/1
6	GOL	D	631	-	-	0/4/4/4	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HEM	C3B-C4B	-7.31	1.45	1.51
3	A	605	HEM	C3B-C4B	-7.20	1.45	1.51
3	A	605	HEM	C2D-C3D	-5.51	1.38	1.54
3	B	605	HEM	C2D-C3D	-4.98	1.39	1.54
3	B	605	HEM	C3D-C4D	-3.27	1.47	1.51
3	A	605	HEM	C2C-C1C	-2.96	1.47	1.52
4	B	606	NIH	C5-C7	-2.93	1.45	1.50
4	A	606	NIH	C5-C7	-2.85	1.45	1.50
3	B	605	HEM	C2C-C1C	-2.67	1.47	1.52
3	B	605	HEM	C3B-CAB	-2.65	1.46	1.51
3	A	605	HEM	C3D-C4D	-2.48	1.48	1.51
3	A	605	HEM	C3B-CAB	-2.32	1.47	1.51
3	B	605	HEM	CAD-C3D	-2.22	1.49	1.54
3	A	605	HEM	C1C-NC	-2.07	1.33	1.36
4	B	606	NIH	F22-C20	2.00	1.40	1.32
3	B	605	HEM	FE-ND	2.02	2.08	1.97
4	B	606	NIH	F23-C20	2.16	1.40	1.32
3	A	605	HEM	CHC-C4B	2.41	1.45	1.38
3	A	605	HEM	CHD-C1D	2.55	1.46	1.38
3	A	605	HEM	CBC-CAC	2.57	1.44	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HEM	FE-NB	2.71	2.11	1.97
3	A	605	HEM	CBB-CAB	2.71	1.45	1.29
3	A	605	HEM	FE-ND	2.73	2.11	1.97
3	B	605	HEM	C4A-CHB	2.94	1.48	1.39
3	B	605	HEM	CHD-C1D	3.16	1.47	1.38
3	B	605	HEM	CBB-CAB	3.16	1.47	1.29
3	B	605	HEM	CBC-CAC	3.23	1.47	1.29
3	B	605	HEM	FE-NC	3.33	2.08	1.95
4	A	606	NIH	C2-N12	3.44	1.40	1.34
3	B	605	HEM	CHD-C4C	3.83	1.45	1.36
3	A	605	HEM	CHD-C4C	3.93	1.45	1.36
3	A	605	HEM	CHC-C1C	4.04	1.45	1.36
3	A	605	HEM	FE-NC	4.18	2.12	1.95
3	B	605	HEM	CHC-C1C	4.35	1.46	1.36

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	606	NIH	N3-C2-N1	-6.38	119.87	126.67
3	A	605	HEM	C3B-CAB-CBB	-5.68	115.74	124.46
4	B	606	NIH	C5-C4-N3	-4.70	119.55	125.06
4	B	606	NIH	N3-C2-N1	-4.37	122.01	126.67
4	A	606	NIH	C5-C4-N3	-3.78	120.63	125.06
4	B	606	NIH	F27-C24-C16	-3.28	105.93	112.95
10	C	1630	NAG	C3-C4-C5	-3.00	104.96	110.20
10	D	2630	NAG	O3-C3-C2	-2.87	103.43	109.11
3	A	605	HEM	CBD-CAD-C3D	-2.77	105.49	113.55
3	B	605	HEM	CBD-CAD-C3D	-2.69	105.71	113.55
10	D	2630	NAG	C3-C4-C5	-2.64	105.59	110.20
3	B	605	HEM	C3B-CAB-CBB	-2.62	120.44	124.46
3	B	605	HEM	CBA-CAA-C2A	-2.51	108.03	112.53
10	C	1620	NAG	C4-C3-C2	-2.48	107.37	111.23
10	C	1620	NAG	C2-N2-C7	-2.45	119.89	123.04
4	A	606	NIH	F26-C24-C16	-2.43	107.76	112.95
4	B	606	NIH	C13-N12-C2	-2.32	120.10	123.35
4	B	606	NIH	C19-C18-C20	-2.31	116.52	119.59
10	C	1630	NAG	O7-C7-C8	-2.24	117.95	122.06
3	B	605	HEM	C3B-C4B-CHC	-2.23	120.03	123.16
10	C	1620	NAG	O4-C4-C3	-2.20	105.38	110.34
3	A	605	HEM	C3C-CAC-CBC	-2.13	121.20	124.46
3	A	605	HEM	CAA-CBA-CGA	-2.12	108.86	112.75
4	B	606	NIH	F23-C20-C18	-2.10	108.47	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	2620	NAG	O5-C5-C6	-2.08	102.85	107.35
10	D	2630	NAG	O6-C6-C5	-2.06	104.52	111.33
4	B	606	NIH	F22-C20-C18	-2.03	108.60	112.95
3	B	605	HEM	C2C-C1C-NC	2.01	113.61	110.21
10	C	1630	NAG	O7-C7-N2	2.05	126.03	121.86
3	A	605	HEM	CMD-C2D-C3D	2.08	123.54	114.35
3	B	605	HEM	CMD-C2D-C3D	2.11	123.67	114.35
4	B	606	NIH	C17-C18-C20	2.15	122.45	119.59
3	B	605	HEM	C3C-CAC-CBC	2.18	127.80	124.46
10	D	2630	NAG	O4-C4-C5	2.29	115.31	109.24
4	A	606	NIH	O11-N8-C7	2.30	127.11	120.06
4	B	606	NIH	C4-N3-C2	2.73	121.16	115.95
10	D	2620	NAG	C1-O5-C5	3.02	116.09	112.25
4	A	606	NIH	C4-N3-C2	3.06	121.79	115.95
10	C	1620	NAG	C1-O5-C5	3.47	116.65	112.25
10	C	1630	NAG	O4-C4-C3	3.59	118.42	110.34
4	B	606	NIH	C6-N1-C2	3.70	120.69	115.31
3	B	605	HEM	CAD-C3D-C4D	4.04	126.71	112.47
4	A	606	NIH	C6-N1-C2	4.25	121.49	115.31
3	A	605	HEM	CAD-C3D-C2D	4.42	125.93	113.22
3	A	605	HEM	CAD-C3D-C4D	4.76	129.25	112.47
3	B	605	HEM	CMB-C2B-C3B	5.11	129.28	116.53
10	C	1630	NAG	C1-O5-C5	5.51	119.24	112.25
3	B	605	HEM	CAD-C3D-C2D	5.61	129.34	113.22
3	B	605	HEM	CMC-C2C-C3C	5.82	131.06	116.53
3	A	605	HEM	CMC-C2C-C3C	6.01	131.54	116.53
3	A	605	HEM	CMB-C2B-C3B	6.59	132.97	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	HEM	10	0
4	A	606	NIH	1	0
3	B	605	HEM	17	0
4	B	606	NIH	1	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	102/108 (94%)	0.43	3 (2%)	55	56	4, 8, 21, 44	0
1	B	105/108 (97%)	0.41	3 (2%)	55	56	6, 11, 26, 35	0
2	C	466/467 (99%)	0.38	8 (1%)	73	73	3, 10, 24, 37	0
2	D	466/467 (99%)	0.59	26 (5%)	28	29	4, 15, 32, 42	0
All	All	1139/1150 (99%)	0.47	40 (3%)	48	49	3, 12, 29, 44	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	11.9
2	D	578	ALA	6.3
2	C	355	PRO	4.9
2	D	217	HIS	4.4
2	D	269	PRO	4.3
2	D	267	LEU	4.3
2	D	113	VAL	4.0
2	C	113	VAL	4.0
2	D	569	ALA	3.8
2	D	270	ARG	3.7
1	B	105	ALA	3.6
2	D	565	SER	3.5
2	D	579	SER	3.5
1	A	4	GLN	3.3
2	D	218	ASP	3.2
2	C	569	ALA	3.1
2	C	578	ALA	3.0
2	D	355	PRO	3.0
2	C	216	LEU	3.0
2	D	541	THR	3.0
2	D	568	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	190	MET	2.8
2	C	217	HIS	2.7
1	B	2	PRO	2.6
2	D	119	CYS	2.6
2	D	350	TYR	2.5
2	D	410	VAL	2.5
2	D	567	LEU	2.5
2	D	141	ALA	2.4
2	D	543	ILE	2.4
2	D	271	TRP	2.4
2	D	356	ASN	2.3
2	D	193	GLN	2.3
2	D	227	SER	2.2
2	D	185	ARG	2.2
2	C	549	ASN	2.2
1	A	5	ASP	2.2
2	D	262	THR	2.2
1	B	5	ASP	2.1
2	C	141	ALA	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	0.11	-	5,6,10,12	0
2	CSO	D	150	7/8	0.94	0.12	-	8,10,16,19	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
11	BMA	D	2642	11/12	0.70	0.22	14.51	24,27,36,41	0
11	BMA	C	1642	11/12	0.76	0.28	8.27	19,23,28,32	0
11	NAG	C	1641	14/15	0.92	0.14	1.11	8,10,12,15	0
11	NAG	D	2641	14/15	0.89	0.14	-0.10	9,11,13,17	0
11	MAN	D	2643	11/12	0.42	0.33	-	36,43,46,46	0
11	FUC	D	2645	10/11	0.83	0.22	-	23,25,28,30	0
11	MAN	D	2644	11/12	0.61	0.24	-	21,24,25,29	0
11	MAN	C	1644	11/12	0.87	0.13	-	24,25,27,28	0
11	NAG	C	1640	14/15	0.92	0.14	-	10,11,14,15	0
11	FUC	C	1645	10/11	0.88	0.23	-	17,20,21,22	0
11	MAN	C	1643	11/12	0.70	0.26	-	36,42,46,48	0
11	NAG	D	2640	14/15	0.92	0.14	-	10,12,13,17	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^{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
9	ACT	D	1581	4/4	0.78	0.22	9.73	22,27,27,28	0
4	NIH	A	606	27/27	0.84	0.30	9.67	4,6,7,8	27
4	NIH	B	606	27/27	0.78	0.31	5.38	10,12,13,14	27
3	HEM	A	605	43/43	0.93	0.15	1.13	4,5,7,10	0
3	HEM	B	605	43/43	0.94	0.14	0.44	5,7,9,12	0
10	NAG	D	2620	14/15	0.83	0.19	0.09	22,23,25,27	0
8	CL	D	1580	1/1	0.99	0.13	0.03	6,6,6,6	0
10	NAG	C	1630	14/15	0.83	0.16	-0.03	19,21,24,25	0
10	NAG	C	1620	14/15	0.92	0.14	-0.15	15,17,19,20	0
8	CL	C	1580	1/1	1.00	0.13	-0.82	4,4,4,4	0
7	CA	D	1579	1/1	0.99	0.07	-3.71	7,7,7,7	0
7	CA	C	1579	1/1	0.99	0.06	-5.84	4,4,4,4	0
5	SO4	C	1581	5/5	0.95	0.16	-	34,34,36,37	0
5	SO4	B	1003	5/5	0.60	0.40	-	29,29,31,31	5
9	ACT	D	1582	4/4	0.52	0.27	-	39,39,40,40	0
9	ACT	C	1582	4/4	0.86	0.16	-	35,37,38,38	0
10	NAG	D	2630	14/15	0.71	0.20	-	31,34,36,37	0
6	GOL	D	631	6/6	0.63	0.24	-	32,34,36,37	0
9	ACT	D	1583	4/4	0.85	0.14	-	34,34,34,36	0
9	ACT	C	1583	4/4	0.91	0.12	-	25,26,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	GOL	C	631	6/6	0.86	0.19	-	35,39,41,46	0

6.5 Other polymers (i)

There are no such residues in this entry.