



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:30 PM GMT

PDB ID : 4F4O
Title : Structure of the Haptoglobin-Haemoglobin Complex
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Deposited on : 2012-05-11
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

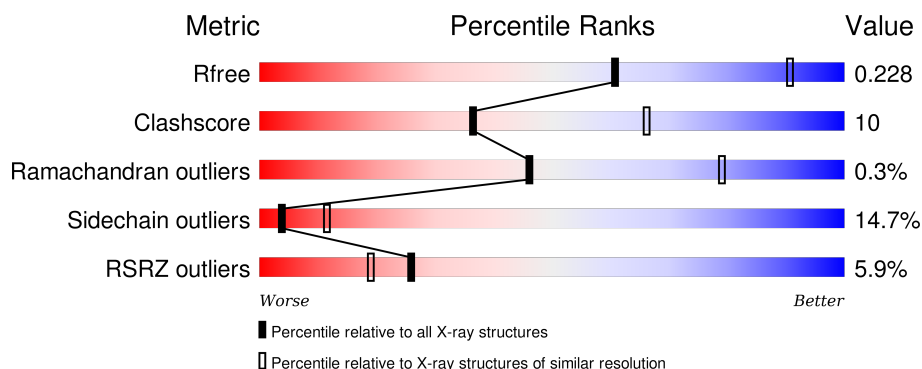
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	141	<div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	D	141	<div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	G	141	<div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	J	141	<div> <div>23%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	B	146	<div> <div>75%</div> <div>22%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	146	
2	H	146	
2	K	146	
3	C	347	
3	F	347	
3	I	347	
3	L	347	

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
5	OXY	A	202	-	-	-	X
5	OXY	G	202	-	-	-	X
5	OXY	K	202	-	-	-	X
8	NAG	C	1005	-	-	-	X
8	NAG	F	1005	-	-	-	X
8	FUC	F	1006	-	-	-	X
8	NAG	I	1005	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19196 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	D	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	G	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	J	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			

- Molecule 2 is a protein called Hemoglobin subunit beta.

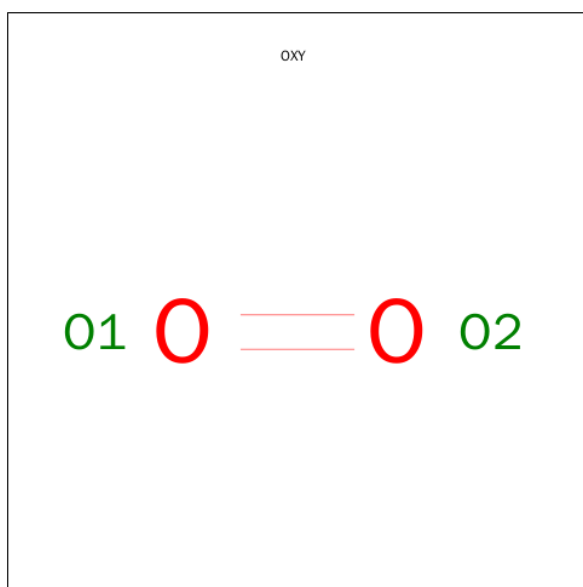
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			
2	E	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			
2	H	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			
2	K	146	Total	C	N	O	S	0	1	0
			1144	731	205	206	2			

- Molecule 3 is a protein called Haptoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			
3	F	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			
3	I	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			
3	L	309	Total	C	N	O	S	0	0	0
			2428	1546	411	457	14			

-
- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



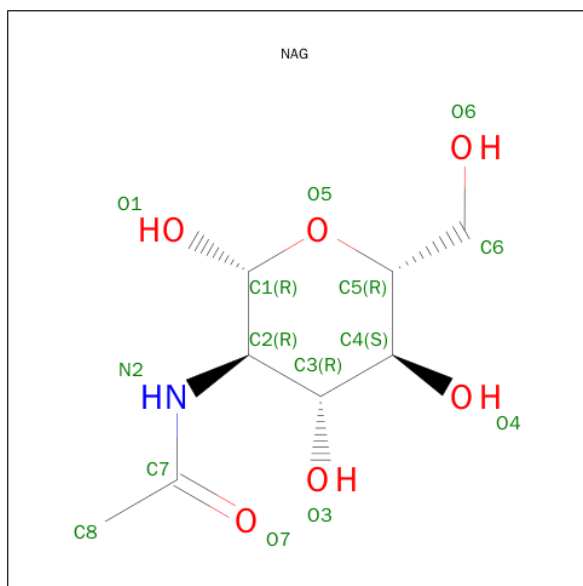
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	D	1	Total O 2 2	0	0
5	E	1	Total O 2 2	0	0
5	G	1	Total O 2 2	0	0
5	H	1	Total O 2 2	0	0
5	J	1	Total O 2 2	0	0
5	K	1	Total O 2 2	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	2	Total C N O 28 16 2 10	0	0
6	F	2	Total C N O 28 16 2 10	0	0
6	I	2	Total C N O 28 16 2 10	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	I	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	2	Total	C	N	O	0	0
			24	14	1	9		
8	F	2	Total	C	N	O	0	0
			24	14	1	9		
8	I	2	Total	C	N	O	0	0
			24	14	1	9		

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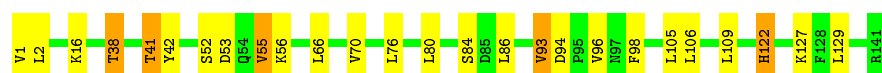
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	2	Total	C	N	O	0	0
			24	14	1	9		

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 ($\text{RSRZ} > 2$). 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.

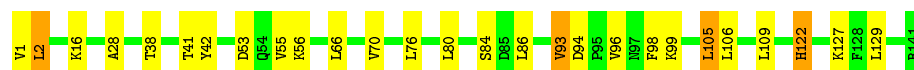
- Molecule 1: Hemoglobin subunit alpha

Chain A: 




- Molecule 1: Hemoglobin subunit alpha

Chain D: 




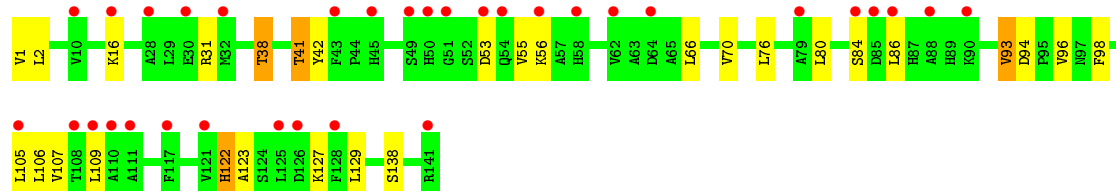
- Molecule 1: Hemoglobin subunit alpha

Chain G: 



- Molecule 1: Hemoglobin subunit alpha

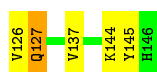
Chain J: 



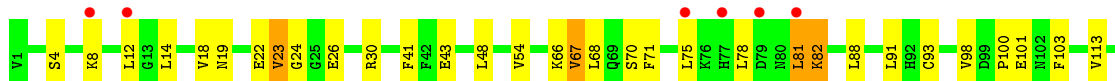
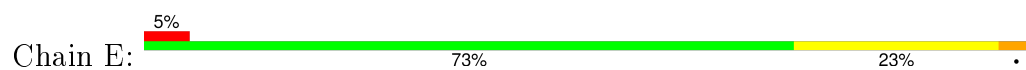
- Molecule 2: Hemoglobin subunit beta

Chain B: 

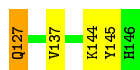
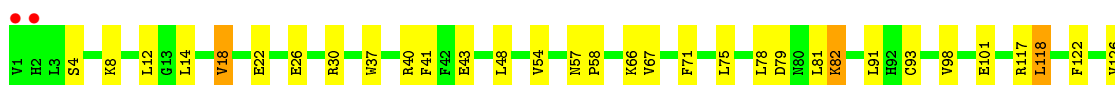
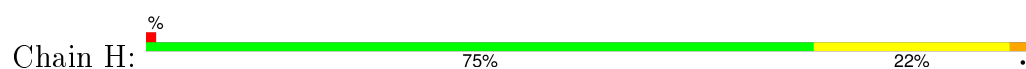




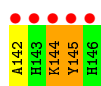
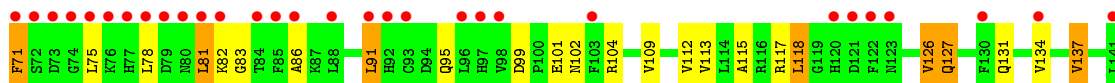
• Molecule 2: Hemoglobin subunit beta



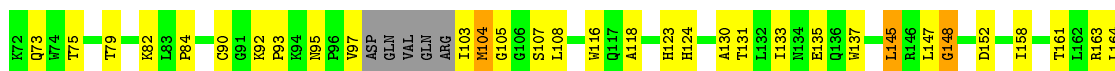
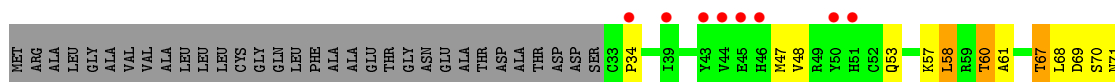
• Molecule 2: Hemoglobin subunit beta



• Molecule 2: Hemoglobin subunit beta

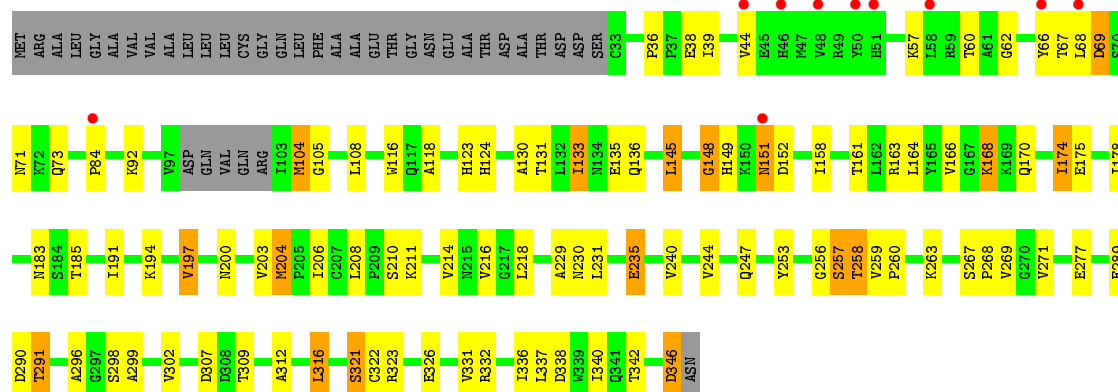


• Molecule 3: Haptoglobin

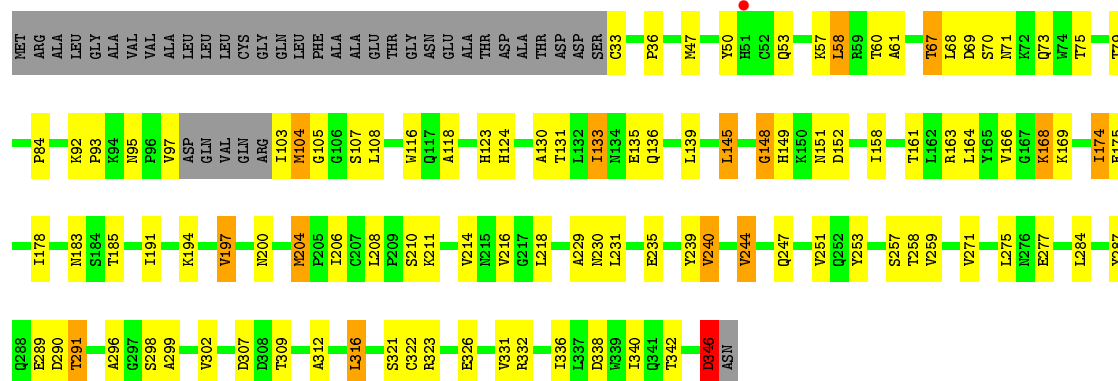




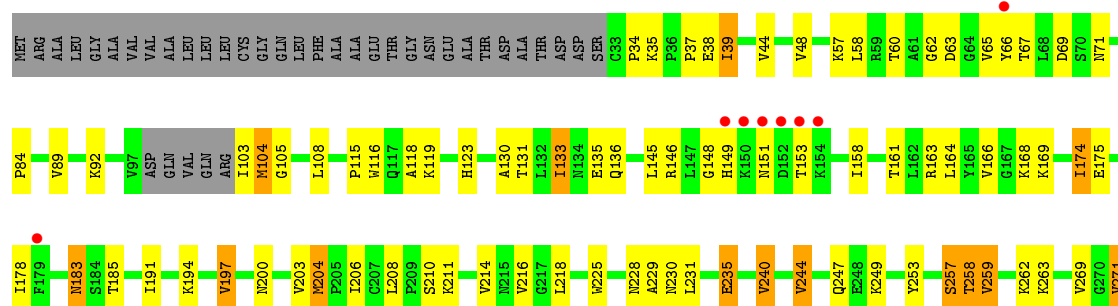
• Molecule 3: Haptoglobin



• Molecule 3: Haptoglobin



• Molecule 3: Haptoglobin





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.88Å 197.78Å 322.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 49.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.90) 99.0 (49.44-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.211 , 0.229 0.208 , 0.228	Depositor DCC
R_{free} test set	2250 reflections (2.18%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 103264 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19196	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: FUC, HEM, OXY, NAG

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	0.59	0/1091	0.70	0/1480
1	D	0.61	0/1091	0.68	0/1480
1	G	0.56	0/1091	0.67	0/1480
1	J	0.35	0/1091	0.58	0/1480
2	B	0.57	0/1169	0.68	0/1580
2	E	0.48	0/1169	0.65	0/1580
2	H	0.63	0/1169	0.69	0/1580
2	K	0.44	0/1169	0.55	0/1580
3	C	0.57	0/2487	0.79	1/3377 (0.0%)
3	F	0.61	1/2487 (0.0%)	0.81	3/3377 (0.1%)
3	I	0.62	0/2487	0.81	3/3377 (0.1%)
3	L	0.51	0/2487	0.75	1/3377 (0.0%)
All	All	0.56	1/18988 (0.0%)	0.73	8/25748 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	151	ASN	C-N	-5.51	1.21	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	346	ASP	CB-CG-OD2	5.56	123.30	118.30
3	F	322	CYS	CA-CB-SG	-5.23	104.59	114.00
3	I	136	GLN	N-CA-C	5.18	125.00	111.00
3	F	322	CYS	C-N-CA	-5.15	108.83	121.70
3	I	322	CYS	CA-CB-SG	-5.09	104.83	114.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	148	GLY	Peptide
3	C	257	SER	Peptide
3	F	148	GLY	Peptide
3	F	257	SER	Peptide
3	I	148	GLY	Peptide

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	1064	0	1060	12	0
1	D	1064	0	1060	12	0
1	G	1064	0	1060	11	0
1	J	1064	0	1060	14	0
2	B	1144	0	1141	21	0
2	E	1144	0	1141	22	0
2	H	1144	0	1141	21	0
2	K	1144	0	1141	35	0
3	C	2428	0	2396	61	0
3	F	2428	0	2394	54	0
3	I	2428	0	2395	57	0
3	L	2428	0	2397	66	0
4	A	43	0	30	1	0
4	B	43	0	30	4	0
4	D	43	0	30	0	0
4	E	43	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	43	0	30	0	0
4	H	43	0	30	4	0
4	J	43	0	30	0	0
4	K	43	0	30	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
5	J	2	0	0	0	0
5	K	2	0	0	0	0
6	C	28	0	25	1	0
6	F	28	0	25	1	0
6	I	28	0	25	1	0
7	C	28	0	26	1	0
7	F	28	0	26	0	0
7	I	28	0	26	0	0
7	L	28	0	26	1	0
8	C	24	0	22	0	0
8	F	24	0	22	2	0
8	I	24	0	22	0	0
8	L	24	0	22	5	0
All	All	19196	0	18893	362	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 10.

The worst 5 of 362 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:K:101[B]:GLU:HG3	3:L:230:ASN:HD22	1.12	1.12
2:E:101[B]:GLU:HG3	3:F:230:ASN:HD22	1.08	1.11
2:H:101[B]:GLU:HG3	3:I:230:ASN:HD22	1.10	1.08
2:B:101[B]:GLU:HG3	3:C:230:ASN:HD22	1.12	1.07
3:F:92:LYS:H	3:F:204:MET:HE2	1.32	0.95

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	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
1	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	G	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
1	J	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
2	B	145/146 (99%)	143 (99%)	2 (1%)	0	100	100
2	E	145/146 (99%)	142 (98%)	3 (2%)	0	100	100
2	H	145/146 (99%)	143 (99%)	2 (1%)	0	100	100
2	K	145/146 (99%)	142 (98%)	3 (2%)	0	100	100
3	C	305/347 (88%)	288 (94%)	15 (5%)	2 (1%)	26	63
3	F	305/347 (88%)	284 (93%)	20 (7%)	1 (0%)	46	79
3	I	305/347 (88%)	287 (94%)	15 (5%)	3 (1%)	19	54
3	L	305/347 (88%)	285 (93%)	18 (6%)	2 (1%)	26	63
All	All	2356/2536 (93%)	2250 (96%)	98 (4%)	8 (0%)	46	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	258	THR
3	L	169	LYS
3	L	258	THR
3	C	169	LYS
3	C	258	THR

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	111/111 (100%)	97 (87%)	14 (13%)	5	16
1	D	111/111 (100%)	97 (87%)	14 (13%)	5	16
1	G	111/111 (100%)	97 (87%)	14 (13%)	5	16
1	J	111/111 (100%)	97 (87%)	14 (13%)	5	16
2	B	120/119 (101%)	101 (84%)	19 (16%)	3	9
2	E	120/119 (101%)	102 (85%)	18 (15%)	3	11
2	H	120/119 (101%)	103 (86%)	17 (14%)	4	12
2	K	120/119 (101%)	100 (83%)	20 (17%)	3	8
3	C	268/296 (90%)	225 (84%)	43 (16%)	3	9
3	F	268/296 (90%)	230 (86%)	38 (14%)	4	12
3	I	268/296 (90%)	225 (84%)	43 (16%)	3	9
3	L	268/296 (90%)	229 (85%)	39 (15%)	4	12
All	All	1996/2104 (95%)	1703 (85%)	293 (15%)	4	11

5 of 293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	235	GLU
2	H	43	GLU
3	L	197	VAL
3	F	277	GLU
1	G	38	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	230	ASN
3	L	230	ASN
3	I	230	ASN
1	D	122	HIS
1	G	122	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

14 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$
6	NAG	C	1001	3,6	14,14,15	2.30	6 (42%)	15,19,21	2.90	8 (53%)
6	NAG	C	1002	6	14,14,15	2.34	7 (50%)	15,19,21	1.82	2 (13%)
8	NAG	C	1005	8,3	14,14,15	1.98	5 (35%)	15,19,21	2.56	5 (33%)
8	FUC	C	1006	8	10,10,11	2.17	4 (40%)	14,14,16	3.37	4 (28%)
6	NAG	F	1001	3,6	14,14,15	2.36	6 (42%)	15,19,21	3.13	10 (66%)
6	NAG	F	1002	6	14,14,15	2.00	6 (42%)	15,19,21	1.59	3 (20%)
8	NAG	F	1005	8,3	14,14,15	1.94	6 (42%)	15,19,21	2.41	5 (33%)
8	FUC	F	1006	8	10,10,11	2.03	4 (40%)	14,14,16	2.93	4 (28%)
6	NAG	I	1001	3,6	14,14,15	2.08	6 (42%)	15,19,21	2.73	7 (46%)
6	NAG	I	1002	6	14,14,15	2.19	7 (50%)	15,19,21	1.76	2 (13%)
8	NAG	I	1005	8,3	14,14,15	1.96	5 (35%)	15,19,21	2.29	4 (26%)
8	FUC	I	1006	8	10,10,11	2.18	5 (50%)	14,14,16	3.66	5 (35%)
8	NAG	L	1003	8,3	14,14,15	0.39	0	15,19,21	1.48	3 (20%)
8	FUC	L	1004	8	10,10,11	0.47	0	14,14,16	1.19	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
6	NAG	C	1001	3,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1002	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1005	8,3	-	0/6/23/26	0/1/1/1
8	FUC	C	1006	8	-	0/0/17/20	0/1/1/1
6	NAG	F	1001	3,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1002	6	-	0/6/23/26	0/1/1/1
8	NAG	F	1005	8,3	-	0/6/23/26	0/1/1/1
8	FUC	F	1006	8	-	0/0/17/20	0/1/1/1
6	NAG	I	1001	3,6	-	0/6/23/26	0/1/1/1
6	NAG	I	1002	6	-	0/6/23/26	0/1/1/1
8	NAG	I	1005	8,3	-	0/6/23/26	0/1/1/1
8	FUC	I	1006	8	-	0/0/17/20	0/1/1/1
8	NAG	L	1003	8,3	-	0/6/23/26	0/1/1/1
8	FUC	L	1004	8	-	0/0/17/20	0/1/1/1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1006	FUC	C2-C3	-4.57	1.46	1.52
8	C	1006	FUC	C2-C3	-4.37	1.46	1.52
8	C	1006	FUC	C4-C3	-3.26	1.43	1.52
6	C	1002	NAG	C4-C3	-3.20	1.44	1.52
8	F	1006	FUC	C2-C3	-3.05	1.48	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1006	FUC	C1-O5-C5	-7.86	100.24	112.38
8	C	1006	FUC	C1-O5-C5	-7.21	101.24	112.38
8	F	1006	FUC	C1-O5-C5	-7.12	101.38	112.38
8	F	1005	NAG	C2-N2-C7	-6.73	114.39	123.04
8	C	1005	NAG	C2-N2-C7	-6.43	114.77	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1001	NAG	1	0
6	C	1002	NAG	1	0
6	F	1001	NAG	1	0
6	F	1002	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	1006	FUC	2	0
6	I	1001	NAG	1	0
6	I	1002	NAG	1	0
8	L	1003	NAG	1	0
8	L	1004	FUC	4	0

5.6 Ligand geometry [i](#)

24 ligands 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
4	HEM	A	201	1,5	30,50,50	2.34	8 (26%)	24,82,82	2.57	10 (41%)
5	OXY	A	202	4	1,1,1	0.32	0	0,0,0	0.00	-
4	HEM	B	201	2,5	30,50,50	2.16	9 (30%)	24,82,82	2.38	9 (37%)
5	OXY	B	202	4	1,1,1	0.31	0	0,0,0	0.00	-
7	NAG	C	1003	3	14,14,15	2.05	5 (35%)	15,19,21	2.19	6 (40%)
7	NAG	C	1004	3	14,14,15	2.36	7 (50%)	15,19,21	2.50	8 (53%)
4	HEM	D	201	1,5	30,50,50	2.31	9 (30%)	24,82,82	2.47	8 (33%)
5	OXY	D	202	4	1,1,1	0.34	0	0,0,0	0.00	-
4	HEM	E	201	2,5	30,50,50	2.23	9 (30%)	24,82,82	2.38	8 (33%)
5	OXY	E	202	4	1,1,1	0.31	0	0,0,0	0.00	-
7	NAG	F	1003	3	14,14,15	2.19	6 (42%)	15,19,21	1.42	3 (20%)
7	NAG	F	1004	3	14,14,15	1.72	6 (42%)	15,19,21	1.31	1 (6%)
4	HEM	G	201	1,5	30,50,50	2.12	11 (36%)	24,82,82	2.48	10 (41%)
5	OXY	G	202	4	1,1,1	0.33	0	0,0,0	0.00	-
4	HEM	H	201	2,5	30,50,50	2.25	10 (33%)	24,82,82	2.41	9 (37%)
5	OXY	H	202	4	1,1,1	0.28	0	0,0,0	0.00	-
7	NAG	I	1003	3	14,14,15	1.97	5 (35%)	15,19,21	1.72	3 (20%)
7	NAG	I	1004	3	14,14,15	1.79	5 (35%)	15,19,21	1.83	3 (20%)
4	HEM	J	201	1,5	30,50,50	2.24	10 (33%)	24,82,82	2.49	9 (37%)
5	OXY	J	202	4	1,1,1	0.31	0	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	K	201	2,5	30,50,50	2.41	11 (36%)	24,82,82	2.40	7 (29%)
5	OXY	K	202	4	1,1,1	0.27	0	0,0,0	0.00	-
7	NAG	L	1001	3	14,14,15	2.33	7 (50%)	15,19,21	2.25	3 (20%)
7	NAG	L	1002	3	14,14,15	0.40	0	15,19,21	1.46	3 (20%)

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	201	1,5	-	0/10/54/54	0/0/8/8
5	OXY	A	202	4	-	0/0/0/0	0/0/0/0
4	HEM	B	201	2,5	-	0/10/54/54	0/0/8/8
5	OXY	B	202	4	-	0/0/0/0	0/0/0/0
7	NAG	C	1003	3	-	0/6/23/26	0/1/1/1
7	NAG	C	1004	3	-	0/6/23/26	0/1/1/1
4	HEM	D	201	1,5	-	0/10/54/54	0/0/8/8
5	OXY	D	202	4	-	0/0/0/0	0/0/0/0
4	HEM	E	201	2,5	-	0/10/54/54	0/0/8/8
5	OXY	E	202	4	-	0/0/0/0	0/0/0/0
7	NAG	F	1003	3	-	0/6/23/26	0/1/1/1
7	NAG	F	1004	3	-	0/6/23/26	0/1/1/1
4	HEM	G	201	1,5	-	0/10/54/54	0/0/8/8
5	OXY	G	202	4	-	0/0/0/0	0/0/0/0
4	HEM	H	201	2,5	-	0/10/54/54	0/0/8/8
5	OXY	H	202	4	-	0/0/0/0	0/0/0/0
7	NAG	I	1003	3	-	0/6/23/26	0/1/1/1
7	NAG	I	1004	3	-	0/6/23/26	0/1/1/1
4	HEM	J	201	1,5	-	0/10/54/54	0/0/8/8
5	OXY	J	202	4	-	0/0/0/0	0/0/0/0
4	HEM	K	201	2,5	-	0/10/54/54	0/0/8/8
5	OXY	K	202	4	-	0/0/0/0	0/0/0/0
7	NAG	L	1001	3	-	0/6/23/26	0/1/1/1
7	NAG	L	1002	3	-	0/6/23/26	0/1/1/1

The worst 5 of 118 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	201	HEM	C3B-C4B	-7.54	1.45	1.51
4	D	201	HEM	C3B-C4B	-7.16	1.45	1.51
4	E	201	HEM	C3B-C4B	-7.15	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	201	HEM	C3B-C4B	-7.09	1.45	1.51
4	K	201	HEM	C3B-C4B	-6.86	1.45	1.51

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1003	NAG	C2-N2-C7	-6.09	115.21	123.04
7	L	1001	NAG	C1-O5-C5	-5.67	105.06	112.25
7	I	1003	NAG	C2-N2-C7	-4.58	117.16	123.04
4	A	201	HEM	CAA-CBA-CGA	-4.15	105.14	112.75
7	F	1003	NAG	C2-N2-C7	-3.77	118.20	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	HEM	1	0
4	B	201	HEM	4	0
7	C	1003	NAG	1	0
4	E	201	HEM	5	0
4	H	201	HEM	4	0
4	K	201	HEM	2	0
7	L	1002	NAG	1	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	141/141 (100%)	-0.13	0	100 100	37, 56, 86, 124	0
1	D	141/141 (100%)	-0.09	0	100 100	40, 57, 84, 103	0
1	G	141/141 (100%)	-0.06	0	100 100	41, 60, 96, 132	0
1	J	141/141 (100%)	1.05	33 (23%)	1 0	110, 156, 201, 300	0
2	B	146/146 (100%)	-0.15	0	100 100	40, 84, 129, 196	0
2	E	146/146 (100%)	0.21	8 (5%)	29 22	47, 93, 138, 233	0
2	H	146/146 (100%)	-0.09	2 (1%)	78 76	48, 85, 131, 204	0
2	K	146/146 (100%)	2.19	67 (45%)	0 0	127, 182, 250, 268	0
3	C	309/347 (89%)	0.13	8 (2%)	59 54	45, 81, 121, 186	0
3	F	309/347 (89%)	0.15	10 (3%)	51 43	42, 72, 118, 165	1 (0%)
3	I	309/347 (89%)	-0.02	1 (0%)	94 94	45, 67, 106, 133	0
3	L	309/347 (89%)	0.19	11 (3%)	46 38	66, 103, 141, 187	1 (0%)
All	All	2384/2536 (94%)	0.24	140 (5%)	26 19	37, 81, 176, 300	2 (0%)

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	75	LEU	8.5
2	K	11	VAL	8.1
2	K	45	PHE	7.4
2	K	146	HIS	7.0
2	K	1	VAL	6.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
8	FUC	F	1006	10/11	0.72	0.47	8.26	149,149,149,149	0
8	NAG	I	1005	14/15	0.81	0.35	4.89	141,141,141,141	0
8	NAG	F	1005	14/15	0.79	0.42	3.14	135,135,135,135	0
8	NAG	C	1005	14/15	0.77	0.37	2.76	138,138,138,138	0
8	NAG	L	1003	14/15	0.77	0.28	0.63	212,212,212,212	0
8	FUC	C	1006	10/11	0.92	0.21	0.33	138,138,138,138	0
8	FUC	I	1006	10/11	0.87	0.25	0.22	148,148,148,148	0
8	FUC	L	1004	10/11	0.82	0.28	-	188,188,188,188	0
6	NAG	I	1002	14/15	0.84	0.32	-	168,168,168,168	0
6	NAG	F	1001	14/15	0.74	0.20	-	118,118,118,118	0
6	NAG	I	1001	14/15	0.72	0.19	-	126,126,126,126	0
6	NAG	F	1002	14/15	0.79	0.25	-	161,161,161,161	0
6	NAG	C	1002	14/15	0.80	0.34	-	180,180,180,180	0
6	NAG	C	1001	14/15	0.79	0.16	-	122,122,122,122	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
5	OXY	A	202	2/2	0.99	0.38	11.24	92,92,92,96	0
5	OXY	G	202	2/2	0.99	0.49	10.42	101,101,101,105	0
5	OXY	H	202	2/2	0.99	0.24	1.61	174,174,174,176	0
4	HEM	H	201	43/43	0.97	0.25	1.37	83,87,101,109	0
5	OXY	D	202	2/2	1.00	0.22	1.26	84,84,84,88	0
4	HEM	E	201	43/43	0.96	0.23	0.55	95,101,114,121	0
5	OXY	K	202	2/2	0.98	0.47	0.49	292,292,292,295	0
4	HEM	B	201	43/43	0.97	0.21	0.44	76,80,95,103	0
4	HEM	J	201	43/43	0.93	0.34	0.31	183,186,190,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	HEM	D	201	43/43	0.98	0.19	0.06	45,51,57,59	0
4	HEM	G	201	43/43	0.98	0.19	-0.14	41,58,62,64	0
4	HEM	A	201	43/43	0.99	0.18	-0.34	45,54,62,63	0
4	HEM	K	201	43/43	0.93	0.32	-0.54	167,186,195,199	0
5	OXY	E	202	2/2	0.99	0.16	-0.62	146,146,146,148	0
5	OXY	B	202	2/2	1.00	0.18	-0.69	121,121,121,123	0
5	OXY	J	202	2/2	0.97	0.21	-1.05	225,225,225,229	0
7	NAG	F	1003	14/15	0.72	0.54	-	174,174,174,174	0
7	NAG	L	1002	14/15	0.81	0.29	-	171,171,171,171	0
7	NAG	F	1004	14/15	0.71	0.30	-	144,144,144,144	0
7	NAG	I	1003	14/15	0.67	0.41	-	164,164,164,164	0
7	NAG	C	1003	14/15	0.48	0.46	-	172,172,172,172	0
7	NAG	L	1001	14/15	0.71	0.17	-	138,138,138,138	0
7	NAG	C	1004	14/15	0.84	0.25	-	159,159,159,159	0
7	NAG	I	1004	14/15	0.64	0.29	-	150,150,150,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.