



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:15 PM GMT

PDB ID : 3WCV  
Title : The structure of a deoxygenated 400 kda hemoglobin provides a more accurate description of the cooperative mechanism of giant hemoglobins: CA bound form  
Authors : Numoto, N.; Nakagawa, T.; Ohara, R.; Hasegawa, T.; Kita, A.; Yoshida, T.; Maruyama, T.; Imai, K.; Fukumori, Y.; Miki, K.  
Deposited on : 2013-06-01  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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

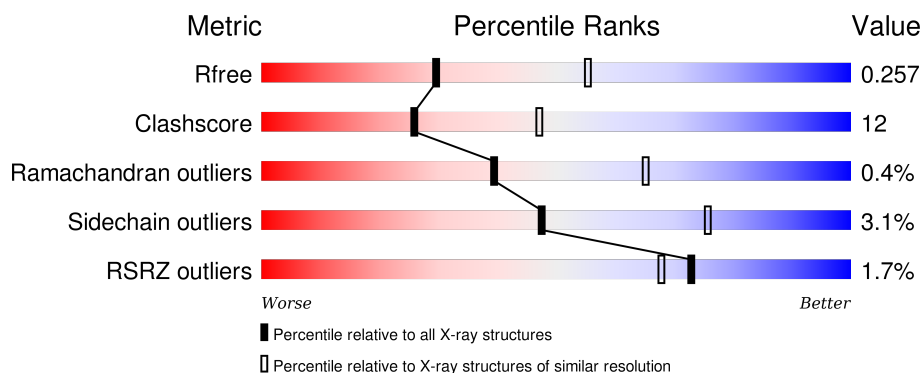
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	<div> <div></div> <div>75%</div> <div>23%</div> <div>•</div> </div>
1	E	146	<div> <div>2%</div> <div>80%</div> <div>18%</div> <div>•</div> </div>
2	B	144	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>•</div> </div>
2	F	144	<div> <div>2%</div> <div>81%</div> <div>19%</div> <div></div> </div>
3	C	150	<div> <div>2%</div> <div>61%</div> <div>33%</div> <div>• •</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	G	150	 4% 73% 27% •
4	D	149	 3% 66% 30% ••
4	H	149	 79% 20% •

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
8	FUC	H	208	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9684 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 A1 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	0	0
			1151	736	198	209	8			
1	E	146	Total	C	N	O	S	0	0	0
			1151	736	198	209	8			

- Molecule 2 is a protein called A2 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1120	697	206	210	7			
2	F	144	Total	C	N	O	S	0	0	0
			1120	697	206	210	7			

- Molecule 3 is a protein called B2 globin chain of giant V2 hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	150	Total	C	N	O	S	0	0	0
			1158	718	211	221	8			
3	G	150	Total	C	N	O	S	0	0	0
			1158	718	211	221	8			

- Molecule 4 is a protein called B1 globin chain of giant V2 hemoglobin.

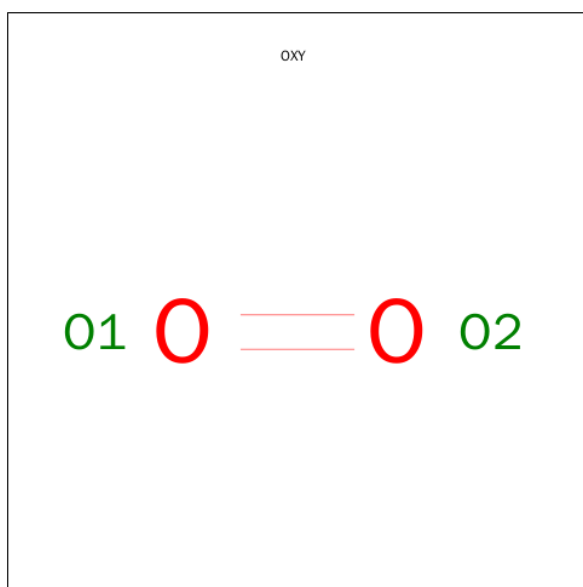
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	147	Total	C	N	O	S	0	0	0
			1125	719	194	205	7			
4	H	148	Total	C	N	O	S	0	0	0
			1134	724	195	208	7			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula:  $O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	C	1	Total O 2 2	0	0
6	D	1	Total O 2 2	0	0
6	E	1	Total O 2 2	0	0
6	F	1	Total O 2 2	0	0
6	G	1	Total O 2 2	0	0
6	H	1	Total O 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Ca 2 2	0	0
7	A	1	Total Ca 1 1	0	0
7	F	3	Total Ca 3 3	0	0

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

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

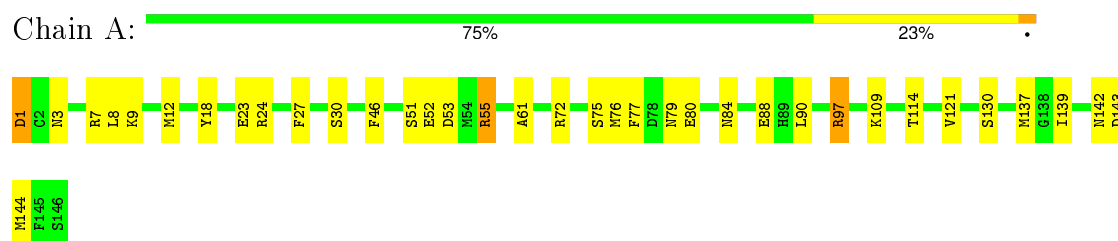
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	11	Total	O	0	0
			11	11		
9	B	2	Total	O	0	0
			2	2		
9	C	7	Total	O	0	0
			7	7		
9	D	9	Total	O	0	0
			9	9		
9	E	11	Total	O	0	0
			11	11		
9	F	9	Total	O	0	0
			9	9		
9	G	3	Total	O	0	0
			3	3		
9	H	7	Total	O	0	0
			7	7		

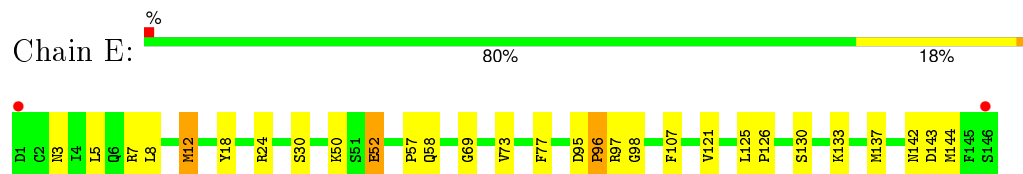
### 3 Residue-property plots

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.

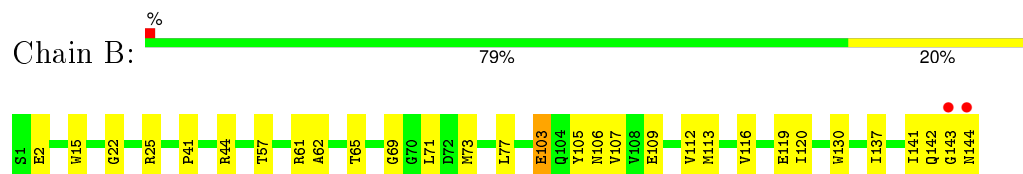
- Molecule 1: A1 globin chain of giant V2 hemoglobin



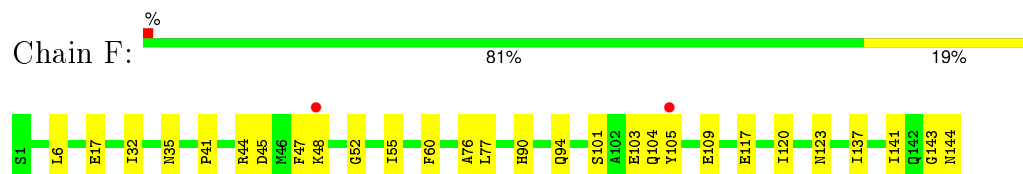
- Molecule 1: A1 globin chain of giant V2 hemoglobin



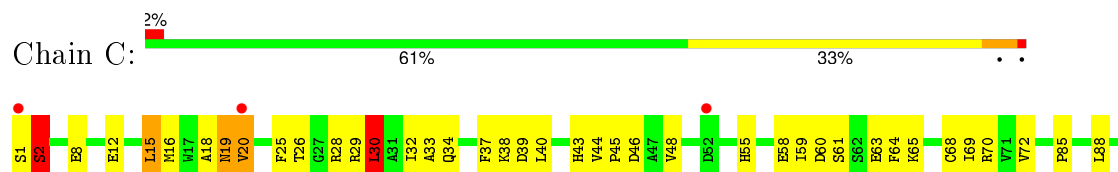
- Molecule 2: A2 globin chain of giant V2 hemoglobin



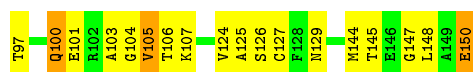
- Molecule 2: A2 globin chain of giant V2 hemoglobin



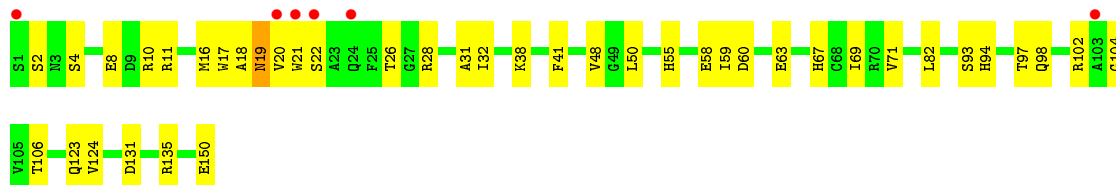
- Molecule 3: B2 globin chain of giant V2 hemoglobin



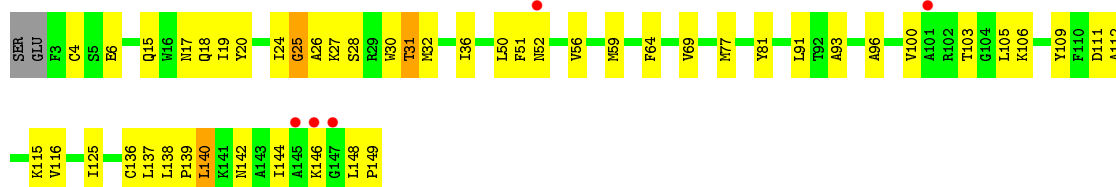




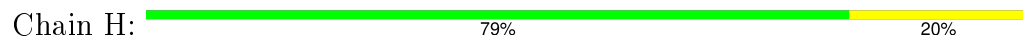
- Molecule 3: B2 globin chain of giant V2 hemoglobin



- Molecule 4: B1 globin chain of giant V2 hemoglobin



- Molecule 4: B1 globin chain of giant V2 hemoglobin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.94Å 108.94Å 195.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.33 – 2.60 36.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.33-2.60) 99.9 (36.33-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.235 , 0.267 0.230 , 0.257	Depositor DCC
$R_{free}$ test set	2037 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.6	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 34.6	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 40167 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9684	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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: NAG, CA, OXY, 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	0.51	0/1178	0.63	0/1585
1	E	0.46	0/1178	0.61	0/1585
2	B	0.42	1/1143 (0.1%)	0.57	0/1543
2	F	0.43	0/1143	0.61	0/1543
3	C	0.67	1/1181 (0.1%)	0.75	4/1597 (0.3%)
3	G	0.40	0/1181	0.58	0/1597
4	D	0.44	0/1149	0.67	3/1559 (0.2%)
4	H	0.49	0/1158	0.61	0/1571
All	All	0.49	2/9311 (0.0%)	0.63	7/12580 (0.1%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	SER	C-O	14.79	1.51	1.23
2	B	119	GLU	CD-OE2	5.64	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	30	LEU	CA-CB-CG	8.16	134.07	115.30
3	C	30	LEU	CB-CG-CD2	-6.57	99.83	111.00
4	D	25	GLY	N-CA-C	6.28	128.80	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	15	LEU	CA-CB-CG	-6.14	101.18	115.30
4	D	140	LEU	CB-CG-CD1	-5.82	101.10	111.00
4	D	140	LEU	CA-CB-CG	5.78	128.60	115.30
3	C	105	VAL	N-CA-C	-5.29	96.72	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	2	SER	Mainchain

## 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	1151	0	1123	35	0
1	E	1151	0	1123	26	0
2	B	1120	0	1077	23	0
2	F	1120	0	1077	16	0
3	C	1158	0	1115	61	0
3	G	1158	0	1115	39	0
4	D	1125	0	1126	37	0
4	H	1134	0	1132	27	0
5	A	43	0	30	2	0
5	B	43	0	30	0	0
5	C	43	0	30	1	0
5	D	43	0	30	0	0
5	E	43	0	30	1	0
5	F	43	0	30	0	0
5	G	43	0	30	0	0
5	H	43	0	30	1	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	2	0	0	0	0
6	H	2	0	0	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	F	3	0	0	0	0
8	D	71	0	61	1	0
8	H	71	0	61	3	0
9	A	11	0	0	1	0
9	B	2	0	0	0	0
9	C	7	0	0	2	0
9	D	9	0	0	0	0
9	E	11	0	0	0	0
9	F	9	0	0	0	0
9	G	3	0	0	1	0
9	H	7	0	0	0	0
All	All	9684	0	9250	234	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 12.

All (234) 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:C:1:SER:CB	3:C:2:SER:HA	1.76	1.10
3:C:1:SER:HB3	3:C:2:SER:CA	1.79	1.10
3:G:20:VAL:CG1	3:G:32:ILE:HD11	1.87	1.03
3:G:20:VAL:HG12	3:G:32:ILE:HD11	1.48	0.95
4:H:50:LEU:HD13	4:H:105:LEU:HD23	1.51	0.93
4:D:19:ILE:HD12	4:D:32:MET:HE3	1.55	0.89
4:H:61:SER:HB2	8:H:208:FUC:H61	1.54	0.89
4:D:27:LYS:O	4:D:31:THR:HG22	1.75	0.86
3:G:20:VAL:HG11	3:G:32:ILE:HD11	1.58	0.83
1:A:137:MET:HE1	1:A:143:ASP:HA	1.58	0.83
1:A:142:ASN:OD1	1:A:144:MET:HG2	1.79	0.82
3:G:20:VAL:HG12	3:G:20:VAL:O	1.82	0.79
3:C:18:ALA:HA	9:C:307:HOH:O	1.86	0.76
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.51	0.76
3:C:104:GLY:O	3:C:106:THR:HG23	1.87	0.75
1:A:53:ASP:OD1	1:A:55:ARG:HG3	1.87	0.75
3:C:147:GLY:O	3:C:148:LEU:HD23	1.87	0.74
3:G:22:SER:HB3	3:G:28:ARG:NH1	2.04	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:ILE:O	2:F:141:ILE:HG13	1.89	0.72
3:C:1:SER:HB3	3:C:2:SER:HA	0.85	0.71
1:A:80:GLU:HG3	1:A:84:ASN:ND2	2.04	0.71
4:D:96:ALA:O	4:D:100:VAL:HG23	1.92	0.70
2:B:73:MET:CE	3:C:69:ILE:HG22	2.23	0.69
4:D:100:VAL:HA	4:D:148:LEU:HD21	1.75	0.69
4:D:15:GLN:O	4:D:18:GLN:HB2	1.93	0.69
3:G:20:VAL:HG21	3:G:124:VAL:HG22	1.76	0.68
1:E:18:TYR:HD2	4:H:22:ALA:HB2	1.59	0.68
4:H:46:GLU:HG3	4:H:109:TYR:OH	1.93	0.68
2:B:41:PRO:O	2:B:44:ARG:HG3	1.92	0.68
3:C:61:SER:O	3:C:65:LYS:HG3	1.94	0.68
1:A:8:LEU:O	1:A:12:MET:HG2	1.94	0.67
3:G:55:HIS:ND1	3:G:63:GLU:HG3	2.10	0.66
3:C:19:ASN:HD22	3:C:20:VAL:N	1.94	0.66
3:C:20:VAL:HG13	3:C:20:VAL:O	1.94	0.66
1:A:121:VAL:HG11	1:E:30:SER:HB3	1.79	0.66
4:H:50:LEU:HD13	4:H:105:LEU:CD2	2.25	0.65
3:G:55:HIS:CG	3:G:63:GLU:HG3	2.32	0.65
3:C:19:ASN:ND2	3:C:20:VAL:N	2.45	0.65
4:H:32:MET:HE3	4:H:124:LEU:HD13	1.80	0.64
1:A:139:ILE:HD12	5:A:201:HEM:HBB2	1.80	0.63
2:B:73:MET:HE1	3:C:70:ARG:HG2	1.81	0.63
4:D:52:ASN:HA	4:D:56:VAL:HG12	1.81	0.62
3:C:20:VAL:CG2	3:C:124:VAL:HG22	2.30	0.62
3:G:22:SER:HB3	3:G:28:ARG:CZ	2.30	0.61
3:C:29:ARG:HB3	3:C:72:VAL:HG11	1.82	0.61
4:H:61:SER:CB	8:H:208:FUC:H61	2.29	0.61
4:H:19:ILE:HD12	4:H:32:MET:HE3	1.82	0.61
3:G:20:VAL:HG12	3:G:32:ILE:CD1	2.27	0.61
3:C:55:HIS:CG	3:C:63:GLU:HG3	2.35	0.61
4:D:28:SER:HA	4:D:31:THR:HG23	1.83	0.61
4:D:106:LYS:HG3	4:D:109:TYR:CE2	2.36	0.61
2:F:143:GLY:O	2:F:144:ASN:HB2	2.01	0.60
2:B:73:MET:HE2	3:C:69:ILE:HG22	1.81	0.60
4:D:142:ASN:O	4:D:146:LYS:HB2	2.01	0.60
3:C:44:VAL:HG12	3:C:46:ASP:OD1	2.02	0.60
1:A:12:MET:HE3	3:C:20:VAL:HA	1.84	0.59
4:D:138:LEU:HB3	4:D:139:PRO:HD3	1.84	0.59
2:B:73:MET:HE1	3:C:70:ARG:CG	2.32	0.58
3:C:85:PRO:HA	3:C:88:LEU:HB3	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:GLY:HA2	2:B:25:ARG:HD2	1.85	0.58
1:A:75:SER:O	4:D:26:ALA:HB2	2.03	0.58
3:G:50:LEU:CD2	3:G:104:GLY:HA3	2.33	0.58
4:H:32:MET:CE	4:H:124:LEU:HD13	2.33	0.58
3:G:106:THR:HB	3:G:150:GLU:O	2.04	0.58
4:H:44:LYS:HE3	4:H:108:VAL:HG12	1.84	0.58
3:G:55:HIS:CE1	3:G:63:GLU:HG3	2.39	0.57
3:C:144:MET:SD	5:C:200:HEM:HBB2	2.44	0.57
2:B:77:LEU:HD21	3:C:69:ILE:CD1	2.34	0.57
4:D:105:LEU:O	4:D:149:PRO:HD2	2.05	0.57
4:H:82:LEU:HA	4:H:88:LEU:HD22	1.86	0.57
2:B:22:GLY:HA2	2:B:25:ARG:CD	2.35	0.57
3:G:21:TRP:CE3	3:G:21:TRP:O	2.58	0.56
2:B:105:TYR:CE2	2:B:142:GLN:HG2	2.40	0.56
4:D:32:MET:O	4:D:36:ILE:HG13	2.05	0.56
2:F:76:ALA:HB1	3:G:26:THR:HG23	1.86	0.56
4:H:61:SER:HB2	8:H:208:FUC:C6	2.31	0.56
3:C:20:VAL:HG21	3:C:124:VAL:HG22	1.88	0.56
4:H:67:HIS:O	4:H:71:VAL:HG23	2.06	0.56
2:B:73:MET:HE3	3:C:69:ILE:HG22	1.89	0.55
1:A:12:MET:CE	3:C:20:VAL:HA	2.37	0.55
2:B:62:ALA:O	2:B:65:THR:HB	2.06	0.55
2:F:77:LEU:HD21	3:G:69:ILE:CD1	2.37	0.55
4:D:106:LYS:HE3	4:D:109:TYR:OH	2.06	0.55
3:C:20:VAL:HG13	3:C:32:ILE:HD11	1.88	0.55
3:C:101:GLU:N	3:C:101:GLU:OE2	2.40	0.55
2:B:77:LEU:CD2	3:C:26:THR:HG21	2.37	0.54
1:E:24:ARG:HH12	4:H:80:ASN:ND2	2.05	0.54
2:F:101:SER:OG	2:F:104:GLN:HG3	2.09	0.53
1:A:12:MET:CE	3:C:28:ARG:HD2	2.39	0.53
2:F:103:GLU:OE1	2:F:103:GLU:HA	2.08	0.53
2:B:69:GLY:O	2:B:73:MET:HG3	2.09	0.52
4:D:15:GLN:HB3	4:D:125:ILE:HG21	1.90	0.52
3:G:131:ASP:HB3	3:G:135:ARG:HH22	1.74	0.52
3:G:50:LEU:HD21	3:G:104:GLY:HA3	1.90	0.52
1:A:72:ARG:NH2	1:A:90:LEU:HD21	2.24	0.52
4:D:111:ASP:O	4:D:115:LYS:HG3	2.10	0.52
4:D:17:ASN:HA	4:D:20:TYR:O	2.09	0.52
3:G:17:TRP:O	3:G:19:ASN:N	2.43	0.52
1:A:1:ASP:HB3	1:A:130:SER:HB3	1.92	0.52
3:C:107:LYS:HE2	3:C:145:THR:O	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TYR:CE1	1:A:24:ARG:HG3	2.45	0.52
4:D:19:ILE:HD12	4:D:32:MET:CE	2.34	0.52
2:B:103:GLU:O	2:B:107:VAL:HG23	2.10	0.52
1:A:84:ASN:O	1:A:88:GLU:HG3	2.09	0.51
2:B:143:GLY:O	2:B:144:ASN:HB2	2.10	0.51
4:D:28:SER:HA	4:D:31:THR:CG2	2.40	0.51
2:B:137:ILE:O	2:B:141:ILE:HG13	2.11	0.51
1:A:97:ARG:HG3	1:A:97:ARG:NH1	2.24	0.51
3:C:18:ALA:HB2	9:C:306:HOH:O	2.11	0.51
2:F:32:ILE:O	2:F:35:ASN:HB3	2.11	0.51
1:A:30:SER:HB3	1:E:121:VAL:HG11	1.93	0.51
3:C:20:VAL:CG1	3:C:20:VAL:O	2.58	0.51
1:E:95:ASP:C	1:E:97:ARG:H	2.14	0.51
3:C:104:GLY:O	3:C:105:VAL:C	2.49	0.51
1:E:95:ASP:O	1:E:97:ARG:N	2.45	0.51
1:E:24:ARG:NH1	4:H:80:ASN:ND2	2.59	0.50
1:A:27:PHE:CE2	1:A:114:THR:HG22	2.47	0.50
2:F:41:PRO:O	2:F:44:ARG:HG2	2.12	0.50
3:C:150:GLU:OE2	3:C:150:GLU:CA	2.60	0.50
2:F:105:TYR:O	2:F:109:GLU:HG3	2.12	0.50
1:A:79:ASN:ND2	4:D:30:TRP:HH2	2.10	0.50
1:A:12:MET:HE2	3:C:28:ARG:HD2	1.94	0.49
4:H:105:LEU:HD22	5:H:201:HEM:HAC	1.95	0.49
3:C:12:GLU:OE1	3:C:129:ASN:ND2	2.45	0.49
3:C:39:ASP:O	3:C:43:HIS:ND1	2.43	0.49
1:A:46:PHE:HB2	1:A:51:SER:HB3	1.94	0.49
3:C:59:ILE:HA	3:C:64:PHE:CD2	2.48	0.49
3:G:2:SER:C	3:G:4:SER:H	2.15	0.49
1:E:95:ASP:N	1:E:96:PRO:HD2	2.28	0.48
2:F:143:GLY:O	2:F:144:ASN:CB	2.61	0.48
3:G:17:TRP:C	3:G:19:ASN:N	2.68	0.47
1:E:107:PHE:CE1	5:E:200:HEM:HAB	2.49	0.47
2:B:109:GLU:O	2:B:113:MET:HG3	2.15	0.47
3:G:38:LYS:HG2	3:G:59:ILE:HD13	1.95	0.47
3:C:20:VAL:HG13	3:C:32:ILE:CD1	2.45	0.47
3:G:20:VAL:CG1	3:G:20:VAL:O	2.56	0.47
1:A:9:LYS:HD3	3:C:124:VAL:O	2.14	0.47
3:C:30:LEU:O	3:C:34:GLN:HG3	2.14	0.47
3:C:126:SER:O	3:C:127:CYS:HB2	2.15	0.47
3:G:67:HIS:O	3:G:71:VAL:HG23	2.15	0.47
3:C:55:HIS:ND1	3:C:63:GLU:HG3	2.30	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ALA:CB	3:C:68:CYS:HB3	2.44	0.47
1:E:52:GLU:H	1:E:52:GLU:CD	2.19	0.46
1:A:80:GLU:HG3	1:A:84:ASN:HD21	1.79	0.46
3:G:17:TRP:C	3:G:19:ASN:H	2.19	0.46
3:G:93:SER:O	3:G:97:THR:HG23	2.16	0.46
3:G:10:ARG:HG2	3:G:82:LEU:HB3	1.97	0.46
4:D:50:LEU:HD13	4:D:105:LEU:CD1	2.46	0.46
3:C:25:PHE:CZ	4:D:28:SER:OG	2.69	0.46
4:D:4:CYS:HB3	4:D:136:CYS:HA	1.98	0.45
1:E:57:PRO:HG2	1:E:58:GLN:NE2	2.32	0.45
4:D:27:LYS:O	4:D:31:THR:CG2	2.56	0.45
9:A:301:HOH:O	1:E:121:VAL:HG13	2.17	0.45
3:C:33:ALA:HB3	3:C:68:CYS:HB3	1.98	0.45
2:B:57:THR:O	2:B:61:ARG:HG3	2.16	0.45
4:D:50:LEU:HD13	4:D:105:LEU:HD12	1.98	0.45
1:A:9:LYS:HE3	3:C:125:ALA:C	2.37	0.45
1:E:12:MET:CE	1:E:12:MET:HA	2.47	0.45
4:D:112:ALA:O	4:D:116:VAL:HG23	2.17	0.45
4:D:51:PHE:HB2	4:D:56:VAL:HB	1.99	0.44
4:D:148:LEU:O	4:D:149:PRO:O	2.35	0.44
4:D:137:LEU:O	4:D:140:LEU:HB2	2.18	0.44
3:G:102:ARG:HB3	9:G:303:HOH:O	2.17	0.44
4:H:15:GLN:O	4:H:18:GLN:HB2	2.18	0.44
2:F:90:HIS:O	2:F:94:GLN:HG3	2.18	0.44
3:G:22:SER:CB	3:G:28:ARG:NH1	2.78	0.44
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.24	0.43
2:F:45:ASP:HA	2:F:48:LYS:HE3	2.00	0.43
1:A:3:ASN:O	1:A:7:ARG:HG3	2.17	0.43
4:H:11:ILE:O	4:H:15:GLN:HG3	2.18	0.43
3:C:104:GLY:O	3:C:106:THR:N	2.51	0.43
4:D:93:ALA:O	4:D:96:ALA:HB3	2.19	0.43
1:A:30:SER:CB	1:E:121:VAL:HG11	2.49	0.43
1:E:142:ASN:C	1:E:144:MET:H	2.21	0.43
3:G:20:VAL:CG1	3:G:32:ILE:CD1	2.78	0.43
1:E:137:MET:CE	1:E:143:ASP:HA	2.49	0.43
4:D:148:LEU:HB3	4:D:149:PRO:HD2	2.00	0.43
4:H:15:GLN:HB3	4:H:125:ILE:HG21	2.01	0.43
1:A:142:ASN:CG	1:A:144:MET:HG2	2.37	0.43
1:E:130:SER:O	1:E:133:LYS:HB2	2.19	0.43
1:E:50:LYS:HD3	1:E:58:GLN:OE1	2.18	0.43
1:A:139:ILE:CD1	5:A:201:HEM:HBB2	2.47	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:THR:HA	3:C:100:GLN:HB2	2.01	0.42
4:D:59:MET:HG2	4:D:64:PHE:CE2	2.53	0.42
2:B:106:ASN:O	2:B:109:GLU:HB2	2.18	0.42
3:G:94:HIS:O	3:G:98:GLN:HG3	2.20	0.42
1:E:8:LEU:HD11	3:G:31:ALA:HB3	2.01	0.42
1:E:125:LEU:HB3	1:E:126:PRO:HD3	2.02	0.42
1:A:121:VAL:HG11	1:E:30:SER:CB	2.48	0.42
3:C:40:LEU:HD12	3:C:40:LEU:O	2.18	0.42
3:C:45:PRO:O	3:C:48:VAL:HG23	2.19	0.42
1:E:3:ASN:O	1:E:7:ARG:HG3	2.20	0.42
2:F:47:PHE:HB2	2:F:52:GLY:HA3	2.02	0.42
3:G:41:PHE:CG	3:G:48:VAL:HG22	2.54	0.42
3:C:12:GLU:O	3:C:16:MET:HG3	2.20	0.42
3:C:40:LEU:HD11	3:C:44:VAL:HG21	2.02	0.42
4:D:77:MET:O	4:D:81:TYR:HD2	2.02	0.42
1:A:97:ARG:CG	1:A:97:ARG:NH1	2.81	0.41
3:C:65:LYS:O	3:C:69:ILE:HG13	2.20	0.41
3:G:63:GLU:H	3:G:63:GLU:CD	2.23	0.41
3:G:38:LYS:HG2	3:G:59:ILE:CD1	2.50	0.41
3:C:150:GLU:OE2	3:C:150:GLU:HA	2.19	0.41
2:B:71:LEU:HD11	2:B:112:VAL:HG21	2.02	0.41
2:B:15:TRP:HB2	2:B:130:TRP:HH2	1.85	0.41
1:E:69:GLY:O	1:E:73:VAL:HG23	2.20	0.41
1:A:61:ALA:HB1	4:D:91:LEU:HD23	2.02	0.41
2:F:55:ILE:HG22	2:F:60:PHE:CE2	2.54	0.41
3:C:55:HIS:CE1	3:C:63:GLU:HG3	2.56	0.41
1:E:95:ASP:C	1:E:97:ARG:N	2.73	0.41
4:H:41:PHE:CE2	4:H:48:GLU:HA	2.55	0.41
3:C:19:ASN:HD22	3:C:20:VAL:H	1.68	0.41
4:H:130:PRO:O	4:H:134:ARG:HG3	2.20	0.41
4:D:105:LEU:HB3	4:D:148:LEU:HD13	2.03	0.41
3:C:8:GLU:CD	3:C:8:GLU:H	2.24	0.41
2:F:6:LEU:HD22	4:H:124:LEU:HD21	2.03	0.41
3:C:37:PHE:O	3:C:38:LYS:C	2.59	0.41
4:H:141:LYS:HB3	4:H:141:LYS:HE3	1.82	0.41
4:H:143:ALA:O	4:H:146:LYS:HB2	2.20	0.41
1:A:76:MET:CE	4:D:69:VAL:HG11	2.51	0.41
3:G:8:GLU:HA	3:G:11:ARG:HD2	2.02	0.41
1:E:5:LEU:HD12	3:G:123:GLN:OE1	2.20	0.41
2:B:77:LEU:HD21	3:C:26:THR:HG21	2.04	0.40
4:H:19:ILE:HD12	4:H:32:MET:CE	2.50	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:44:LYS:NZ	4:H:108:VAL:HG11	2.36	0.40
3:G:21:TRP:HE3	3:G:21:TRP:O	2.01	0.40
1:E:137:MET:HE1	1:E:143:ASP:HA	2.03	0.40
1:A:23:GLU:HA	1:A:23:GLU:OE1	2.20	0.40
2:B:116:VAL:O	2:B:120:ILE:HG12	2.20	0.40
8:D:204:NAG:O3	8:D:205:MAN:H2	2.21	0.40
3:C:58:GLU:HG2	3:C:61:SER:HB3	2.03	0.40
4:H:19:ILE:HD13	4:H:125:ILE:HG13	2.03	0.40
3:G:16:MET:O	3:G:19:ASN:HB2	2.21	0.40
2:F:17:GLU:HG2	2:F:120:ILE:HG22	2.02	0.40
4:D:144:ILE:O	4:D:144:ILE:HG22	2.22	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	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
1	E	144/146 (99%)	139 (96%)	3 (2%)	2 (1%)	14	28
2	B	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
2	F	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
3	C	148/150 (99%)	137 (93%)	10 (7%)	1 (1%)	26	51
3	G	148/150 (99%)	140 (95%)	7 (5%)	1 (1%)	26	51
4	D	145/149 (97%)	138 (95%)	6 (4%)	1 (1%)	26	51
4	H	146/149 (98%)	144 (99%)	2 (1%)	0	100	100
All	All	1159/1178 (98%)	1101 (95%)	53 (5%)	5 (0%)	39	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	25	GLY
3	G	18	ALA
3	C	103	ALA
1	E	96	PRO
1	E	98	GLY

### 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	120/120 (100%)	114 (95%)	6 (5%)	30	56
1	E	120/120 (100%)	117 (98%)	3 (2%)	55	81
2	B	116/116 (100%)	114 (98%)	2 (2%)	68	88
2	F	116/116 (100%)	114 (98%)	2 (2%)	68	88
3	C	124/124 (100%)	117 (94%)	7 (6%)	26	50
3	G	124/124 (100%)	121 (98%)	3 (2%)	57	82
4	D	120/122 (98%)	116 (97%)	4 (3%)	45	73
4	H	121/122 (99%)	118 (98%)	3 (2%)	55	81
All	All	961/964 (100%)	931 (97%)	30 (3%)	47	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	52	GLU
1	A	55	ARG
1	A	77	PHE
1	A	97	ARG
1	A	109	LYS
2	B	2	GLU
2	B	103	GLU
3	C	15	LEU
3	C	19	ASN
3	C	20	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	30	LEU
3	C	60	ASP
3	C	100	GLN
3	C	150	GLU
4	D	6	GLU
4	D	24	ILE
4	D	31	THR
4	D	103	THR
1	E	12	MET
1	E	52	GLU
1	E	77	PHE
2	F	117	GLU
2	F	123	ASN
3	G	19	ASN
3	G	58	GLU
3	G	60	ASP
4	H	2	GLU
4	H	42	LYS
4	H	140	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	103	ASN
2	B	131	GLN
3	C	14	GLN
3	C	19	ASN
3	C	115	GLN
4	D	52	ASN
4	D	127	ASN
1	E	103	ASN
2	F	131	GLN
2	F	142	GLN
3	G	3	ASN
3	G	14	GLN
4	H	52	ASN
4	H	80	ASN

### 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 ⓘ

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
8	NAG	D	203	8,4	14,14,15	0.59	0	15,19,21	1.19	1 (6%)
8	NAG	D	204	8	14,14,15	1.07	1 (7%)	15,19,21	1.40	3 (20%)
8	MAN	D	205	8	11,11,12	0.96	0	14,15,17	1.23	2 (14%)
8	MAN	D	206	8	11,11,12	0.90	0	14,15,17	0.79	1 (7%)
8	MAN	D	207	8	11,11,12	0.77	0	14,15,17	1.21	2 (14%)
8	FUC	D	208	8	10,10,11	0.63	0	14,14,16	0.79	0
8	NAG	H	203	8,4	14,14,15	1.03	2 (14%)	15,19,21	1.26	2 (13%)
8	NAG	H	204	8	14,14,15	0.80	0	15,19,21	0.94	1 (6%)
8	MAN	H	205	8	11,11,12	1.26	1 (9%)	14,15,17	2.18	2 (14%)
8	MAN	H	206	8	11,11,12	1.04	1 (9%)	14,15,17	1.12	2 (14%)
8	MAN	H	207	8	11,11,12	1.02	1 (9%)	14,15,17	0.93	1 (7%)
8	FUC	H	208	8	10,10,11	0.41	0	14,14,16	0.81	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
8	NAG	D	203	8,4	-	0/6/23/26	0/1/1/1
8	NAG	D	204	8	-	0/6/23/26	0/1/1/1
8	MAN	D	205	8	-	0/2/19/22	0/1/1/1
8	MAN	D	206	8	-	0/2/19/22	0/1/1/1
8	MAN	D	207	8	-	0/2/19/22	0/1/1/1
8	FUC	D	208	8	-	0/0/17/20	0/1/1/1
8	NAG	H	203	8,4	-	0/6/23/26	0/1/1/1
8	NAG	H	204	8	-	0/6/23/26	0/1/1/1
8	MAN	H	205	8	-	0/2/19/22	0/1/1/1
8	MAN	H	206	8	-	0/2/19/22	0/1/1/1
8	MAN	H	207	8	-	0/2/19/22	0/1/1/1
8	FUC	H	208	8	-	0/0/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	203	NAG	C8-C7	2.03	1.54	1.50
8	H	206	MAN	C2-C3	2.11	1.55	1.52
8	H	207	MAN	C2-C3	2.32	1.55	1.52
8	D	204	NAG	C1-C2	2.74	1.56	1.52
8	H	203	NAG	C1-C2	2.81	1.56	1.52
8	H	205	MAN	C2-C3	3.28	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	203	NAG	C2-N2-C7	-3.23	118.89	123.04
8	D	204	NAG	C2-N2-C7	-3.21	118.91	123.04
8	H	203	NAG	C4-C3-C2	-3.01	106.55	111.23
8	H	203	NAG	C2-N2-C7	-2.79	119.46	123.04
8	D	204	NAG	C4-C3-C2	-2.59	107.21	111.23
8	H	204	NAG	C2-N2-C7	-2.49	119.84	123.04
8	H	208	FUC	C1-C2-C3	2.06	111.98	109.54
8	D	206	MAN	C1-O5-C5	2.22	115.07	112.25
8	H	206	MAN	C1-C2-C3	2.33	112.30	109.54
8	D	205	MAN	C2-C3-C4	2.33	115.00	111.04
8	D	207	MAN	C1-C2-C3	2.57	112.59	109.54
8	H	205	MAN	C2-C3-C4	2.62	115.49	111.04
8	D	204	NAG	C1-O5-C5	2.74	115.73	112.25
8	D	207	MAN	C1-O5-C5	2.84	115.86	112.25
8	H	207	MAN	C1-O5-C5	2.88	115.90	112.25
8	H	206	MAN	C1-O5-C5	3.25	116.37	112.25
8	D	205	MAN	C1-C2-C3	3.50	113.68	109.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	205	MAN	C1-C2-C3	7.21	118.07	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	204	NAG	1	0
8	D	205	MAN	1	0
8	H	208	FUC	3	0

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	A	201	1,6	30,50,50	2.99	6 (20%)	24,82,82	2.94	8 (33%)
6	OXY	A	202	5	1,1,1	0.07	0	0,0,0	0.00	-
5	HEM	B	201	2,6	30,50,50	2.94	9 (30%)	24,82,82	2.82	8 (33%)
6	OXY	B	202	5	1,1,1	0.12	0	0,0,0	0.00	-
5	HEM	C	200	3,6	30,50,50	2.80	8 (26%)	24,82,82	3.13	8 (33%)
6	OXY	C	201	5	1,1,1	0.12	0	0,0,0	0.00	-
5	HEM	D	201	4,6	30,50,50	2.80	7 (23%)	24,82,82	2.99	8 (33%)
6	OXY	D	202	5	1,1,1	0.16	0	0,0,0	0.00	-
5	HEM	E	200	1,6	30,50,50	2.93	8 (26%)	24,82,82	2.94	8 (33%)
6	OXY	E	201	5	1,1,1	0.10	0	0,0,0	0.00	-
5	HEM	F	201	2,6	30,50,50	3.00	8 (26%)	24,82,82	2.94	9 (37%)
6	OXY	F	202	5	1,1,1	0.11	0	0,0,0	0.00	-
5	HEM	G	200	3,6	30,50,50	2.95	7 (23%)	24,82,82	3.03	8 (33%)
6	OXY	G	201	5	1,1,1	0.13	0	0,0,0	0.00	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEM	H	201	4,6	30,50,50	2.89	8 (26%)	24,82,82	2.95	8 (33%)
6	OXY	H	202	5	1,1,1	0.11	0	0,0,0	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	201	1,6	-	0/10/54/54	0/0/8/8
6	OXY	A	202	5	-	0/0/0/0	0/0/0/0
5	HEM	B	201	2,6	-	0/10/54/54	0/0/8/8
6	OXY	B	202	5	-	0/0/0/0	0/0/0/0
5	HEM	C	200	3,6	-	0/10/54/54	0/0/8/8
6	OXY	C	201	5	-	0/0/0/0	0/0/0/0
5	HEM	D	201	4,6	-	0/10/54/54	0/0/8/8
6	OXY	D	202	5	-	0/0/0/0	0/0/0/0
5	HEM	E	200	1,6	-	0/10/54/54	0/0/8/8
6	OXY	E	201	5	-	0/0/0/0	0/0/0/0
5	HEM	F	201	2,6	-	0/10/54/54	0/0/8/8
6	OXY	F	202	5	-	0/0/0/0	0/0/0/0
5	HEM	G	200	3,6	-	0/10/54/54	0/0/8/8
6	OXY	G	201	5	-	0/0/0/0	0/0/0/0
5	HEM	H	201	4,6	-	0/10/54/54	0/0/8/8
6	OXY	H	202	5	-	0/0/0/0	0/0/0/0

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	201	HEM	C3B-C4B	-10.99	1.42	1.51
5	F	201	HEM	C3B-C4B	-10.77	1.42	1.51
5	G	200	HEM	C3B-C4B	-10.46	1.42	1.51
5	E	200	HEM	C3B-C4B	-10.05	1.42	1.51
5	H	201	HEM	C3B-C4B	-10.04	1.42	1.51
5	C	200	HEM	C3B-C4B	-9.70	1.43	1.51
5	D	201	HEM	C3B-C4B	-9.42	1.43	1.51
5	B	201	HEM	C3B-C4B	-9.39	1.43	1.51
5	B	201	HEM	C3C-CAC	-8.59	1.35	1.51
5	A	201	HEM	C3C-CAC	-8.43	1.35	1.51
5	G	200	HEM	C3C-CAC	-8.24	1.35	1.51
5	E	200	HEM	C3C-CAC	-8.17	1.36	1.51
5	H	201	HEM	C3C-CAC	-7.97	1.36	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	201	HEM	C3C-CAC	-7.97	1.36	1.51
5	C	200	HEM	C3C-CAC	-7.72	1.36	1.51
5	F	201	HEM	C3C-CAC	-7.61	1.37	1.51
5	B	201	HEM	C2D-C3D	-5.90	1.36	1.54
5	F	201	HEM	C2D-C3D	-5.87	1.36	1.54
5	G	200	HEM	C2D-C3D	-5.82	1.37	1.54
5	A	201	HEM	C2D-C3D	-5.81	1.37	1.54
5	E	200	HEM	C2D-C3D	-5.73	1.37	1.54
5	C	200	HEM	C2D-C3D	-5.72	1.37	1.54
5	H	201	HEM	C2D-C3D	-5.62	1.37	1.54
5	D	201	HEM	C2D-C3D	-5.59	1.37	1.54
5	F	201	HEM	C3B-CAB	-3.90	1.44	1.51
5	E	200	HEM	C3D-C4D	-3.83	1.46	1.51
5	A	201	HEM	C3B-CAB	-3.68	1.44	1.51
5	B	201	HEM	C3B-CAB	-3.39	1.45	1.51
5	B	201	HEM	C3D-C4D	-3.24	1.47	1.51
5	F	201	HEM	C2C-C1C	-3.19	1.46	1.52
5	B	201	HEM	C2C-C1C	-3.03	1.46	1.52
5	E	200	HEM	C2C-C1C	-3.02	1.46	1.52
5	G	200	HEM	C3B-CAB	-3.00	1.45	1.51
5	H	201	HEM	C2C-C1C	-2.99	1.46	1.52
5	F	201	HEM	C3D-C4D	-2.94	1.47	1.51
5	G	200	HEM	C3D-C4D	-2.92	1.47	1.51
5	G	200	HEM	C2C-C1C	-2.90	1.47	1.52
5	H	201	HEM	C3B-CAB	-2.88	1.45	1.51
5	C	200	HEM	C3D-C4D	-2.72	1.48	1.51
5	C	200	HEM	C3B-CAB	-2.71	1.46	1.51
5	D	201	HEM	C2C-C1C	-2.54	1.47	1.52
5	E	200	HEM	C3B-CAB	-2.45	1.46	1.51
5	A	201	HEM	C4C-NC	-2.42	1.33	1.36
5	D	201	HEM	C3B-CAB	-2.39	1.46	1.51
5	D	201	HEM	C3D-C4D	-2.38	1.48	1.51
5	B	201	HEM	C4A-CHB	-2.33	1.33	1.39
5	C	200	HEM	C4A-CHB	-2.31	1.33	1.39
5	H	201	HEM	C4A-CHB	-2.30	1.33	1.39
5	A	201	HEM	CMB-C2B	-2.29	1.47	1.53
5	G	200	HEM	C4A-CHB	-2.25	1.33	1.39
5	E	200	HEM	C4A-CHB	-2.18	1.33	1.39
5	C	200	HEM	C2C-C1C	-2.13	1.48	1.52
5	F	201	HEM	C4A-CHB	-2.11	1.34	1.39
5	H	201	HEM	C2B-C1B	-2.05	1.45	1.51
5	B	201	HEM	CMB-C2B	-2.01	1.48	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	200	HEM	C1C-NC	2.20	1.38	1.36
5	C	200	HEM	C1C-NC	2.35	1.38	1.36
5	F	201	HEM	C1C-NC	2.48	1.39	1.36
5	B	201	HEM	C1C-NC	2.50	1.39	1.36
5	H	201	HEM	C1C-NC	2.87	1.39	1.36
5	D	201	HEM	C1C-NC	3.33	1.40	1.36

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	201	HEM	CMA-C3A-C4A	-2.95	123.48	128.36
5	C	200	HEM	CMA-C3A-C4A	-2.81	123.71	128.36
5	F	201	HEM	CMA-C3A-C4A	-2.80	123.73	128.36
5	H	201	HEM	CMA-C3A-C4A	-2.78	123.77	128.36
5	E	200	HEM	CMA-C3A-C4A	-2.75	123.81	128.36
5	D	201	HEM	CMA-C3A-C4A	-2.54	124.17	128.36
5	G	200	HEM	CMA-C3A-C4A	-2.44	124.32	128.36
5	B	201	HEM	CMA-C3A-C4A	-2.35	124.48	128.36
5	F	201	HEM	CAA-CBA-CGA	2.04	116.48	112.75
5	A	201	HEM	C2D-C3D-C4D	2.97	106.54	101.50
5	D	201	HEM	C2D-C3D-C4D	3.08	106.72	101.50
5	H	201	HEM	C2D-C3D-C4D	3.12	106.78	101.50
5	B	201	HEM	C2D-C3D-C4D	3.19	106.91	101.50
5	G	200	HEM	C2D-C3D-C4D	3.23	106.97	101.50
5	C	200	HEM	C2D-C3D-C4D	3.23	106.97	101.50
5	F	201	HEM	C2D-C3D-C4D	3.25	107.01	101.50
5	E	200	HEM	C2D-C3D-C4D	3.32	107.14	101.50
5	E	200	HEM	CAD-C3D-C4D	3.53	124.91	112.47
5	C	200	HEM	CAD-C3D-C4D	3.53	124.94	112.47
5	D	201	HEM	CMD-C2D-C3D	3.61	130.32	114.35
5	G	200	HEM	CAD-C3D-C4D	3.66	125.38	112.47
5	A	201	HEM	CAD-C3D-C4D	3.67	125.41	112.47
5	C	200	HEM	CMD-C2D-C3D	3.67	130.59	114.35
5	B	201	HEM	CMD-C2D-C3D	3.68	130.63	114.35
5	H	201	HEM	CMD-C2D-C3D	3.68	130.63	114.35
5	F	201	HEM	CMD-C2D-C3D	3.69	130.65	114.35
5	E	200	HEM	CMD-C2D-C3D	3.71	130.75	114.35
5	G	200	HEM	CMD-C2D-C3D	3.72	130.80	114.35
5	B	201	HEM	CAD-C3D-C4D	3.75	125.69	112.47
5	A	201	HEM	CMD-C2D-C3D	3.76	131.00	114.35
5	D	201	HEM	CAD-C3D-C4D	3.79	125.83	112.47
5	F	201	HEM	CAD-C3D-C4D	3.83	126.00	112.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	HEM	CAD-C3D-C4D	4.00	126.59	112.47
5	F	201	HEM	CMC-C2C-C3C	4.16	126.92	116.53
5	B	201	HEM	CMC-C2C-C3C	4.21	127.05	116.53
5	C	200	HEM	CMC-C2C-C3C	4.26	127.17	116.53
5	E	200	HEM	CMC-C2C-C3C	4.26	127.17	116.53
5	H	201	HEM	CMC-C2C-C3C	4.30	127.27	116.53
5	D	201	HEM	CMC-C2C-C3C	4.52	127.81	116.53
5	F	201	HEM	CMB-C2B-C3B	4.64	128.11	116.53
5	B	201	HEM	CMB-C2B-C3B	4.64	128.12	116.53
5	H	201	HEM	CAD-C3D-C2D	4.66	126.63	113.22
5	H	201	HEM	CMB-C2B-C3B	4.66	128.18	116.53
5	D	201	HEM	CMB-C2B-C3B	4.68	128.20	116.53
5	G	200	HEM	CMB-C2B-C3B	4.72	128.32	116.53
5	G	200	HEM	CMC-C2C-C3C	4.73	128.35	116.53
5	E	200	HEM	CMB-C2B-C3B	4.74	128.36	116.53
5	F	201	HEM	CAD-C3D-C2D	4.79	127.00	113.22
5	C	200	HEM	CMB-C2B-C3B	4.81	128.54	116.53
5	A	201	HEM	CMC-C2C-C3C	4.83	128.57	116.53
5	B	201	HEM	CAD-C3D-C2D	4.94	127.41	113.22
5	D	201	HEM	CAD-C3D-C2D	4.95	127.45	113.22
5	G	200	HEM	CAD-C3D-C2D	5.02	127.65	113.22
5	E	200	HEM	CAD-C3D-C2D	5.13	127.95	113.22
5	A	201	HEM	CAD-C3D-C2D	5.16	128.05	113.22
5	C	200	HEM	CAD-C3D-C2D	5.17	128.09	113.22
5	A	201	HEM	CMB-C2B-C3B	5.25	129.63	116.53
5	A	201	HEM	C3C-CAC-CBC	8.47	137.46	124.46
5	B	201	HEM	C3C-CAC-CBC	8.83	138.01	124.46
5	E	200	HEM	C3C-CAC-CBC	9.50	139.02	124.46
5	F	201	HEM	C3C-CAC-CBC	9.52	139.06	124.46
5	H	201	HEM	C3C-CAC-CBC	9.70	139.33	124.46
5	D	201	HEM	C3C-CAC-CBC	9.92	139.68	124.46
5	G	200	HEM	C3C-CAC-CBC	10.00	139.80	124.46
5	C	200	HEM	C3C-CAC-CBC	10.57	140.67	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	201	HEM	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	200	HEM	1	0
5	E	200	HEM	1	0
5	H	201	HEM	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	146/146 (100%)	-0.49	0 100 100	27, 43, 69, 79	0
1	E	146/146 (100%)	-0.44	2 (1%) 78 74	27, 51, 71, 86	0
2	B	144/144 (100%)	-0.05	2 (1%) 78 74	38, 67, 92, 106	0
2	F	144/144 (100%)	-0.16	2 (1%) 78 74	32, 57, 85, 101	0
3	C	150/150 (100%)	0.08	3 (2%) 68 63	39, 67, 108, 131	0
3	G	150/150 (100%)	0.06	6 (4%) 42 34	40, 64, 98, 132	0
4	D	147/149 (98%)	-0.17	5 (3%) 49 41	37, 56, 101, 122	0
4	H	148/149 (99%)	-0.48	0 100 100	35, 55, 78, 100	0
All	All	1175/1178 (99%)	-0.21	20 (1%) 73 68	27, 57, 96, 132	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	1	SER	5.7
2	B	144	ASN	4.0
4	D	101	ALA	3.4
3	C	20	VAL	2.9
3	C	1	SER	2.9
3	G	21	TRP	2.8
4	D	146	LYS	2.6
3	G	20	VAL	2.5
3	C	52	ASP	2.5
1	E	1	ASP	2.4
2	B	143	GLY	2.4
4	D	145	ALA	2.4
2	F	105	TYR	2.3
4	D	147	GLY	2.3
3	G	103	ALA	2.2
4	D	52	ASN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	G	22	SER	2.1
3	G	24	GLN	2.1
2	F	48	LYS	2.0
1	E	146	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	FUC	H	208	10/11	0.89	0.36	10.02	111,113,114,116	0
8	FUC	D	208	10/11	0.78	0.23	1.78	100,101,103,105	0
8	NAG	H	203	14/15	0.85	0.15	-	112,116,119,125	0
8	MAN	H	205	11/12	0.37	0.64	-	155,161,165,166	0
8	MAN	D	205	11/12	0.20	0.58	-	161,166,168,172	0
8	MAN	H	206	11/12	0.08	0.90	-	168,169,170,170	0
8	MAN	D	206	11/12	0.07	0.91	-	175,176,178,178	0
8	NAG	D	203	14/15	0.85	0.19	-	108,119,124,133	0
8	MAN	H	207	11/12	-0.14	0.90	-	169,170,171,171	0
8	NAG	H	204	14/15	0.78	0.33	-	131,134,138,146	0
8	MAN	D	207	11/12	0.52	0.47	-	167,169,169,170	0
8	NAG	D	204	14/15	0.68	0.37	-	141,145,148,155	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	HEM	C	200	43/43	0.94	0.20	0.56	66,70,75,79	0
6	OXY	E	201	2/2	0.99	0.13	0.28	54,54,54,61	0
5	HEM	G	200	43/43	0.94	0.19	0.27	65,68,75,76	0
5	HEM	D	201	43/43	0.95	0.18	0.11	51,58,60,61	0
5	HEM	H	201	43/43	0.97	0.15	0.09	51,54,62,65	0
5	HEM	E	200	43/43	0.97	0.13	-0.24	46,48,53,56	0
5	HEM	B	201	43/43	0.97	0.17	-0.26	59,63,69,73	0
5	HEM	F	201	43/43	0.95	0.18	-0.52	51,57,62,67	0
5	HEM	A	201	43/43	0.98	0.12	-0.53	31,37,47,53	0
7	CA	B	203	1/1	0.88	0.07	-	77,77,77,77	0
7	CA	F	203	1/1	0.75	0.08	-	60,60,60,60	0
7	CA	A	203	1/1	0.70	0.12	-	56,56,56,56	1
6	OXY	G	201	2/2	0.97	0.14	-	70,70,70,70	0
7	CA	F	204	1/1	0.69	0.14	-	83,83,83,83	0
7	CA	F	205	1/1	0.94	0.07	-	81,81,81,81	0
6	OXY	C	201	2/2	0.98	0.19	-	78,78,78,84	0
6	OXY	A	202	2/2	0.99	0.12	-	40,40,40,41	0
6	OXY	B	202	2/2	0.99	0.12	-	70,70,70,70	0
6	OXY	F	202	2/2	0.98	0.14	-	66,66,66,67	0
6	OXY	D	202	2/2	0.99	0.12	-	58,58,58,64	0
6	OXY	H	202	2/2	0.98	0.18	-	65,65,65,71	0
7	CA	B	204	1/1	0.92	0.06	-	91,91,91,91	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.