



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:43 AM GMT

PDB ID : 4F4O  
Title : Structure of the Haptoglobin-HaemoglobinComplex  
Authors : Andersen, C.B.F.; Torvund-Jensen, M.; Nielsen, M.J.; Oliveira, C.L.P.; Hersleth, H.P.; Andersen, N.H.; Pedersen, J.S.; Andersen, G.R.; Moestrup, S.K.  
Deposited on : 2012-05-11  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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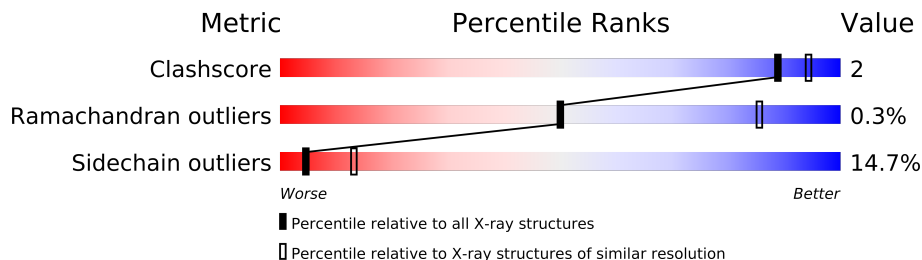
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	141	
1	D	141	
1	G	141	
1	J	141	
2	B	146	
2	E	146	
2	H	146	
2	K	146	
3	C	347	
3	F	347	
3	I	347	
3	L	347	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19196 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

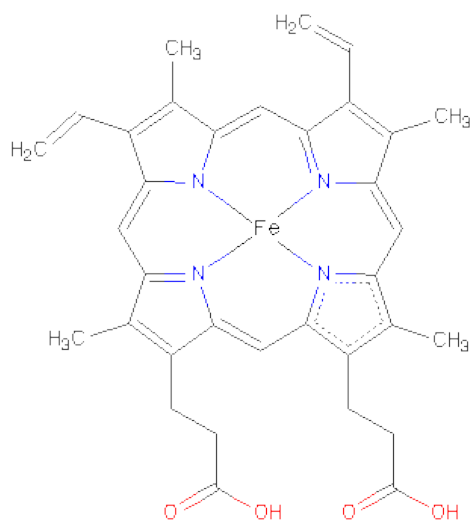
- Molecule 2 is a protein called Hemoglobin subunit beta.

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			

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



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

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

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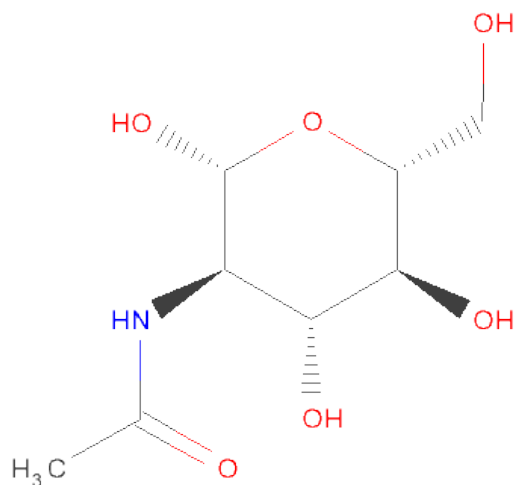
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	D	1	Total O 2 2	0	0
5	E	1	Total O 2 2	0	0
5	G	1	Total O 2 2	0	0
5	H	1	Total O 2 2	0	0
5	J	1	Total O 2 2	0	0
5	K	1	Total O 2 2	0	0

- 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:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

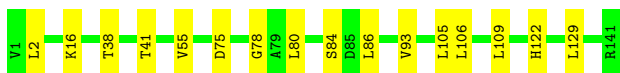
### 3 Residue-property plots

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.

Note EDS failed to run properly.

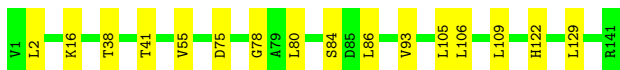
- Molecule 1: Hemoglobin subunit alpha

Chain A: 



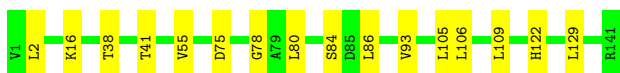
- Molecule 1: Hemoglobin subunit alpha

Chain D: 



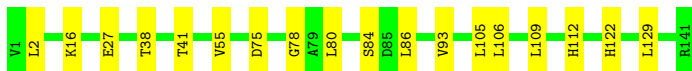
- Molecule 1: Hemoglobin subunit alpha

Chain G: 



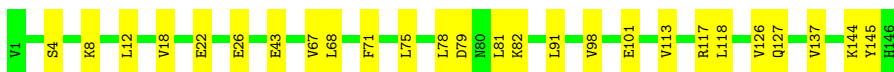
- Molecule 1: Hemoglobin subunit alpha

Chain J: 



- Molecule 2: Hemoglobin subunit beta

Chain B: 



- Molecule 2: Hemoglobin subunit beta

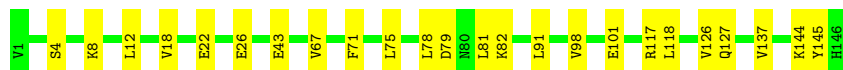
Chain E: 





- Molecule 2: Hemoglobin subunit beta

Chain H: 



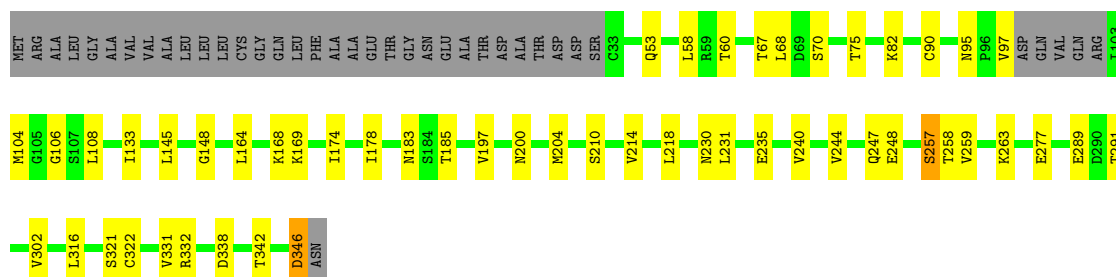
- Molecule 2: Hemoglobin subunit beta

Chain K: 



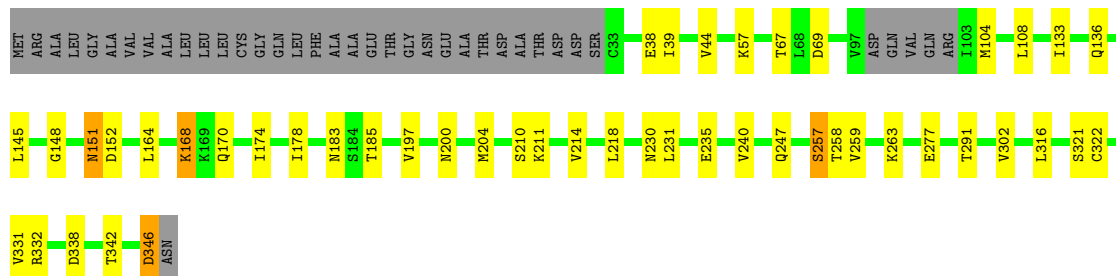
- Molecule 3: Haptoglobin

Chain C: 



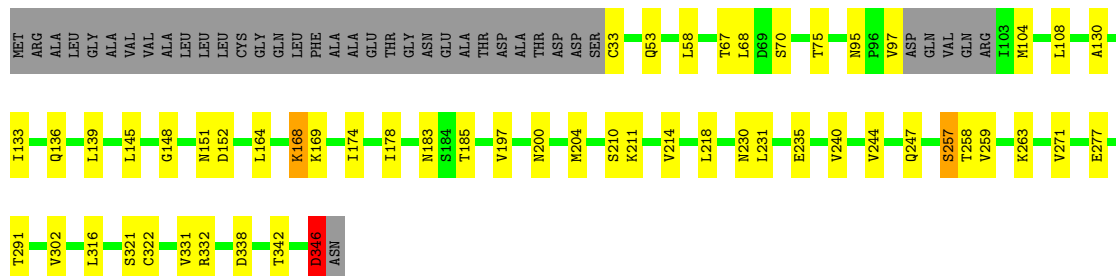
- Molecule 3: Haptoglobin

Chain F: 



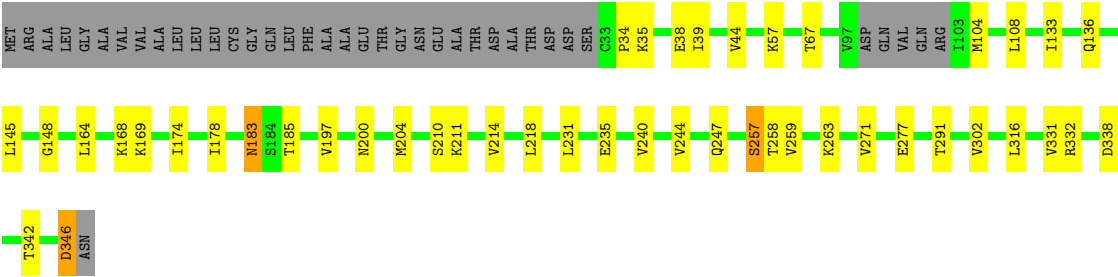
- Molecule 3: Haptoglobin

Chain I: 



- Molecule 3: Haptoglobin

Chain L: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.88Å 197.78Å 322.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.0 (20.00-2.90)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.211 , 0.229	Depositor
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.173	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 103264 reflections	Xtriage
Total number of atoms	19196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

All (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
3	C	322	CYS	C-N-CA	-5.06	109.06	121.70
3	F	136	GLN	N-CA-C	5.04	124.61	111.00
3	L	136	GLN	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (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
3	I	257	SER	Peptide
3	L	148	GLY	Peptide
3	L	257	SER	Peptide
3	L	34	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1064	0	0	1	0
1	D	1064	0	0	1	0
1	G	1064	0	0	1	0
1	J	1064	0	0	2	0
2	B	1144	0	0	5	0
2	E	1144	0	0	5	0
2	H	1144	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1144	0	0	6	0
3	C	2428	0	0	5	0
3	F	2428	0	0	6	0
3	I	2428	0	0	5	0
3	L	2428	0	0	3	0
4	A	43	0	0	0	0
4	B	43	0	0	0	0
4	D	43	0	0	0	0
4	E	43	0	0	0	0
4	G	43	0	0	0	0
4	H	43	0	0	0	0
4	J	43	0	0	0	0
4	K	43	0	0	0	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	0	1	0
6	F	28	0	0	1	0
6	I	28	0	0	1	0
7	C	28	0	0	0	0
7	F	28	0	0	0	0
7	I	28	0	0	0	0
7	L	28	0	0	1	0
8	C	24	0	0	0	0
8	F	24	0	0	0	0
8	I	24	0	0	0	0
8	L	24	0	0	1	0
All	All	19196	0	0	45	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:22:GLU:OE1	2:H:117:ARG:NH2	2.09	0.86
2:K:26:GLU:OE2	2:K:117:ARG:NH1	2.19	0.74
2:H:98:VAL:O	2:H:145:TYR:OH	2.07	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:151:ASN:OD1	3:F:152:ASP:N	2.25	0.70
3:C:257:SER:OG	3:C:263:LYS:NZ	2.25	0.70
3:C:346:ASP:N	3:C:346:ASP:OD1	2.26	0.69
2:B:22:GLU:OE1	2:B:117:ARG:NH2	2.25	0.69
2:B:98:VAL:O	2:B:145:TYR:OH	2.10	0.68
3:I:346:ASP:OD1	3:I:346:ASP:N	2.27	0.68
3:F:346:ASP:OD1	3:F:346:ASP:N	2.27	0.67
3:L:346:ASP:OD1	3:L:346:ASP:N	2.29	0.66
2:E:22:GLU:OE1	2:E:117:ARG:NH2	2.30	0.65
2:E:26:GLU:OE2	2:E:117:ARG:NH1	2.31	0.64
3:I:257:SER:OG	3:I:263:LYS:NZ	2.30	0.64
3:L:257:SER:OG	3:L:263:LYS:NZ	2.30	0.63
3:F:257:SER:OG	3:F:263:LYS:NZ	2.33	0.60
2:E:98:VAL:O	2:E:145:TYR:OH	2.20	0.59
2:B:26:GLU:OE2	2:B:117:ARG:NH1	2.39	0.55
6:C:1001:NAG:O3	6:C:1002:NAG:N2	2.40	0.54
2:K:26:GLU:OE1	2:K:30:ARG:NH2	2.42	0.52
2:K:101[B]:GLU:OE2	8:L:1003:NAG:O7	2.29	0.51
3:L:183:ASN:CG	7:L:1002:NAG:O7	2.50	0.50
2:H:26:GLU:OE2	2:H:117:ARG:NH1	2.44	0.50
2:B:79:ASP:OD1	2:B:79:ASP:N	2.46	0.48
2:K:47:ASP:OD2	2:K:49:SER:OG	2.32	0.47
3:C:106:GLY:N	3:C:289:GLU:OE1	2.48	0.47
1:J:27:GLU:OE1	1:J:112:HIS:NE2	2.48	0.46
1:G:75:ASP:OD1	1:G:78:GLY:N	2.48	0.46
2:H:79:ASP:N	2:H:79:ASP:OD1	2.49	0.45
6:I:1001:NAG:O3	6:I:1002:NAG:N2	2.50	0.45
2:H:101[B]:GLU:CG	3:I:230:ASN:ND2	2.80	0.45
2:E:79:ASP:N	2:E:79:ASP:OD1	2.49	0.45
6:F:1001:NAG:O3	6:F:1002:NAG:N2	2.49	0.45
2:E:101[B]:GLU:CG	3:F:230:ASN:ND2	2.80	0.45
1:D:75:ASP:OD1	1:D:78:GLY:N	2.51	0.43
2:K:98:VAL:O	2:K:145:TYR:OH	2.36	0.43
2:B:101[B]:GLU:CG	3:C:230:ASN:ND2	2.83	0.42
1:A:75:ASP:OD1	1:A:78:GLY:N	2.53	0.42
3:I:130:ALA:O	3:I:139:LEU:O	2.37	0.42
3:I:151:ASN:OD1	3:I:152:ASP:N	2.53	0.41
1:J:75:ASP:OD1	1:J:78:GLY:N	2.53	0.41
3:F:168:LYS:O	3:F:170:GLN:N	2.53	0.41
2:K:79:ASP:OD1	2:K:79:ASP:N	2.53	0.41
3:C:248:GLU:OE1	3:C:248:GLU:N	2.53	0.40
3:F:151:ASN:OD1	3:F:152:ASP:OD1	2.40	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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%)	30	72
3	F	305/347 (88%)	284 (93%)	20 (7%)	1 (0%)	50	85
3	I	305/347 (88%)	287 (94%)	15 (5%)	3 (1%)	22	63
3	L	305/347 (88%)	285 (93%)	18 (6%)	2 (1%)	30	72
All	All	2356/2536 (93%)	2250 (96%)	98 (4%)	8 (0%)	50	85

All (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
3	I	168	LYS
3	I	169	LYS
3	I	258	THR



### 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	111/111 (100%)	97 (87%)	14 (13%)	7	18
1	D	111/111 (100%)	97 (87%)	14 (13%)	7	18
1	G	111/111 (100%)	97 (87%)	14 (13%)	7	18
1	J	111/111 (100%)	97 (87%)	14 (13%)	7	18
2	B	120/119 (101%)	101 (84%)	19 (16%)	4	11
2	E	120/119 (101%)	102 (85%)	18 (15%)	4	12
2	H	120/119 (101%)	103 (86%)	17 (14%)	5	13
2	K	120/119 (101%)	100 (83%)	20 (17%)	3	9
3	C	268/296 (90%)	225 (84%)	43 (16%)	3	10
3	F	268/296 (90%)	230 (86%)	38 (14%)	5	13
3	I	268/296 (90%)	225 (84%)	43 (16%)	3	10
3	L	268/296 (90%)	229 (85%)	39 (15%)	5	13
All	All	1996/2104 (95%)	1703 (85%)	293 (15%)	4	13

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	16	LYS
1	A	38	THR
1	A	41	THR
1	A	55	VAL
1	A	80	LEU
1	A	84	SER
1	A	86	LEU
1	A	93	VAL
1	A	105	LEU
1	A	106	LEU
1	A	109	LEU
1	A	122	HIS
1	A	129	LEU
2	B	4	SER

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Mol	Chain	Res	Type
2	B	8	LYS
2	B	12	LEU
2	B	18	VAL
2	B	43	GLU
2	B	67	VAL
2	B	68	LEU
2	B	71	PHE
2	B	75	LEU
2	B	78	LEU
2	B	81	LEU
2	B	82	LYS
2	B	91	LEU
2	B	113	VAL
2	B	118	LEU
2	B	126	VAL
2	B	127	GLN
2	B	137	VAL
2	B	144	LYS
3	C	53	GLN
3	C	58	LEU
3	C	60	THR
3	C	67	THR
3	C	68	LEU
3	C	70	SER
3	C	75	THR
3	C	82	LYS
3	C	90	CYS
3	C	95	ASN
3	C	97	VAL
3	C	104	MET
3	C	108	LEU
3	C	133	ILE
3	C	145	LEU
3	C	164	LEU
3	C	168	LYS
3	C	174	ILE
3	C	178	ILE
3	C	183	ASN
3	C	185	THR
3	C	197	VAL
3	C	200	ASN
3	C	204	MET

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Mol	Chain	Res	Type
3	C	210	SER
3	C	214	VAL
3	C	218	LEU
3	C	231	LEU
3	C	235	GLU
3	C	240	VAL
3	C	244	VAL
3	C	247	GLN
3	C	259	VAL
3	C	277	GLU
3	C	291	THR
3	C	302	VAL
3	C	316	LEU
3	C	321	SER
3	C	331	VAL
3	C	332	ARG
3	C	338	ASP
3	C	342	THR
3	C	346	ASP
1	D	2	LEU
1	D	16	LYS
1	D	38	THR
1	D	41	THR
1	D	55	VAL
1	D	80	LEU
1	D	84	SER
1	D	86	LEU
1	D	93	VAL
1	D	105	LEU
1	D	106	LEU
1	D	109	LEU
1	D	122	HIS
1	D	129	LEU
2	E	4	SER
2	E	8	LYS
2	E	12	LEU
2	E	23	VAL
2	E	43	GLU
2	E	67	VAL
2	E	71	PHE
2	E	75	LEU
2	E	78	LEU

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Mol	Chain	Res	Type
2	E	81	LEU
2	E	82	LYS
2	E	91	LEU
2	E	113	VAL
2	E	118	LEU
2	E	126	VAL
2	E	127	GLN
2	E	137	VAL
2	E	144	LYS
3	F	38	GLU
3	F	39	ILE
3	F	44	VAL
3	F	57	LYS
3	F	67	THR
3	F	69	ASP
3	F	104	MET
3	F	108	LEU
3	F	133	ILE
3	F	145	LEU
3	F	164	LEU
3	F	168	LYS
3	F	174	ILE
3	F	178	ILE
3	F	183	ASN
3	F	185	THR
3	F	197	VAL
3	F	200	ASN
3	F	204	MET
3	F	210	SER
3	F	211	LYS
3	F	214	VAL
3	F	218	LEU
3	F	231	LEU
3	F	235	GLU
3	F	240	VAL
3	F	247	GLN
3	F	259	VAL
3	F	277	GLU
3	F	291	THR
3	F	302	VAL
3	F	316	LEU
3	F	321	SER

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Mol	Chain	Res	Type
3	F	331	VAL
3	F	332	ARG
3	F	338	ASP
3	F	342	THR
3	F	346	ASP
1	G	2	LEU
1	G	16	LYS
1	G	38	THR
1	G	41	THR
1	G	55	VAL
1	G	80	LEU
1	G	84	SER
1	G	86	LEU
1	G	93	VAL
1	G	105	LEU
1	G	106	LEU
1	G	109	LEU
1	G	122	HIS
1	G	129	LEU
2	H	4	SER
2	H	8	LYS
2	H	12	LEU
2	H	18	VAL
2	H	43	GLU
2	H	67	VAL
2	H	71	PHE
2	H	75	LEU
2	H	78	LEU
2	H	81	LEU
2	H	82	LYS
2	H	91	LEU
2	H	118	LEU
2	H	126	VAL
2	H	127	GLN
2	H	137	VAL
2	H	144	LYS
3	I	33	CYS
3	I	53	GLN
3	I	58	LEU
3	I	67	THR
3	I	68	LEU
3	I	70	SER

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Mol	Chain	Res	Type
3	I	75	THR
3	I	95	ASN
3	I	97	VAL
3	I	104	MET
3	I	108	LEU
3	I	133	ILE
3	I	145	LEU
3	I	164	LEU
3	I	168	LYS
3	I	174	ILE
3	I	178	ILE
3	I	183	ASN
3	I	185	THR
3	I	197	VAL
3	I	200	ASN
3	I	204	MET
3	I	210	SER
3	I	211	LYS
3	I	214	VAL
3	I	218	LEU
3	I	231	LEU
3	I	235	GLU
3	I	240	VAL
3	I	244	VAL
3	I	247	GLN
3	I	259	VAL
3	I	271	VAL
3	I	277	GLU
3	I	291	THR
3	I	302	VAL
3	I	316	LEU
3	I	321	SER
3	I	331	VAL
3	I	332	ARG
3	I	338	ASP
3	I	342	THR
3	I	346	ASP
1	J	2	LEU
1	J	16	LYS
1	J	38	THR
1	J	41	THR
1	J	55	VAL

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Mol	Chain	Res	Type
1	J	80	LEU
1	J	84	SER
1	J	86	LEU
1	J	93	VAL
1	J	105	LEU
1	J	106	LEU
1	J	109	LEU
1	J	122	HIS
1	J	129	LEU
2	K	4	SER
2	K	12	LEU
2	K	23	VAL
2	K	43	GLU
2	K	61	LYS
2	K	67	VAL
2	K	68	LEU
2	K	71	PHE
2	K	75	LEU
2	K	78	LEU
2	K	81	LEU
2	K	91	LEU
2	K	104	ARG
2	K	112	VAL
2	K	118	LEU
2	K	126	VAL
2	K	127	GLN
2	K	137	VAL
2	K	144	LYS
2	K	145	TYR
3	L	35	LYS
3	L	38	GLU
3	L	39	ILE
3	L	44	VAL
3	L	57	LYS
3	L	67	THR
3	L	104	MET
3	L	108	LEU
3	L	133	ILE
3	L	145	LEU
3	L	164	LEU
3	L	168	LYS
3	L	174	ILE

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Mol	Chain	Res	Type
3	L	178	ILE
3	L	183	ASN
3	L	185	THR
3	L	197	VAL
3	L	200	ASN
3	L	204	MET
3	L	210	SER
3	L	211	LYS
3	L	214	VAL
3	L	218	LEU
3	L	231	LEU
3	L	235	GLU
3	L	240	VAL
3	L	244	VAL
3	L	247	GLN
3	L	259	VAL
3	L	271	VAL
3	L	277	GLU
3	L	291	THR
3	L	302	VAL
3	L	316	LEU
3	L	331	VAL
3	L	332	ARG
3	L	338	ASP
3	L	342	THR
3	L	346	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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	12,14,15	2.68	5 (41%)	15,19,21	2.60	8 (53%)
6	NAG	C	1002	6	12,14,15	2.63	6 (50%)	15,19,21	1.60	2 (13%)
8	NAG	C	1005	8,3	12,14,15	2.17	5 (41%)	15,19,21	2.09	5 (33%)
8	FUC	C	1006	8	9,10,11	2.55	4 (44%)	10,14,16	3.04	2 (20%)
6	NAG	F	1001	3,6	12,14,15	2.84	5 (41%)	15,19,21	3.07	9 (60%)
6	NAG	F	1002	6	12,14,15	2.17	6 (50%)	15,19,21	1.44	1 (6%)
8	NAG	F	1005	8,3	12,14,15	2.20	6 (50%)	15,19,21	2.12	5 (33%)
8	FUC	F	1006	8	9,10,11	2.23	4 (44%)	10,14,16	2.33	2 (20%)
6	NAG	I	1001	3,6	12,14,15	2.33	4 (33%)	15,19,21	3.07	7 (46%)
6	NAG	I	1002	6	12,14,15	2.38	6 (50%)	15,19,21	1.47	1 (6%)
8	NAG	I	1005	8,3	12,14,15	2.11	6 (50%)	15,19,21	2.05	3 (20%)
8	FUC	I	1006	8	9,10,11	2.60	5 (55%)	10,14,16	3.21	2 (20%)
8	NAG	L	1003	8,3	12,14,15	0.51	0	15,19,21	1.20	2 (13%)
8	FUC	L	1004	8	9,10,11	0.59	0	10,14,16	0.90	1 (10%)

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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1001	NAG	C2-N2	7.04	1.54	1.46
6	C	1001	NAG	C2-N2	6.37	1.53	1.46
8	I	1006	FUC	O5-C5	5.76	1.56	1.45
6	C	1002	NAG	C2-N2	5.70	1.53	1.46
8	C	1006	FUC	O5-C5	5.58	1.55	1.45
6	I	1001	NAG	C2-N2	5.21	1.52	1.46
6	I	1002	NAG	C2-N2	4.42	1.51	1.46
8	F	1006	FUC	O5-C5	4.25	1.53	1.45
8	C	1005	NAG	O5-C5	4.05	1.52	1.45
8	F	1005	NAG	C2-N2	3.99	1.51	1.46
8	I	1005	NAG	O5-C5	3.94	1.52	1.45
6	F	1001	NAG	C7-N2	3.94	1.50	1.34
6	C	1002	NAG	O5-C5	3.86	1.52	1.45
6	I	1002	NAG	O5-C5	3.75	1.52	1.45
6	F	1002	NAG	C2-N2	3.68	1.50	1.46
6	C	1001	NAG	C7-N2	3.62	1.49	1.34
6	I	1001	NAG	C7-N2	3.52	1.48	1.34
8	C	1006	FUC	C4-C3	-3.22	1.43	1.52
6	C	1002	NAG	C4-C3	-3.16	1.44	1.52
8	I	1005	NAG	O4-C4	3.11	1.50	1.43
8	F	1005	NAG	C7-N2	3.06	1.46	1.34
6	F	1002	NAG	O5-C5	3.06	1.51	1.45
8	C	1005	NAG	C2-N2	3.03	1.49	1.46
8	C	1005	NAG	C7-N2	3.00	1.46	1.34
8	F	1005	NAG	O5-C5	3.00	1.51	1.45
8	I	1006	FUC	C3-C2	-3.00	1.46	1.52
8	F	1006	FUC	O3-C3	2.99	1.50	1.43
8	I	1005	NAG	C7-N2	2.99	1.46	1.34
6	I	1001	NAG	O4-C4	2.96	1.50	1.43
6	C	1002	NAG	C7-N2	2.93	1.46	1.34
6	F	1002	NAG	C4-C3	-2.92	1.44	1.52
8	F	1006	FUC	C4-C3	-2.90	1.44	1.52
6	C	1001	NAG	O4-C4	2.89	1.50	1.43
8	C	1005	NAG	O4-C4	2.87	1.49	1.43
8	C	1006	FUC	C3-C2	-2.87	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	1002	NAG	C4-C3	-2.83	1.44	1.52
6	I	1002	NAG	C7-N2	2.81	1.45	1.34
6	C	1001	NAG	C3-C2	-2.74	1.47	1.52
6	F	1002	NAG	C7-N2	2.73	1.45	1.34
8	I	1006	FUC	C4-C3	-2.71	1.45	1.52
8	F	1005	NAG	C4-C3	-2.66	1.45	1.52
6	C	1002	NAG	O3-C3	2.60	1.49	1.43
6	F	1001	NAG	C3-C2	-2.54	1.47	1.52
6	F	1002	NAG	O3-C3	2.46	1.48	1.43
8	I	1005	NAG	C2-N2	2.44	1.49	1.46
6	F	1001	NAG	O4-C4	2.43	1.48	1.43
8	F	1005	NAG	O3-C3	2.40	1.48	1.43
6	I	1002	NAG	O4-C4	2.40	1.48	1.43
8	C	1005	NAG	C4-C3	-2.35	1.46	1.52
6	I	1002	NAG	O3-C3	2.35	1.48	1.43
6	F	1002	NAG	O4-C4	2.27	1.48	1.43
8	I	1006	FUC	O3-C3	2.22	1.48	1.43
8	F	1005	NAG	O4-C4	2.22	1.48	1.43
8	I	1006	FUC	O4-C4	2.20	1.48	1.43
8	C	1006	FUC	O4-C4	2.19	1.48	1.43
6	I	1001	NAG	O3-C3	2.19	1.48	1.43
6	F	1001	NAG	O5-C5	2.18	1.49	1.45
6	C	1002	NAG	O4-C4	2.15	1.48	1.43
8	I	1005	NAG	C4-C3	-2.11	1.46	1.52
8	F	1006	FUC	C3-C2	-2.05	1.48	1.52
8	I	1005	NAG	O3-C3	2.05	1.47	1.43
6	C	1001	NAG	O5-C5	2.02	1.49	1.45

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1006	FUC	O5-C5-C6	8.55	121.78	108.03
8	C	1006	FUC	O5-C5-C6	8.10	121.05	108.03
6	I	1001	NAG	O5-C5-C6	-6.61	100.04	106.98
6	F	1001	NAG	O5-C5-C6	-5.88	100.81	106.98
8	F	1006	FUC	O5-C5-C6	5.74	117.26	108.03
8	F	1005	NAG	C2-N2-C7	-5.18	114.39	123.09
6	F	1001	NAG	C2-N2-C7	5.02	131.52	123.09
8	C	1005	NAG	C2-N2-C7	-4.95	114.77	123.09
8	I	1006	FUC	C6-C5-C4	-4.94	105.04	113.06
8	C	1006	FUC	C6-C5-C4	-4.83	105.22	113.06
8	I	1005	NAG	C2-N2-C7	-4.65	115.29	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1001	NAG	O3-C3-C2	-4.53	99.56	109.09
6	C	1002	NAG	C2-N2-C7	-4.45	115.62	123.09
6	F	1001	NAG	O7-C7-C8	-4.36	113.53	122.04
8	I	1005	NAG	O5-C5-C4	4.34	116.16	110.65
6	I	1001	NAG	O4-C4-C3	4.22	119.81	110.35
6	C	1001	NAG	C2-N2-C7	4.14	130.04	123.09
6	I	1001	NAG	C8-C7-N2	4.14	124.19	116.11
6	C	1001	NAG	O7-C7-C8	-4.09	114.06	122.04
8	C	1005	NAG	O5-C5-C4	4.06	115.81	110.65
6	I	1001	NAG	O7-C7-C8	-4.06	114.12	122.04
6	I	1001	NAG	O3-C3-C4	3.88	119.06	110.35
6	I	1002	NAG	C2-N2-C7	-3.88	116.58	123.09
6	F	1001	NAG	O3-C3-C2	-3.80	101.10	109.09
8	F	1006	FUC	C6-C5-C4	-3.73	107.00	113.06
6	I	1001	NAG	O3-C3-C2	-3.72	101.27	109.09
6	C	1001	NAG	O4-C4-C3	3.70	118.64	110.35
8	F	1005	NAG	O5-C5-C4	3.64	115.28	110.65
6	F	1001	NAG	O4-C4-C3	3.48	118.17	110.35
6	F	1002	NAG	C2-N2-C7	-3.45	117.29	123.09
6	C	1002	NAG	O5-C5-C6	3.06	110.19	106.98
6	I	1001	NAG	O5-C5-C4	2.98	114.43	110.65
6	F	1001	NAG	C3-C2-N2	-2.95	107.27	111.76
6	C	1001	NAG	C8-C7-N2	2.63	121.25	116.11
6	C	1001	NAG	O5-C5-C6	-2.57	104.28	106.98
6	F	1001	NAG	O3-C3-C4	2.56	116.10	110.35
6	C	1001	NAG	O3-C3-C4	2.55	116.07	110.35
8	C	1005	NAG	O3-C3-C2	-2.53	103.78	109.09
6	F	1001	NAG	C8-C7-N2	2.40	120.80	116.11
8	F	1005	NAG	C8-C7-N2	2.37	120.73	116.11
8	F	1005	NAG	O5-C5-C6	-2.32	104.55	106.98
8	L	1003	NAG	O5-C5-C6	2.27	109.36	106.98
8	I	1005	NAG	O4-C4-C5	2.27	115.25	109.28
8	L	1004	FUC	C6-C5-C4	-2.21	109.48	113.06
6	F	1001	NAG	C6-C5-C4	2.08	118.02	113.00
8	C	1005	NAG	O4-C4-C5	2.05	114.68	109.28
8	C	1005	NAG	C4-C3-C2	2.03	116.29	111.32
6	C	1001	NAG	C4-C3-C2	2.03	116.28	111.32
8	L	1003	NAG	C8-C7-N2	2.02	120.06	116.11
8	F	1005	NAG	O6-C6-C5	2.00	118.24	111.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry

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	49,50,50	2.38	13 (26%)	46,82,82	2.30	14 (30%)
5	OXY	A	202	4	1,1,1	0.42	0	0,0,0	0.00	-
4	HEM	B	201	2,5	49,50,50	2.57	19 (38%)	46,82,82	2.27	11 (23%)
5	OXY	B	202	4	1,1,1	0.44	0	0,0,0	0.00	-
7	NAG	C	1003	3	12,14,15	2.35	5 (41%)	15,19,21	1.93	6 (40%)
7	NAG	C	1004	3	12,14,15	2.50	8 (66%)	15,19,21	2.99	9 (60%)
4	HEM	D	201	1,5	49,50,50	2.18	14 (28%)	46,82,82	2.05	8 (17%)
5	OXY	D	202	4	1,1,1	0.38	0	0,0,0	0.00	-
4	HEM	E	201	2,5	49,50,50	2.37	16 (32%)	46,82,82	2.21	10 (21%)
5	OXY	E	202	4	1,1,1	0.44	0	0,0,0	0.00	-
7	NAG	F	1003	3	12,14,15	2.21	5 (41%)	15,19,21	1.69	3 (20%)
7	NAG	F	1004	3	12,14,15	1.55	5 (41%)	15,19,21	1.28	1 (6%)
4	HEM	G	201	1,5	49,50,50	2.13	14 (28%)	46,82,82	2.30	11 (23%)
5	OXY	G	202	4	1,1,1	0.41	0	0,0,0	0.00	-
4	HEM	H	201	2,5	49,50,50	2.30	15 (30%)	46,82,82	2.34	10 (21%)
5	OXY	H	202	4	1,1,1	0.49	0	0,0,0	0.00	-
7	NAG	I	1003	3	12,14,15	2.25	5 (41%)	15,19,21	1.44	3 (20%)
7	NAG	I	1004	3	12,14,15	1.56	3 (25%)	15,19,21	1.82	3 (20%)
4	HEM	J	201	1,5	49,50,50	2.16	14 (28%)	46,82,82	2.23	9 (19%)
5	OXY	J	202	4	1,1,1	0.45	0	0,0,0	0.00	-
4	HEM	K	201	2,5	49,50,50	2.53	15 (30%)	46,82,82	2.28	13 (28%)
5	OXY	K	202	4	1,1,1	0.51	0	0,0,0	0.00	-
7	NAG	L	1001	3	12,14,15	2.70	7 (58%)	15,19,21	1.51	2 (13%)
7	NAG	L	1002	3	12,14,15	0.52	0	15,19,21	1.21	2 (13%)

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	-	0/14/114/114	0/0/8/8
5	OXY	A	202	4	-	0/0/0/0	0/0/0/0
4	HEM	B	201	2,5	-	0/14/114/114	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	-	1/6/23/26	0/1/1/1
4	HEM	D	201	1,5	-	0/14/114/114	0/0/8/8
5	OXY	D	202	4	-	0/0/0/0	0/0/0/0
4	HEM	E	201	2,5	-	0/14/114/114	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	-	0/14/114/114	0/0/8/8
5	OXY	G	202	4	-	0/0/0/0	0/0/0/0
4	HEM	H	201	2,5	-	0/14/114/114	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	-	0/14/114/114	0/0/8/8
5	OXY	J	202	4	-	0/0/0/0	0/0/0/0
4	HEM	K	201	2,5	-	0/14/114/114	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

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	201	HEM	C2B-C1B	7.43	1.46	1.44
4	B	201	HEM	C2B-C1B	6.63	1.46	1.44
4	K	201	HEM	C3D-C2D	6.22	1.54	1.43
4	A	201	HEM	C2B-C1B	6.00	1.46	1.44
4	B	201	HEM	C3D-C2D	5.71	1.53	1.43
4	A	201	HEM	C3B-C2B	-5.67	1.33	1.43
4	A	201	HEM	C3D-C2D	5.63	1.53	1.43
4	A	201	HEM	FE-NC	5.48	2.18	1.97
4	H	201	HEM	C3D-C2D	5.45	1.53	1.43
4	J	201	HEM	C3D-C2D	5.41	1.53	1.43
7	L	1001	NAG	C2-N2	5.40	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	201	HEM	C3B-C2B	-5.27	1.34	1.43
4	E	201	HEM	C3D-C2D	5.26	1.53	1.43
4	B	201	HEM	C3C-CAC	5.20	1.56	1.40
4	D	201	HEM	C3D-C2D	5.10	1.52	1.43
4	E	201	HEM	C2B-C1B	5.06	1.45	1.44
4	H	201	HEM	C3C-CAC	5.06	1.56	1.40
4	G	201	HEM	C3D-C2D	5.02	1.52	1.43
4	K	201	HEM	C3B-CAB	5.01	1.56	1.40
4	E	201	HEM	C3C-CAC	4.97	1.56	1.40
4	J	201	HEM	C3B-C2B	-4.91	1.35	1.43
4	J	201	HEM	C3C-C2C	-4.89	1.35	1.43
4	K	201	HEM	C3C-CAC	4.88	1.55	1.40
4	H	201	HEM	C3C-C2C	-4.87	1.35	1.43
4	B	201	HEM	C3C-C2C	-4.87	1.35	1.43
4	B	201	HEM	C3B-CAB	4.87	1.55	1.40
4	E	201	HEM	C3C-C2C	-4.85	1.35	1.43
4	B	201	HEM	C3B-C2B	-4.80	1.35	1.43
4	H	201	HEM	C3B-CAB	4.78	1.55	1.40
4	E	201	HEM	C3B-CAB	4.75	1.55	1.40
4	J	201	HEM	C3C-CAC	4.75	1.55	1.40
4	A	201	HEM	C3C-CAC	4.75	1.55	1.40
4	D	201	HEM	C2B-C1B	4.72	1.45	1.44
4	D	201	HEM	C3C-C2C	-4.70	1.35	1.43
4	K	201	HEM	C3C-C2C	-4.70	1.35	1.43
4	D	201	HEM	C3C-CAC	4.67	1.55	1.40
4	G	201	HEM	C3C-CAC	4.67	1.55	1.40
4	D	201	HEM	C3B-C2B	-4.61	1.35	1.43
4	A	201	HEM	C3C-C2C	-4.59	1.35	1.43
4	K	201	HEM	FE-NC	4.59	2.15	1.97
4	E	201	HEM	C3B-C2B	-4.59	1.35	1.43
4	J	201	HEM	C3B-CAB	4.59	1.54	1.40
4	H	201	HEM	C3B-C2B	-4.57	1.35	1.43
4	B	201	HEM	C4A-C3A	4.50	1.45	1.40
4	H	201	HEM	C4A-C3A	4.48	1.45	1.40
4	G	201	HEM	C3C-C2C	-4.41	1.36	1.43
4	G	201	HEM	C3B-CAB	4.38	1.54	1.40
7	C	1003	NAG	C2-N2	4.38	1.51	1.46
4	D	201	HEM	C3B-CAB	4.30	1.53	1.40
7	I	1003	NAG	C2-N2	4.29	1.51	1.46
4	K	201	HEM	C3B-C2B	-4.28	1.36	1.43
4	H	201	HEM	FE-ND	4.26	2.13	1.97
4	E	201	HEM	FE-ND	4.25	2.13	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	201	HEM	C4A-C3A	4.22	1.45	1.40
4	A	201	HEM	C3B-CAB	4.21	1.53	1.40
7	C	1004	NAG	O5-C5	4.19	1.53	1.45
4	K	201	HEM	C4A-C3A	4.19	1.45	1.40
4	J	201	HEM	C4A-C3A	4.01	1.45	1.40
4	K	201	HEM	FE-NB	4.00	2.12	1.97
4	H	201	HEM	FE-NA	3.99	2.09	1.92
4	A	201	HEM	FE-ND	3.94	2.12	1.97
4	E	201	HEM	C3D-C4D	3.87	1.45	1.44
4	D	201	HEM	FE-ND	3.87	2.11	1.97
4	B	201	HEM	FE-NC	3.85	2.12	1.97
4	E	201	HEM	FE-NA	3.84	2.08	1.92
7	C	1003	NAG	O5-C5	3.80	1.52	1.45
7	I	1003	NAG	O5-C5	3.78	1.52	1.45
4	B	201	HEM	C3D-C4D	3.77	1.45	1.44
7	F	1003	NAG	O5-C5	3.73	1.52	1.45
4	D	201	HEM	C4A-C3A	3.72	1.44	1.40
7	L	1001	NAG	C7-N2	3.71	1.49	1.34
4	G	201	HEM	C4A-C3A	3.55	1.44	1.40
7	F	1003	NAG	C2-N2	3.52	1.50	1.46
4	H	201	HEM	C3D-C4D	3.50	1.45	1.44
7	C	1004	NAG	C7-N2	3.47	1.48	1.34
7	C	1004	NAG	O4-C4	3.42	1.51	1.43
4	B	201	HEM	FE-NB	3.37	2.10	1.97
4	D	201	HEM	FE-NC	3.35	2.10	1.97
4	J	201	HEM	FE-NB	3.34	2.10	1.97
4	J	201	HEM	FE-NC	3.34	2.10	1.97
4	A	201	HEM	C4A-C3A	3.33	1.44	1.40
7	C	1003	NAG	C7-N2	3.32	1.47	1.34
4	B	201	HEM	C2D-C1D	3.28	1.45	1.44
4	G	201	HEM	FE-ND	3.26	2.09	1.97
7	I	1004	NAG	C4-C3	-3.18	1.43	1.52
4	E	201	HEM	FE-NC	3.16	2.09	1.97
7	F	1003	NAG	C7-N2	3.12	1.47	1.34
7	L	1001	NAG	O5-C5	3.10	1.51	1.45
4	B	201	HEM	FE-NA	3.08	2.05	1.92
7	I	1003	NAG	C7-N2	3.06	1.46	1.34
4	G	201	HEM	CMC-C2C	3.05	1.56	1.47
4	G	201	HEM	FE-NB	3.04	2.08	1.97
4	A	201	HEM	CMC-C2C	2.93	1.56	1.47
7	L	1001	NAG	C4-C3	-2.93	1.44	1.52
4	H	201	HEM	FE-NC	2.91	2.08	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	201	HEM	FE-NA	2.87	2.04	1.92
4	K	201	HEM	FE-ND	2.83	2.08	1.97
4	D	201	HEM	CMC-C2C	2.83	1.56	1.47
4	G	201	HEM	C3D-C4D	2.83	1.45	1.44
4	B	201	HEM	FE-ND	2.82	2.08	1.97
4	J	201	HEM	FE-ND	2.80	2.08	1.97
4	G	201	HEM	FE-NA	2.77	2.04	1.92
7	C	1004	NAG	C4-C3	-2.76	1.45	1.52
7	I	1004	NAG	C7-N2	2.68	1.45	1.34
4	K	201	HEM	CMB-C2B	2.67	1.55	1.47
7	C	1004	NAG	O3-C3	2.67	1.49	1.43
7	C	1004	NAG	C2-N2	2.66	1.49	1.46
4	B	201	HEM	CMC-C2C	2.62	1.55	1.47
7	F	1003	NAG	C4-C3	-2.61	1.45	1.52
4	E	201	HEM	CMB-C2B	2.58	1.55	1.47
4	B	201	HEM	C1A-C2A	2.56	1.47	1.43
7	L	1001	NAG	O4-C4	2.55	1.49	1.43
4	G	201	HEM	CMB-C2B	2.55	1.55	1.47
7	I	1003	NAG	O3-C3	2.54	1.49	1.43
7	C	1004	NAG	C3-C2	-2.52	1.47	1.52
4	D	201	HEM	CMB-C2B	2.51	1.55	1.47
7	L	1001	NAG	C3-C2	-2.49	1.47	1.52
7	C	1003	NAG	C4-C3	-2.49	1.45	1.52
4	D	201	HEM	C3D-C4D	-2.49	1.43	1.44
4	K	201	HEM	CMC-C2C	2.49	1.55	1.47
4	J	201	HEM	CMB-C2B	2.48	1.55	1.47
4	A	201	HEM	CMB-C2B	2.48	1.55	1.47
4	K	201	HEM	CHB-C1B	2.47	1.39	1.35
4	E	201	HEM	CHA-C4D	2.46	1.39	1.35
4	J	201	HEM	CMC-C2C	2.46	1.55	1.47
4	B	201	HEM	CMD-C2D	2.45	1.55	1.47
4	B	201	HEM	CMB-C2B	2.44	1.55	1.47
4	H	201	HEM	CMC-C2C	2.40	1.54	1.47
7	F	1003	NAG	O3-C3	2.36	1.48	1.43
4	A	201	HEM	CMD-C2D	2.36	1.54	1.47
4	H	201	HEM	FE-NB	2.35	2.06	1.97
4	H	201	HEM	CMD-C2D	2.34	1.54	1.47
4	D	201	HEM	O1A-CGA	2.32	1.30	1.22
4	H	201	HEM	CMB-C2B	2.31	1.54	1.47
4	K	201	HEM	CMD-C2D	2.28	1.54	1.47
4	E	201	HEM	CMD-C2D	2.28	1.54	1.47
4	J	201	HEM	CMD-C2D	2.28	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	HEM	O1A-CGA	2.26	1.30	1.22
4	B	201	HEM	CHB-C1B	2.24	1.39	1.35
4	G	201	HEM	C2B-C1B	2.23	1.45	1.44
4	J	201	HEM	C2B-C1B	2.22	1.45	1.44
7	L	1001	NAG	O3-C3	2.21	1.48	1.43
7	I	1003	NAG	C4-C3	-2.21	1.46	1.52
4	D	201	HEM	CMD-C2D	2.20	1.54	1.47
4	E	201	HEM	CMC-C2C	2.20	1.54	1.47
4	H	201	HEM	C1A-C2A	2.19	1.47	1.43
7	F	1004	NAG	O4-C4	2.18	1.48	1.43
7	F	1004	NAG	O5-C5	2.17	1.49	1.45
4	G	201	HEM	CMD-C2D	2.16	1.54	1.47
7	F	1004	NAG	C4-C3	-2.14	1.46	1.52
7	C	1003	NAG	O3-C3	2.14	1.48	1.43
7	I	1004	NAG	O4-C4	2.14	1.48	1.43
4	E	201	HEM	CAA-C2A	2.11	1.55	1.52
4	J	201	HEM	FE-NA	2.07	2.01	1.92
7	F	1004	NAG	C7-N2	2.05	1.42	1.34
7	F	1004	NAG	C2-N2	-2.02	1.43	1.46
7	C	1004	NAG	O7-C7	2.00	1.27	1.23
4	B	201	HEM	CAA-C2A	2.00	1.55	1.52

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	201	HEM	C3B-C4B-NB	-9.74	107.03	114.00
4	H	201	HEM	C3B-C4B-NB	-9.38	107.29	114.00
4	A	201	HEM	C3B-C4B-NB	-8.99	107.57	114.00
4	J	201	HEM	C3B-C4B-NB	-8.98	107.58	114.00
4	B	201	HEM	C3B-C4B-NB	-8.85	107.67	114.00
4	E	201	HEM	C3B-C4B-NB	-8.47	107.94	114.00
7	C	1004	NAG	O5-C5-C6	8.44	115.84	106.98
4	D	201	HEM	C3B-C4B-NB	-8.08	108.22	114.00
4	K	201	HEM	C3B-C4B-NB	-7.91	108.34	114.00
4	K	201	HEM	C4D-ND-C1D	7.49	112.82	105.16
4	H	201	HEM	C4D-ND-C1D	6.67	111.99	105.16
4	B	201	HEM	C4D-ND-C1D	6.42	111.73	105.16
4	E	201	HEM	C4D-ND-C1D	6.35	111.66	105.16
4	A	201	HEM	C4D-ND-C1D	6.28	111.59	105.16
4	J	201	HEM	C4D-ND-C1D	6.26	111.56	105.16
4	G	201	HEM	C4D-ND-C1D	6.05	111.35	105.16
4	D	201	HEM	C4D-ND-C1D	5.95	111.25	105.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	HEM	CBD-CAD-C3D	-5.34	102.71	114.37
4	G	201	HEM	CBD-CAD-C3D	-4.97	103.53	114.37
7	F	1003	NAG	O5-C5-C6	4.94	112.17	106.98
4	J	201	HEM	CBD-CAD-C3D	-4.79	103.91	114.37
7	C	1003	NAG	C2-N2-C7	-4.69	115.21	123.09
4	D	201	HEM	CBD-CAD-C3D	-4.64	104.23	114.37
4	K	201	HEM	C2D-C1D-ND	-4.40	107.74	112.93
7	I	1004	NAG	C8-C7-N2	4.01	123.95	116.11
7	C	1004	NAG	C2-N2-C7	3.84	129.53	123.09
4	B	201	HEM	C4A-C3A-C2A	3.80	109.64	107.00
4	E	201	HEM	CHC-C4B-NB	3.72	127.67	124.58
4	H	201	HEM	CHC-C4B-NB	3.71	127.67	124.58
4	H	201	HEM	C2D-C1D-ND	-3.65	108.62	112.93
4	B	201	HEM	C2D-C1D-ND	-3.57	108.71	112.93
7	I	1003	NAG	C2-N2-C7	-3.53	117.16	123.09
4	A	201	HEM	C2D-C1D-ND	-3.43	108.88	112.93
4	H	201	HEM	C1B-NB-C4B	3.43	108.67	105.16
7	L	1001	NAG	O7-C7-C8	-3.42	115.37	122.04
4	J	201	HEM	C2D-C1D-ND	-3.38	108.94	112.93
4	E	201	HEM	C2D-C1D-ND	-3.36	108.96	112.93
7	L	1001	NAG	C2-N2-C7	3.35	128.71	123.09
4	B	201	HEM	CHC-C4B-NB	3.32	127.34	124.58
7	I	1004	NAG	O6-C6-C5	3.25	122.53	111.36
4	D	201	HEM	C2D-C1D-ND	-3.23	109.12	112.93
4	G	201	HEM	C1B-NB-C4B	3.17	108.40	105.16
7	I	1004	NAG	O7-C7-C8	-3.06	116.06	122.04
4	H	201	HEM	CMA-C3A-C4A	-3.06	123.91	128.62
4	B	201	HEM	C3A-C4A-NA	-3.05	107.11	109.41
4	H	201	HEM	C4A-C3A-C2A	3.05	109.11	107.00
4	E	201	HEM	C1B-NB-C4B	3.04	108.27	105.16
4	H	201	HEM	C3A-C4A-NA	-3.03	107.12	109.41
4	K	201	HEM	C1B-NB-C4B	3.00	108.23	105.16
4	G	201	HEM	C2D-C1D-ND	-3.00	109.39	112.93
4	B	201	HEM	C1B-NB-C4B	2.94	108.17	105.16
4	K	201	HEM	C3A-C4A-NA	-2.93	107.20	109.41
7	C	1004	NAG	O7-C7-C8	-2.92	116.34	122.04
7	F	1003	NAG	C2-N2-C7	-2.91	118.20	123.09
4	K	201	HEM	CBD-CAD-C3D	-2.91	108.03	114.37
4	E	201	HEM	CMA-C3A-C4A	-2.77	124.36	128.62
4	J	201	HEM	C1B-NB-C4B	2.77	108.00	105.16
7	C	1004	NAG	C6-C5-C4	-2.74	106.37	113.00
4	B	201	HEM	CMA-C3A-C4A	-2.70	124.46	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1004	NAG	C8-C7-N2	2.68	121.35	116.11
4	E	201	HEM	C3A-C4A-NA	-2.68	107.39	109.41
7	I	1003	NAG	O3-C3-C4	2.64	116.27	110.35
7	C	1004	NAG	O6-C6-C5	2.64	120.45	111.36
4	K	201	HEM	CHD-C1D-ND	2.64	126.78	124.58
4	E	201	HEM	C4A-C3A-C2A	2.62	108.82	107.00
4	K	201	HEM	C4C-NC-C1C	2.60	108.24	105.53
4	A	201	HEM	CHC-C4B-NB	2.60	126.74	124.58
4	A	201	HEM	CAA-CBA-CGA	-2.59	105.14	113.47
4	A	201	HEM	C4C-NC-C1C	2.54	108.17	105.53
4	G	201	HEM	CHD-C4C-NC	2.52	126.92	124.73
7	C	1004	NAG	O4-C4-C5	2.52	115.91	109.28
4	K	201	HEM	CBA-CAA-C2A	-2.51	108.26	112.69
4	E	201	HEM	CAD-C3D-C4D	2.49	129.01	124.53
4	G	201	HEM	C4A-CHB-C1B	-2.43	124.27	127.47
4	E	201	HEM	C4C-NC-C1C	2.41	108.04	105.53
7	C	1004	NAG	O7-C7-N2	2.41	126.94	121.90
4	K	201	HEM	CHC-C4B-NB	2.39	126.57	124.58
7	L	1002	NAG	O5-C5-C6	2.36	109.46	106.98
7	C	1004	NAG	O5-C5-C4	2.36	113.65	110.65
4	J	201	HEM	CHC-C4B-NB	2.32	126.51	124.58
7	C	1004	NAG	C4-C3-C2	2.31	116.98	111.32
4	J	201	HEM	C4C-NC-C1C	2.31	107.94	105.53
7	C	1003	NAG	O5-C5-C6	2.30	109.40	106.98
4	A	201	HEM	C1B-NB-C4B	2.30	107.52	105.16
7	C	1003	NAG	O3-C3-C2	-2.27	104.33	109.09
4	H	201	HEM	C4C-NC-C1C	2.26	107.89	105.53
4	J	201	HEM	C3A-C4A-NA	-2.26	107.71	109.41
4	K	201	HEM	C2A-C1A-NA	-2.24	106.62	109.73
4	G	201	HEM	CAA-CBA-CGA	-2.24	106.26	113.47
4	B	201	HEM	CAD-C3D-C4D	2.23	128.54	124.53
4	D	201	HEM	C4C-NC-C1C	2.19	107.82	105.53
4	H	201	HEM	CAD-C3D-C4D	2.19	128.47	124.53
4	G	201	HEM	CHC-C4B-NB	2.19	126.40	124.58
4	A	201	HEM	C4A-CHB-C1B	-2.19	124.59	127.47
4	B	201	HEM	C4C-NC-C1C	2.17	107.80	105.53
7	C	1003	NAG	C8-C7-N2	2.17	120.35	116.11
4	J	201	HEM	CAA-CBA-CGA	-2.16	106.52	113.47
4	A	201	HEM	C1A-C2A-C3A	2.16	109.16	106.92
4	G	201	HEM	C4C-NC-C1C	2.16	107.78	105.53
7	C	1003	NAG	O3-C3-C4	2.15	115.17	110.35
4	D	201	HEM	C1B-NB-C4B	2.14	107.35	105.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	HEM	C3A-C4A-NA	-2.13	107.80	109.41
4	D	201	HEM	CAA-CBA-CGA	-2.11	106.70	113.47
4	A	201	HEM	C2A-C1A-NA	-2.10	106.81	109.73
7	F	1003	NAG	O3-C3-C4	2.10	115.07	110.35
4	K	201	HEM	CHC-C1C-NC	2.09	126.55	124.73
7	C	1003	NAG	O5-C5-C4	2.09	113.30	110.65
4	K	201	HEM	CHA-C4D-ND	2.06	127.14	124.31
4	A	201	HEM	CAD-C3D-C4D	2.05	128.22	124.53
4	B	201	HEM	CBD-CAD-C3D	-2.05	109.90	114.37
4	A	201	HEM	CHD-C1D-ND	2.04	126.28	124.58
4	G	201	HEM	C3A-C4A-NA	-2.04	107.87	109.41
7	L	1002	NAG	C8-C7-N2	2.03	120.07	116.11
7	I	1003	NAG	O5-C5-C6	2.02	109.11	106.98
4	D	201	HEM	C1A-C2A-C3A	2.02	109.01	106.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1004	NAG	C3-C2-N2-C7

There are no ring outliers.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.