



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:01 PM GMT

PDB ID : 3UCP
Title : Outer membrane Endecaheme cytochrome UndA from Shewanella sp. HRCR-6
Authors : Edwards, M.J.; Clarke, T.A.
Deposited on : 2011-10-27
Resolution : 1.76 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

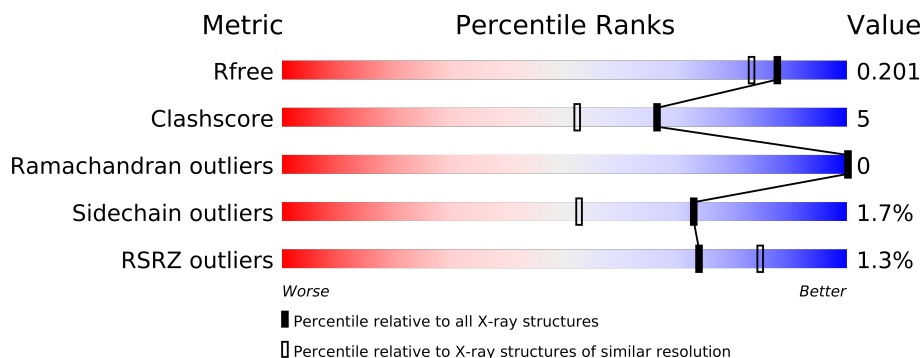
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 1.76 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}	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	874	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HEC	A	911	-	X
5	GOL	A	915	-	X
5	GOL	A	916	-	X
5	GOL	A	918	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7814 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 UndA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	800	5990	3720	1030	1205	35	0	11	0

There are 58 discrepancies between the modelled and reference sequences:

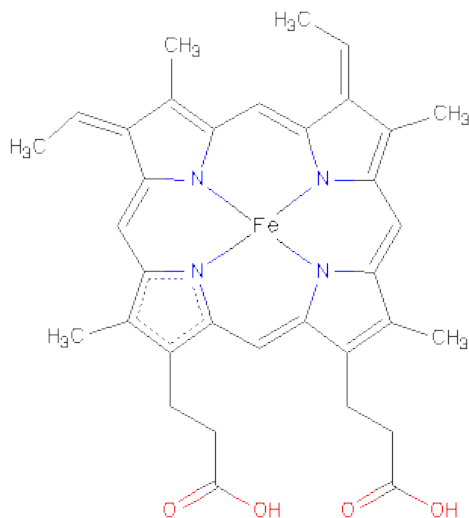
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP F8UWD6
A	1	SER	-	EXPRESSION TAG	UNP F8UWD6
A	2	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	3	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	4	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	5	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	6	SER	-	EXPRESSION TAG	UNP F8UWD6
A	7	VAL	-	EXPRESSION TAG	UNP F8UWD6
A	8	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	9	PHE	-	EXPRESSION TAG	UNP F8UWD6
A	10	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	11	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	12	SER	-	EXPRESSION TAG	UNP F8UWD6
A	13	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	14	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	15	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	16	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	17	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	18	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	19	SER	-	EXPRESSION TAG	UNP F8UWD6
A	20	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	21	THR	-	EXPRESSION TAG	UNP F8UWD6
A	22	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	23	PHE	-	EXPRESSION TAG	UNP F8UWD6
A	24	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	25	ALA	-	EXPRESSION TAG	UNP F8UWD6
A	26	ASP	-	EXPRESSION TAG	UNP F8UWD6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLN	-	EXPRESSION TAG	UNP F8UWD6
A	844	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	845	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	846	GLU	-	EXPRESSION TAG	UNP F8UWD6
A	847	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	848	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	849	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	850	GLU	-	EXPRESSION TAG	UNP F8UWD6
A	851	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	852	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	853	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	854	ILE	-	EXPRESSION TAG	UNP F8UWD6
A	855	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	856	ASN	-	EXPRESSION TAG	UNP F8UWD6
A	857	PRO	-	EXPRESSION TAG	UNP F8UWD6
A	858	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	859	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	860	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	861	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	862	ASP	-	EXPRESSION TAG	UNP F8UWD6
A	863	SER	-	EXPRESSION TAG	UNP F8UWD6
A	864	THR	-	EXPRESSION TAG	UNP F8UWD6
A	865	ARG	-	EXPRESSION TAG	UNP F8UWD6
A	866	THR	-	EXPRESSION TAG	UNP F8UWD6
A	867	GLY	-	EXPRESSION TAG	UNP F8UWD6
A	868	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	869	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	870	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	871	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	872	HIS	-	EXPRESSION TAG	UNP F8UWD6
A	873	HIS	-	EXPRESSION TAG	UNP F8UWD6

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

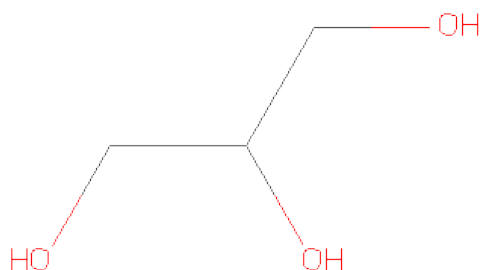
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

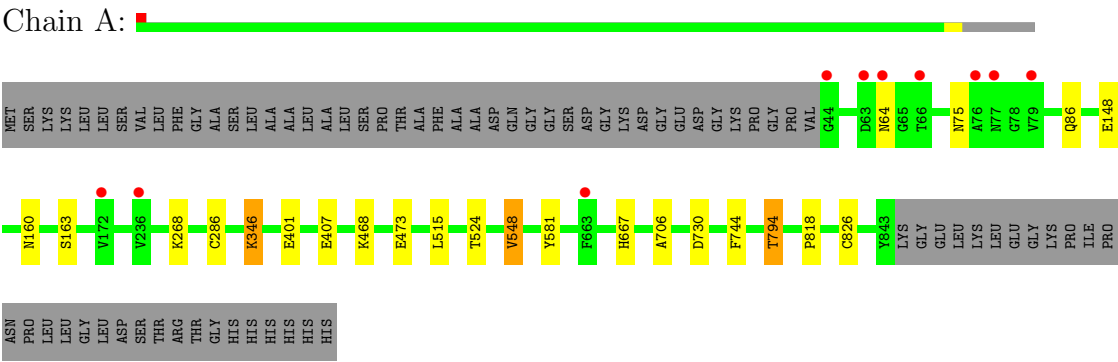
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1318	Total	O	0	0
			1318	1318		

3 Residue-property plots i

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

● Molecule 1: UndA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.64Å 106.09Å 151.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.91 – 1.76 40.91 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.91-1.76) 99.6 (40.91-1.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.144 , 0.177 0.171 , 0.201	Depositor DCC
R_{free} test set	5538 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 110649 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7814	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL, CA, MG, HEC

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	0.71	1/6151 (0.0%)	0.67	1/8368 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	548	VAL	CB-CG2	-5.51	1.41	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	VAL	CB-CA-C	-5.21	101.49	111.40

There are no chirality outliers.

There are no planarity outliers.

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	5990	0	0	21	0
2	A	473	0	331	17	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	30	0	40	4	0
6	A	1318	0	0	13	1
All	All	7814	0	371	33	1

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 5.

All (33) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:826:CYS:SG	2:A:911:HEC:HAC	1.94	1.01
1:A:730[A]:ASP:OD1	6:A:1301:HOH:O	1.83	0.97
5:A:917:GOL:H11	6:A:1405:HOH:O	1.77	0.82
1:A:794:THR:CG2	6:A:1242:HOH:O	2.28	0.80
1:A:346:LYS:CD	6:A:1403:HOH:O	2.31	0.78
1:A:286:CYS:SG	2:A:902:HEC:CBC	2.78	0.71
1:A:286:CYS:SG	2:A:902:HEC:C3C	2.78	0.70
1:A:826:CYS:SG	2:A:911:HEC:C3C	2.80	0.69
1:A:160:ASN:OD1	5:A:918:GOL:H32	2.00	0.61
2:A:902:HEC:HMC1	2:A:902:HEC:HBC3	1.84	0.60
1:A:163[A]:SER:OG	5:A:918:GOL:H31	2.02	0.59
2:A:910:HEC:HBA1	2:A:910:HEC:HMA3	1.87	0.57
2:A:903:HEC:HMB1	2:A:903:HEC:HBB3	1.87	0.56
1:A:346:LYS:NZ	6:A:1403:HOH:O	2.38	0.56
2:A:904:HEC:HBC3	2:A:904:HEC:HMC1	1.89	0.53
2:A:910:HEC:HBB3	2:A:910:HEC:HMB1	1.91	0.53
1:A:346:LYS:CE	6:A:1403:HOH:O	2.58	0.52
1:A:86:GLN:CG	6:A:1272:HOH:O	2.58	0.50
2:A:907:HEC:HBB3	2:A:907:HEC:HMB1	1.93	0.50
1:A:468:LYS:NZ	6:A:1832:HOH:O	2.46	0.48
1:A:401:GLU:OE1	6:A:2260:HOH:O	2.20	0.47
2:A:911:HEC:HMC1	2:A:911:HEC:HBC3	1.97	0.46
1:A:473:GLU:OE2	6:A:2297:HOH:O	2.21	0.45
1:A:160:ASN:CG	6:A:2002:HOH:O	2.54	0.45
1:A:524[B]:THR:CG2	6:A:2033:HOH:O	2.64	0.45
1:A:286:CYS:CB	2:A:902:HEC:CAC	2.93	0.45
2:A:910:HEC:HBA1	2:A:910:HEC:CMA	2.45	0.44
2:A:905:HEC:HMC1	2:A:905:HEC:HBC3	1.99	0.43
1:A:524[B]:THR:CG2	1:A:706:ALA:CB	2.96	0.43
5:A:916:GOL:H11	6:A:2157:HOH:O	2.18	0.41
1:A:744:PHE:CE1	2:A:906:HEC:HBC2	2.56	0.41
2:A:910:HEC:HMC1	2:A:910:HEC:HBC3	2.02	0.40
1:A:667:HIS:CD2	2:A:908:HEC:ND	2.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:1417:HOH:O	6:A:2274:HOH:O[4_555]	2.19	0.01

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	809/874 (93%)	783 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	655/700 (94%)	644 (98%)	11 (2%)	73	52

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	75	ASN
1	A	148	GLU
1	A	268	LYS
1	A	346	LYS
1	A	407	GLU
1	A	515	LEU
1	A	548	VAL
1	A	581	TYR

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Mol	Chain	Res	Type
1	A	794	THR
1	A	818	PRO

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 3 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$
2	HEC	A	901	1	50,50,50	2.68	13 (26%)	56,82,82	2.11	13 (23%)
2	HEC	A	902	1,3	50,50,50	2.62	16 (32%)	56,82,82	1.99	14 (25%)
2	HEC	A	903	1	50,50,50	2.74	15 (30%)	56,82,82	2.12	20 (35%)
2	HEC	A	904	1	50,50,50	2.63	15 (30%)	56,82,82	2.07	15 (26%)
2	HEC	A	905	1	50,50,50	2.81	17 (34%)	56,82,82	2.00	16 (28%)
2	HEC	A	906	1	50,50,50	2.58	13 (26%)	56,82,82	2.29	18 (32%)
2	HEC	A	907	1	50,50,50	2.51	12 (24%)	56,82,82	2.26	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	A	908	1,4	50,50,50	2.49	13 (26%)	56,82,82	1.98	17 (30%)
2	HEC	A	909	1	50,50,50	2.75	16 (32%)	56,82,82	2.50	18 (32%)
2	HEC	A	910	1	50,50,50	2.83	14 (28%)	56,82,82	2.24	17 (30%)
2	HEC	A	911	1	50,50,50	2.66	15 (30%)	56,82,82	2.13	15 (26%)
5	GOL	A	915	-	5,5,5	0.24	0	5,5,5	0.56	0
5	GOL	A	916	-	5,5,5	0.41	0	5,5,5	0.50	0
5	GOL	A	917	-	5,5,5	0.52	0	5,5,5	0.40	0
5	GOL	A	918	-	5,5,5	0.46	0	5,5,5	0.30	0
5	GOL	A	919	-	5,5,5	0.51	0	5,5,5	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	901	1	-	0/10/54/54	0/0/8/8
2	HEC	A	902	1,3	-	0/10/54/54	0/0/8/8
2	HEC	A	903	1	-	0/10/54/54	0/0/8/8
2	HEC	A	904	1	-	0/10/54/54	0/0/8/8
2	HEC	A	905	1	-	0/10/54/54	0/0/8/8
2	HEC	A	906	1	-	0/10/54/54	0/0/8/8
2	HEC	A	907	1	-	0/10/54/54	0/0/8/8
2	HEC	A	908	1,4	-	0/10/54/54	0/0/8/8
2	HEC	A	909	1	-	0/10/54/54	0/0/8/8
2	HEC	A	910	1	-	0/10/54/54	0/0/8/8
2	HEC	A	911	1	-	0/10/54/54	0/0/8/8
5	GOL	A	915	-	-	0/4/4/4	0/0/0/0
5	GOL	A	916	-	-	0/4/4/4	0/0/0/0
5	GOL	A	917	-	-	0/4/4/4	0/0/0/0
5	GOL	A	918	-	-	0/4/4/4	0/0/0/0
5	GOL	A	919	-	-	0/4/4/4	0/0/0/0

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEC	C3C-CAC	10.60	1.57	1.35
2	A	905	HEC	C3C-CAC	10.36	1.56	1.35
2	A	902	HEC	C3C-CAC	10.34	1.56	1.35
2	A	903	HEC	C3B-CAB	10.32	1.56	1.35
2	A	910	HEC	C3B-CAB	10.25	1.56	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	909	HEC	C3C-CAC	10.07	1.56	1.35
2	A	911	HEC	C3C-CAC	9.95	1.55	1.35
2	A	910	HEC	C3C-CAC	9.72	1.55	1.35
2	A	909	HEC	C3B-CAB	9.70	1.55	1.35
2	A	907	HEC	C3C-CAC	9.54	1.55	1.35
2	A	904	HEC	C3C-CAC	9.49	1.55	1.35
2	A	908	HEC	C3B-CAB	9.49	1.55	1.35
2	A	911	HEC	C3B-CAB	9.38	1.54	1.35
2	A	905	HEC	C3B-CAB	9.30	1.54	1.35
2	A	906	HEC	C3C-CAC	9.22	1.54	1.35
2	A	901	HEC	C3B-CAB	9.08	1.54	1.35
2	A	906	HEC	C3B-CAB	9.06	1.54	1.35
2	A	903	HEC	C3C-CAC	9.01	1.54	1.35
2	A	904	HEC	C3B-CAB	8.77	1.53	1.35
2	A	908	HEC	C3C-CAC	8.71	1.53	1.35
2	A	902	HEC	C3B-CAB	8.63	1.53	1.35
2	A	907	HEC	C3B-CAB	8.12	1.52	1.35
2	A	903	HEC	C1D-C2D	5.53	1.47	1.40
2	A	910	HEC	C1C-C2C	5.07	1.46	1.40
2	A	911	HEC	C3D-C2D	5.04	1.52	1.37
2	A	905	HEC	C3D-C2D	5.04	1.52	1.37
2	A	910	HEC	C3D-C2D	4.85	1.52	1.37
2	A	904	HEC	C1D-C2D	4.80	1.46	1.40
2	A	905	HEC	C1B-C2B	4.74	1.46	1.40
2	A	906	HEC	C1B-C2B	4.71	1.46	1.40
2	A	904	HEC	C1C-C2C	4.52	1.45	1.40
2	A	903	HEC	C3D-C2D	4.52	1.51	1.37
2	A	911	HEC	C1C-C2C	4.49	1.45	1.40
2	A	906	HEC	C1C-C2C	4.48	1.45	1.40
2	A	901	HEC	C3D-C2D	4.44	1.50	1.37
2	A	910	HEC	C1B-C2B	4.43	1.45	1.40
2	A	907	HEC	C1C-C2C	4.43	1.45	1.40
2	A	909	HEC	C3D-C2D	4.40	1.50	1.37
2	A	909	HEC	C3B-C4B	4.33	1.47	1.41
2	A	902	HEC	C3D-C2D	4.31	1.50	1.37
2	A	905	HEC	C1C-C2C	4.25	1.45	1.40
2	A	903	HEC	C1C-C2C	4.22	1.45	1.40
2	A	902	HEC	C1C-C2C	4.21	1.45	1.40
2	A	911	HEC	C1B-C2B	4.18	1.45	1.40
2	A	904	HEC	C1B-C2B	4.16	1.45	1.40
2	A	901	HEC	C3B-C2B	-4.15	1.32	1.41
2	A	901	HEC	C1C-C2C	4.14	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	908	HEC	C1C-C2C	4.14	1.45	1.40
2	A	905	HEC	C3B-C4B	4.08	1.46	1.41
2	A	907	HEC	C1D-C2D	3.98	1.45	1.40
2	A	910	HEC	C1D-C2D	3.98	1.45	1.40
2	A	907	HEC	C3D-C2D	3.90	1.49	1.37
2	A	904	HEC	C3D-C2D	3.87	1.49	1.37
2	A	906	HEC	C3B-C4B	3.80	1.46	1.41
2	A	910	HEC	FE-NC	3.72	2.08	1.92
2	A	911	HEC	C1D-C2D	3.67	1.44	1.40
2	A	905	HEC	C1D-C2D	3.63	1.44	1.40
2	A	906	HEC	C3D-C2D	3.59	1.48	1.37
2	A	910	HEC	C3B-C4B	3.57	1.46	1.41
2	A	902	HEC	C1B-C2B	3.54	1.44	1.40
2	A	905	HEC	FE-NA	3.53	2.07	1.92
2	A	909	HEC	C3C-C4C	3.50	1.46	1.41
2	A	906	HEC	C3C-C2C	-3.50	1.34	1.41
2	A	909	HEC	C1C-C2C	3.49	1.44	1.40
2	A	909	HEC	C1B-C2B	3.49	1.44	1.40
2	A	910	HEC	FE-NA	3.47	2.07	1.92
2	A	902	HEC	C1D-C2D	3.45	1.44	1.40
2	A	910	HEC	C3C-C4C	3.44	1.45	1.41
2	A	907	HEC	C3B-C2B	-3.41	1.34	1.41
2	A	907	HEC	C3C-C2C	-3.40	1.34	1.41
2	A	901	HEC	C1D-C2D	3.39	1.44	1.40
2	A	905	HEC	C3C-C4C	3.33	1.45	1.41
2	A	911	HEC	FE-ND	3.33	2.06	1.92
2	A	903	HEC	FE-NA	3.30	2.06	1.92
2	A	908	HEC	C3D-C2D	3.29	1.47	1.37
2	A	904	HEC	FE-NC	3.27	2.06	1.92
2	A	902	HEC	C3C-C4C	3.22	1.45	1.41
2	A	902	HEC	FE-ND	3.22	2.06	1.92
2	A	903	HEC	C3B-C4B	3.22	1.45	1.41
2	A	908	HEC	C1D-C2D	3.19	1.44	1.40
2	A	901	HEC	C1B-C2B	3.19	1.44	1.40
2	A	902	HEC	C3B-C4B	3.15	1.45	1.41
2	A	908	HEC	C3C-C2C	-3.15	1.34	1.41
2	A	901	HEC	FE-NC	3.15	2.05	1.92
2	A	907	HEC	C3B-C4B	3.13	1.45	1.41
2	A	906	HEC	C3B-C2B	-3.09	1.35	1.41
2	A	910	HEC	C4D-ND	3.07	1.42	1.36
2	A	906	HEC	C1D-C2D	3.07	1.44	1.40
2	A	909	HEC	FE-ND	3.07	2.05	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	903	HEC	C1B-C2B	3.07	1.44	1.40
2	A	909	HEC	FE-NB	3.05	2.05	1.92
2	A	909	HEC	C1D-C2D	3.04	1.44	1.40
2	A	903	HEC	FE-NB	3.03	2.05	1.92
2	A	903	HEC	C3B-C2B	-3.01	1.35	1.41
2	A	904	HEC	C4A-NA	3.01	1.41	1.37
2	A	911	HEC	C3C-C4C	3.00	1.45	1.41
2	A	905	HEC	FE-ND	2.98	2.05	1.92
2	A	906	HEC	C1A-NA	2.98	1.41	1.37
2	A	908	HEC	FE-NA	2.94	2.05	1.92
2	A	910	HEC	C3B-C2B	-2.94	1.35	1.41
2	A	909	HEC	C3B-C2B	-2.93	1.35	1.41
2	A	905	HEC	C3C-C2C	-2.91	1.35	1.41
2	A	904	HEC	FE-ND	2.90	2.04	1.92
2	A	902	HEC	C3B-C2B	-2.90	1.35	1.41
2	A	909	HEC	C3C-C2C	-2.90	1.35	1.41
2	A	904	HEC	C3B-C2B	-2.89	1.35	1.41
2	A	903	HEC	C3C-C4C	2.88	1.45	1.41
2	A	908	HEC	C3B-C2B	-2.88	1.35	1.41
2	A	903	HEC	FE-ND	2.87	2.04	1.92
2	A	907	HEC	C1B-C2B	2.86	1.43	1.40
2	A	901	HEC	C3C-C2C	-2.86	1.35	1.41
2	A	908	HEC	C3C-C4C	2.85	1.45	1.41
2	A	903	HEC	FE-NC	2.84	2.04	1.92
2	A	904	HEC	C3C-C4C	2.84	1.45	1.41
2	A	905	HEC	C3B-C2B	-2.83	1.35	1.41
2	A	907	HEC	FE-NA	2.82	2.04	1.92
2	A	902	HEC	C3C-C2C	-2.79	1.35	1.41
2	A	911	HEC	FE-NC	2.77	2.04	1.92
2	A	904	HEC	FE-NB	2.74	2.04	1.92
2	A	911	HEC	C3C-C2C	-2.73	1.35	1.41
2	A	902	HEC	FE-NB	2.73	2.04	1.92
2	A	904	HEC	C3C-C2C	-2.72	1.35	1.41
2	A	910	HEC	C3C-C2C	-2.70	1.35	1.41
2	A	908	HEC	FE-NC	2.67	2.03	1.92
2	A	907	HEC	FE-NC	2.64	2.03	1.92
2	A	901	HEC	C3C-C4C	2.64	1.44	1.41
2	A	906	HEC	FE-NB	2.61	2.03	1.92
2	A	905	HEC	FE-NC	2.58	2.03	1.92
2	A	904	HEC	C3B-C4B	2.56	1.44	1.41
2	A	905	HEC	CAD-C3D	2.56	1.56	1.52
2	A	901	HEC	FE-NA	2.56	2.03	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	907	HEC	C3C-C4C	2.55	1.44	1.41
2	A	909	HEC	C4B-NB	2.54	1.40	1.37
2	A	908	HEC	FE-ND	2.53	2.03	1.92
2	A	911	HEC	FE-NB	2.52	2.03	1.92
2	A	909	HEC	FE-NA	2.48	2.03	1.92
2	A	908	HEC	C1B-C2B	2.46	1.43	1.40
2	A	906	HEC	FE-ND	2.46	2.03	1.92
2	A	902	HEC	FE-NA	2.46	2.02	1.92
2	A	911	HEC	C3B-C2B	-2.45	1.36	1.41
2	A	903	HEC	C3C-C2C	-2.45	1.36	1.41
2	A	906	HEC	C3C-C4C	2.38	1.44	1.41
2	A	909	HEC	FE-NC	2.37	2.02	1.92
2	A	902	HEC	C4A-NA	2.35	1.40	1.37
2	A	909	HEC	CMD-C2D	2.33	1.56	1.51
2	A	908	HEC	FE-NB	2.31	2.02	1.92
2	A	905	HEC	FE-NB	2.29	2.02	1.92
2	A	902	HEC	CMD-C2D	2.28	1.56	1.51
2	A	901	HEC	C3B-C4B	2.25	1.44	1.41
2	A	902	HEC	C1D-ND	2.24	1.41	1.36
2	A	911	HEC	C3B-C4B	2.19	1.44	1.41
2	A	901	HEC	C4B-NB	2.17	1.40	1.37
2	A	905	HEC	CMD-C2D	2.11	1.56	1.51
2	A	905	HEC	C4D-C3D	2.10	1.47	1.43
2	A	911	HEC	CMD-C2D	2.10	1.56	1.51
2	A	903	HEC	C1D-ND	2.10	1.40	1.36
2	A	904	HEC	C1D-ND	2.09	1.40	1.36
2	A	910	HEC	FE-ND	2.08	2.01	1.92
2	A	911	HEC	C1D-ND	2.01	1.40	1.36

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	909	HEC	CBB-CAB-C3B	-7.69	106.78	128.44
2	A	911	HEC	CBB-CAB-C3B	-6.96	108.84	128.44
2	A	904	HEC	CBB-CAB-C3B	-6.87	109.08	128.44
2	A	910	HEC	CBC-CAC-C3C	-6.21	110.97	128.44
2	A	906	HEC	CBB-CAB-C3B	-6.16	111.10	128.44
2	A	907	HEC	CBB-CAB-C3B	-6.08	111.33	128.44
2	A	907	HEC	CMC-C2C-C3C	6.07	132.42	125.72
2	A	905	HEC	CBC-CAC-C3C	-6.02	111.48	128.44
2	A	909	HEC	CMC-C2C-C1C	-6.00	119.39	128.62
2	A	901	HEC	CBC-CAC-C3C	-5.97	111.64	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	907	HEC	CBC-CAC-C3C	-5.85	111.97	128.44
2	A	904	HEC	CBC-CAC-C3C	-5.73	112.30	128.44
2	A	902	HEC	CBB-CAB-C3B	-5.62	112.61	128.44
2	A	908	HEC	CBB-CAB-C3B	-5.62	112.63	128.44
2	A	905	HEC	CBB-CAB-C3B	-5.61	112.65	128.44
2	A	907	HEC	CMC-C2C-C1C	-5.45	120.23	128.62
2	A	911	HEC	CBC-CAC-C3C	-5.44	113.13	128.44
2	A	903	HEC	CBB-CAB-C3B	-5.38	113.28	128.44
2	A	909	HEC	CBC-CAC-C3C	-5.26	113.63	128.44
2	A	910	HEC	CBB-CAB-C3B	-5.24	113.69	128.44
2	A	901	HEC	CMC-C2C-C3C	5.12	131.37	125.72
2	A	901	HEC	CBB-CAB-C3B	-5.11	114.06	128.44
2	A	906	HEC	CBC-CAC-C3C	-5.11	114.07	128.44
2	A	903	HEC	CBC-CAC-C3C	-5.09	114.10	128.44
2	A	909	HEC	CMC-C2C-C3C	5.07	131.32	125.72
2	A	911	HEC	CMC-C2C-C1C	-5.07	120.83	128.62
2	A	908	HEC	CBC-CAC-C3C	-4.93	114.55	128.44
2	A	902	HEC	CBC-CAC-C3C	-4.92	114.59	128.44
2	A	901	HEC	CMC-C2C-C1C	-4.90	121.08	128.62
2	A	906	HEC	CMB-C2B-C1B	-4.80	121.24	128.62
2	A	903	HEC	CMC-C2C-C1C	-4.75	121.31	128.62
2	A	909	HEC	CBA-CAA-C2A	-4.68	103.61	112.35
2	A	909	HEC	CMB-C2B-C1B	-4.68	121.43	128.62
2	A	906	HEC	CMB-C2B-C3B	4.50	130.69	125.72
2	A	906	HEC	C1A-CHA-C4D	-4.26	121.87	127.47
2	A	902	HEC	CMC-C2C-C3C	4.25	130.41	125.72
2	A	902	HEC	C1A-CHA-C4D	-4.11	122.07	127.47
2	A	906	HEC	C4A-CHB-C1B	-4.09	122.09	127.47
2	A	910	HEC	CBA-CAA-C2A	-4.06	104.76	112.35
2	A	910	HEC	C2A-C1A-NA	-4.02	106.62	109.64
2	A	911	HEC	CMC-C2C-C3C	3.98	130.11	125.72
2	A	910	HEC	C3A-C4A-NA	-3.98	106.41	109.41
2	A	902	HEC	C4B-CHC-C1C	-3.96	122.26	127.47
2	A	901	HEC	CBA-CAA-C2A	-3.94	104.98	112.35
2	A	909	HEC	C4B-CHC-C1C	-3.91	122.33	127.47
2	A	903	HEC	C1D-C2D-C3D	-3.90	104.28	107.00
2	A	901	HEC	C4B-CHC-C1C	-3.90	122.34	127.47
2	A	902	HEC	CMB-C2B-C1B	-3.89	122.64	128.62
2	A	905	HEC	CMC-C2C-C1C	-3.87	122.67	128.62
2	A	906	HEC	CBD-CAD-C3D	-3.86	105.89	112.69
2	A	911	HEC	CBA-CAA-C2A	-3.84	105.18	112.35
2	A	910	HEC	CMC-C2C-C1C	-3.80	122.77	128.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	907	HEC	C3A-C4A-NA	-3.78	106.56	109.41
2	A	906	HEC	CMC-C2C-C3C	3.77	129.88	125.72
2	A	904	HEC	CBD-CAD-C3D	-3.77	106.05	112.69
2	A	902	HEC	CMC-C2C-C1C	-3.73	122.88	128.62
2	A	911	HEC	C1A-CHA-C4D	-3.70	122.60	127.47
2	A	904	HEC	C1A-CHA-C4D	-3.69	122.61	127.47
2	A	901	HEC	CBD-CAD-C3D	-3.68	106.21	112.69
2	A	910	HEC	C2C-C1C-NC	-3.65	106.66	109.41
2	A	908	HEC	C4C-CHD-C1D	-3.60	122.74	127.47
2	A	910	HEC	CBD-CAD-C3D	-3.54	106.45	112.69
2	A	903	HEC	C2C-C1C-NC	-3.47	106.79	109.41
2	A	910	HEC	C4A-NA-C1A	3.46	110.78	105.58
2	A	904	HEC	CMC-C2C-C1C	-3.44	123.33	128.62
2	A	908	HEC	CMA-C3A-C2A	3.43	131.41	124.94
2	A	907	HEC	C4A-C3A-C2A	3.42	109.07	106.89
2	A	908	HEC	CMB-C2B-C1B	-3.40	123.40	128.62
2	A	901	HEC	C4A-C3A-C2A	3.37	109.03	106.89
2	A	910	HEC	C3C-C4C-NC	-3.36	106.66	111.52
2	A	909	HEC	CMB-C2B-C3B	3.35	129.42	125.72
2	A	903	HEC	C2A-C1A-NA	-3.33	107.14	109.64
2	A	906	HEC	CMC-C2C-C1C	-3.28	123.58	128.62
2	A	903	HEC	CMB-C2B-C1B	-3.28	123.58	128.62
2	A	904	HEC	C4B-C3B-C2B	3.28	108.77	106.68
2	A	911	HEC	C4B-CHC-C1C	-3.28	123.16	127.47
2	A	902	HEC	CBD-CAD-C3D	-3.24	106.98	112.69
2	A	905	HEC	CMB-C2B-C1B	-3.23	123.65	128.62
2	A	907	HEC	CMB-C2B-C1B	-3.16	123.76	128.62
2	A	905	HEC	C4B-CHC-C1C	-3.16	123.32	127.47
2	A	911	HEC	C4D-ND-C1D	3.15	110.91	106.76
2	A	909	HEC	C4A-C3A-C2A	3.12	108.88	106.89
2	A	907	HEC	C1D-C2D-C3D	-3.11	104.83	107.00
2	A	905	HEC	CMB-C2B-C3B	3.08	129.13	125.72
2	A	909	HEC	C3B-C4B-NB	-3.07	107.08	111.52
2	A	908	HEC	C1D-C2D-C3D	-3.07	104.86	107.00
2	A	903	HEC	CMC-C2C-C3C	3.04	129.08	125.72
2	A	908	HEC	C4A-CHB-C1B	-2.99	123.53	127.47
2	A	904	HEC	C3B-C4B-NB	-2.98	107.22	111.52
2	A	909	HEC	C4D-ND-C1D	2.96	110.66	106.76
2	A	903	HEC	CAD-CBD-CGD	-2.95	104.00	113.47
2	A	903	HEC	C3C-C4C-NC	-2.95	107.26	111.52
2	A	901	HEC	C3A-C4A-NA	-2.94	107.19	109.41
2	A	910	HEC	CMC-C2C-C3C	2.90	128.93	125.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	906	HEC	C4A-C3A-C2A	2.90	108.74	106.89
2	A	906	HEC	C4C-C3C-C2C	2.88	108.51	106.68
2	A	904	HEC	C4D-ND-C1D	2.87	110.54	106.76
2	A	908	HEC	C3C-C4C-NC	-2.86	107.39	111.52
2	A	905	HEC	C4D-ND-C1D	2.85	110.52	106.76
2	A	907	HEC	C4B-CHC-C1C	-2.85	123.72	127.47
2	A	903	HEC	CBA-CAA-C2A	-2.84	107.04	112.35
2	A	905	HEC	CMC-C2C-C3C	2.83	128.85	125.72
2	A	909	HEC	C3C-C4C-NC	-2.82	107.45	111.52
2	A	905	HEC	C4B-C3B-C2B	2.82	108.47	106.68
2	A	904	HEC	CMB-C2B-C1B	-2.80	124.31	128.62
2	A	910	HEC	C4C-NC-C1C	2.80	110.45	106.76
2	A	902	HEC	C1D-C2D-C3D	-2.79	105.06	107.00
2	A	901	HEC	CMB-C2B-C1B	-2.79	124.34	128.62
2	A	902	HEC	CMB-C2B-C3B	2.78	128.79	125.72
2	A	909	HEC	C1A-CHA-C4D	-2.78	123.81	127.47
2	A	911	HEC	CMB-C2B-C1B	-2.78	124.35	128.62
2	A	906	HEC	O2D-CGD-CBD	2.76	123.97	114.22
2	A	908	HEC	C4C-C3C-C2C	2.72	108.41	106.68
2	A	908	HEC	C4B-CHC-C1C	-2.69	123.93	127.47
2	A	904	HEC	C4A-CHB-C1B	-2.68	123.94	127.47
2	A	903	HEC	C3A-C4A-NA	-2.67	107.39	109.41
2	A	911	HEC	C3B-C4B-NB	-2.65	107.70	111.52
2	A	907	HEC	C2D-C1D-ND	2.62	111.39	109.41
2	A	903	HEC	C4A-CHB-C1B	-2.59	124.06	127.47
2	A	902	HEC	C4D-ND-C1D	2.58	110.16	106.76
2	A	901	HEC	C1D-C2D-C3D	-2.54	105.23	107.00
2	A	906	HEC	C4D-ND-C1D	2.52	110.08	106.76
2	A	905	HEC	C3B-C4B-NB	-2.51	107.89	111.52
2	A	901	HEC	C3C-C4C-NC	-2.51	107.89	111.52
2	A	905	HEC	C2C-C1C-NC	-2.51	107.52	109.41
2	A	909	HEC	C3A-C4A-NA	-2.51	107.52	109.41
2	A	911	HEC	C3C-C4C-NC	-2.50	107.90	111.52
2	A	907	HEC	CBD-CAD-C3D	-2.50	108.29	112.69
2	A	909	HEC	CBD-CAD-C3D	-2.50	108.29	112.69
2	A	910	HEC	C4C-C3C-C2C	2.49	108.26	106.68
2	A	909	HEC	C3B-C2B-C1B	2.49	108.72	107.07
2	A	905	HEC	C3C-C4C-NC	-2.48	107.94	111.52
2	A	907	HEC	C4A-NA-C1A	2.46	109.28	105.58
2	A	908	HEC	CMB-C2B-C3B	2.44	128.41	125.72
2	A	911	HEC	C4B-C3B-C2B	2.43	108.23	106.68
2	A	903	HEC	C4C-NC-C1C	2.42	109.95	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	908	HEC	CMA-C3A-C4A	-2.41	121.39	126.16
2	A	905	HEC	C1A-CHA-C4D	-2.40	124.31	127.47
2	A	902	HEC	C4A-C3A-C2A	2.40	108.42	106.89
2	A	906	HEC	CHD-C1D-ND	2.39	128.57	124.58
2	A	910	HEC	CMA-C3A-C2A	2.39	129.44	124.94
2	A	903	HEC	C3B-C4B-NB	-2.38	108.09	111.52
2	A	907	HEC	C3C-C4C-NC	-2.35	108.12	111.52
2	A	909	HEC	C4C-C3C-C2C	2.33	108.17	106.68
2	A	904	HEC	CMB-C2B-C3B	2.28	128.24	125.72
2	A	911	HEC	C2B-C1B-NB	-2.26	107.70	109.41
2	A	904	HEC	C4B-CHC-C1C	-2.26	124.50	127.47
2	A	904	HEC	C2B-C1B-NB	-2.26	107.71	109.41
2	A	911	HEC	C1D-C2D-C3D	-2.25	105.43	107.00
2	A	910	HEC	CAA-CBA-CGA	-2.25	106.25	113.47
2	A	906	HEC	C4C-CHD-C1D	-2.24	124.53	127.47
2	A	910	HEC	C4A-CHB-C1B	-2.23	124.53	127.47
2	A	907	HEC	C2A-C1A-NA	-2.22	107.97	109.64
2	A	910	HEC	C4D-C3D-C2D	-2.22	104.62	106.92
2	A	908	HEC	O2D-CGD-CBD	2.21	122.02	114.22
2	A	905	HEC	CBD-CAD-C3D	-2.20	108.81	112.69
2	A	906	HEC	C2B-C1B-NB	-2.19	107.76	109.41
2	A	901	HEC	C1A-CHA-C4D	-2.18	124.60	127.47
2	A	903	HEC	C4A-NA-C1A	2.18	108.85	105.58
2	A	904	HEC	CHD-C1D-ND	2.18	128.22	124.58
2	A	909	HEC	C4A-CHB-C1B	-2.17	124.62	127.47
2	A	907	HEC	CMB-C2B-C3B	2.15	128.09	125.72
2	A	907	HEC	O2D-CGD-CBD	2.13	121.76	114.22
2	A	908	HEC	O1D-CGD-CBD	-2.13	115.71	123.03
2	A	906	HEC	C4B-CHC-C1C	-2.12	124.68	127.47
2	A	905	HEC	C3C-C2C-C1C	2.11	108.47	107.07
2	A	908	HEC	CMD-C2D-C3D	2.10	128.91	124.94
2	A	902	HEC	C4C-C3C-C2C	2.09	108.01	106.68
2	A	903	HEC	C4A-C3A-C2A	2.08	108.22	106.89
2	A	905	HEC	C4D-C3D-C2D	-2.06	104.78	106.92
2	A	908	HEC	C2A-C1A-NA	-2.05	108.09	109.64
2	A	908	HEC	CAA-C2A-C1A	-2.05	120.97	124.67
2	A	903	HEC	C4D-ND-C1D	2.04	109.45	106.76
2	A	911	HEC	C2C-C1C-NC	-2.04	107.87	109.41
2	A	902	HEC	C3C-C4C-NC	-2.04	108.58	111.52
2	A	904	HEC	C1D-C2D-C3D	-2.03	105.58	107.00
2	A	903	HEC	CMB-C2B-C3B	2.02	127.95	125.72
2	A	903	HEC	CMA-C3A-C2A	2.01	128.74	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	906	HEC	C3B-C4B-NB	-2.01	108.62	111.52

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	800/874 (91%)	0.04	10 (1%) 74 84	7, 19, 39, 58	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	ASN	3.0
1	A	236	VAL	2.5
1	A	76	ALA	2.5
1	A	64	ASN	2.4
1	A	79	VAL	2.3
1	A	63	ASP	2.2
1	A	663	PHE	2.2
1	A	44	GLY	2.2
1	A	66	THR	2.1
1	A	172	VAL	2.0

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 ⓘ

There are no carbohydrates in this entry.

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	916	6/6	0.23	22.86	37,41,43,49	0
5	GOL	A	918	6/6	0.16	3.79	49,53,56,60	0
5	GOL	A	915	6/6	0.14	2.88	33,36,42,43	0
2	HEC	A	911	43/43	0.12	2.08	19,25,40,50	0
5	GOL	A	917	6/6	0.16	1.96	39,45,46,47	0
2	HEC	A	902	43/43	0.14	1.32	13,16,24,34	0
3	CA	A	912	1/1	0.11	0.84	20,20,20,20	0
2	HEC	A	906	43/43	0.14	0.72	7,9,12,14	0
2	HEC	A	908	43/43	0.14	0.61	5,8,10,15	0
2	HEC	A	910	43/43	0.11	0.46	12,20,47,56	0
2	HEC	A	905	43/43	0.09	0.42	14,18,24,26	0
4	MG	A	913	1/1	0.12	0.14	10,10,10,10	0
2	HEC	A	904	43/43	0.08	0.10	9,13,18,24	0
5	GOL	A	919	6/6	0.12	0.07	30,41,42,45	0
2	HEC	A	903	43/43	0.11	0.03	10,13,16,23	0
2	HEC	A	901	43/43	0.13	-0.07	8,12,27,32	0
2	HEC	A	909	43/43	0.09	-0.19	9,12,15,19	0
2	HEC	A	907	43/43	0.10	-0.30	5,9,12,13	0
4	MG	A	914	1/1	0.05	-0.83	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.