



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:54 PM GMT

PDB ID : 1Z1N  
Title : Crystal Structure of the sixteen heme cytochrome from *Desulfovibrio gigas*  
Authors : Santos-Silva, T.; Dias, J.M.; Romao, M.J.  
Deposited on : 2005-03-04  
Resolution : 2.10 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.

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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 : 1.7 (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

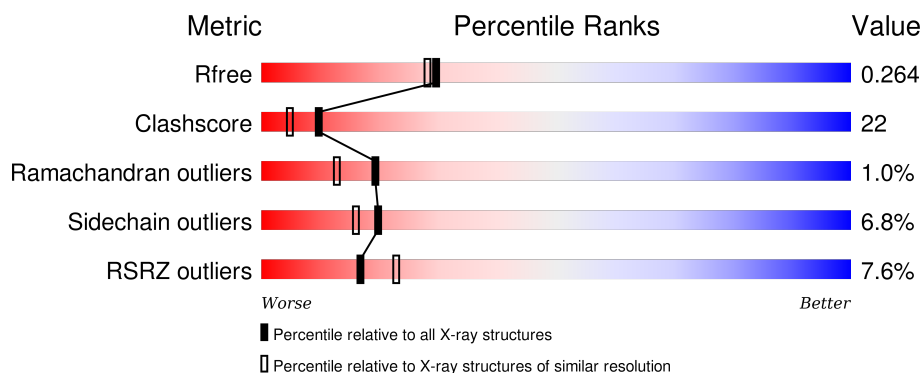
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	X	560	

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
2	NAG	X	900	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	X	803	-	-	X	-
5	GOL	X	804	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4998 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 sixteen heme cytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	516	Total	C	N	O	S	0	0	0
			3837	2355	703	739	40			

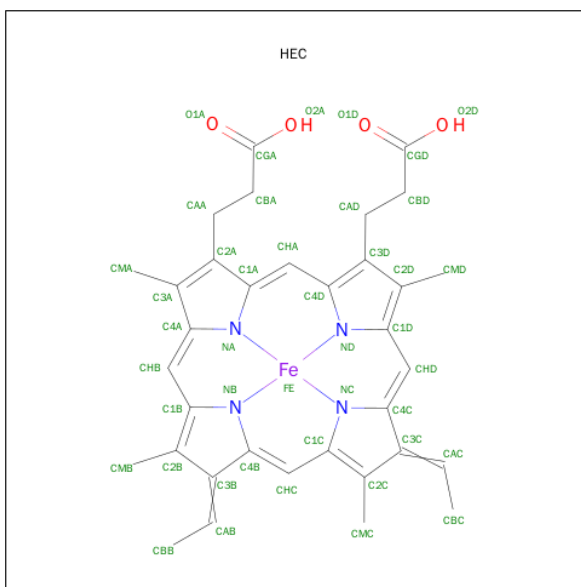
- Molecule 2 is a polymer of unknown type called SUGAR (N-ACETYL-D-GLUCOSAMINE).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	3	Total	Zn	0	0
			3	3		

- Molecule 4 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).

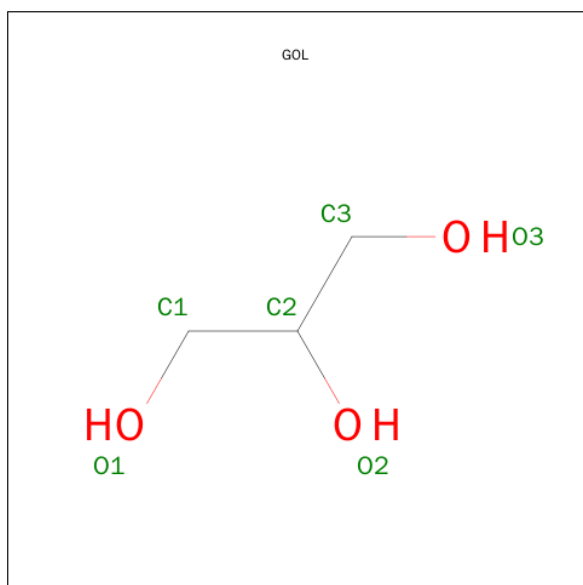
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	X	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



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

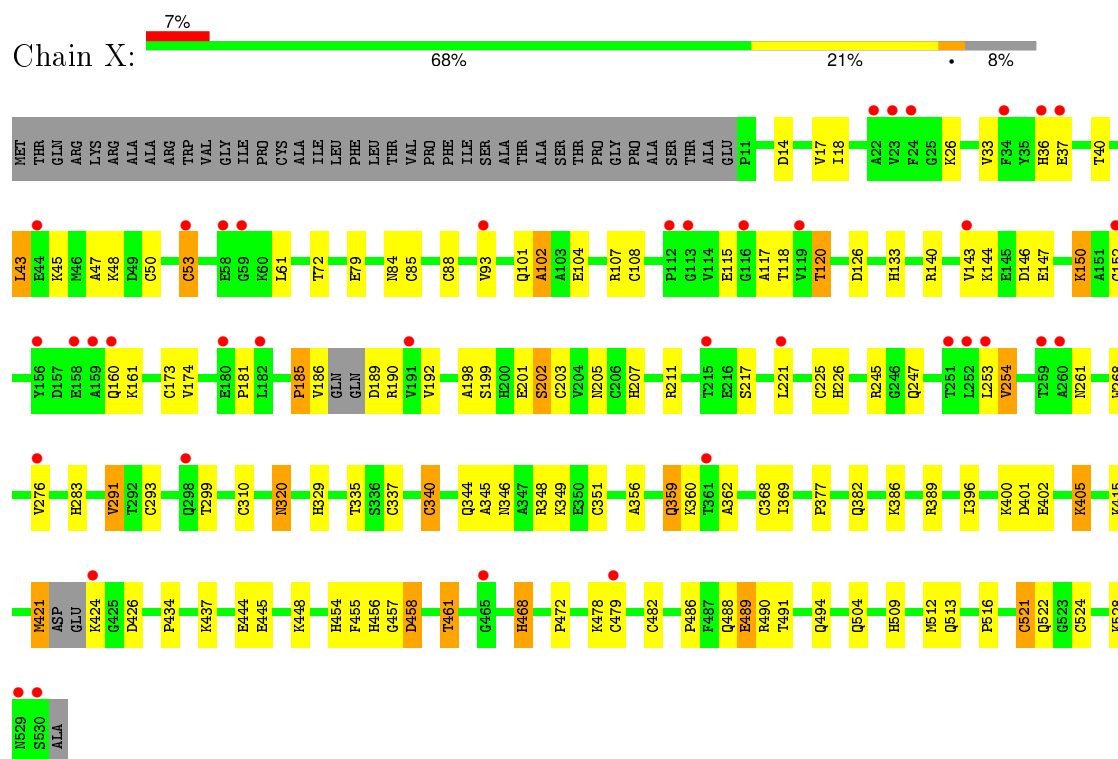
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	X	412	Total O 412 412	0	0

### 3 Residue-property plots [i](#)

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

- Molecule 1: sixteen heme cytochrome



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.89Å 90.80Å 83.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 24.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.00-2.10) 98.2 (24.81-2.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.194 , 0.260 0.204 , 0.264	Depositor DCC
$R_{free}$ test set	1979 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.1	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 39580 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NAA, NAG, 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	X	1.00	6/3925 (0.2%)	0.98	8/5326 (0.2%)

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
1	X	0	1
2	X	1	0
All	All	1	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	479	CYS	CB-SG	6.77	1.93	1.82
1	X	276	VAL	CB-CG2	6.29	1.66	1.52
1	X	53	CYS	CB-SG	-5.78	1.72	1.81
1	X	340	CYS	CB-SG	5.38	1.91	1.82
1	X	455	PHE	CE1-CZ	5.08	1.47	1.37
1	X	521	CYS	CB-SG	-5.08	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	389	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	X	389	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	X	448	LYS	CD-CE-NZ	-7.46	94.53	111.70
1	X	291	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	X	291	VAL	CB-CA-C	-7.21	97.70	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	126	ASP	CB-CG-OD1	6.43	124.09	118.30
1	X	457	GLY	N-CA-C	-5.93	98.27	113.10
1	X	254	VAL	CB-CA-C	-5.54	100.87	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	900	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	424	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	3837	0	3662	154	2
2	X	28	0	25	1	0
3	X	3	0	0	0	0
4	X	688	0	495	112	2
5	X	30	0	40	6	0
6	X	412	0	0	20	2
All	All	4998	0	4222	182	3

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 22.

All (182) 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)
1:X:50:CYS:SG	4:X:601:HEC:HAB	1.37	1.63
1:X:152:CYS:SG	4:X:604:HEC:HAC	1.54	1.44
1:X:524:CYS:SG	4:X:616:HEC:CAC	2.12	1.36
1:X:85:CYS:SG	4:X:602:HEC:CAB	2.14	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:88:CYS:SG	4:X:602:HEC:HAC	1.67	1.33
1:X:203:CYS:SG	4:X:606:HEC:HAB	1.69	1.33
1:X:293:CYS:SG	4:X:608:HEC:CAC	2.15	1.32
1:X:152:CYS:SG	4:X:604:HEC:CAC	2.24	1.25
1:X:50:CYS:SG	4:X:601:HEC:CAB	2.24	1.24
1:X:225:CYS:SG	4:X:607:HEC:CAC	2.27	1.23
1:X:53:CYS:SG	4:X:601:HEC:CAC	2.27	1.21
1:X:421:MET:O	6:X:1312:HOH:O	1.61	1.19
1:X:521:CYS:SG	4:X:616:HEC:HAB	1.73	1.16
1:X:108:CYS:SG	4:X:603:HEC:CAC	2.37	1.11
1:X:85:CYS:SG	4:X:602:HEC:HAB	1.93	1.07
1:X:340:CYS:SG	4:X:610:HEC:HAC	1.90	1.06
1:X:482:CYS:SG	4:X:614:HEC:HAC	1.91	1.05
1:X:261:ASN:OD1	6:X:1190:HOH:O	1.73	1.04
1:X:337:CYS:SG	4:X:610:HEC:HAB	2.00	1.00
1:X:108:CYS:SG	4:X:603:HEC:HAC	2.03	0.95
4:X:614:HEC:O1D	5:X:803:GOL:H32	1.65	0.95
1:X:53:CYS:SG	4:X:601:HEC:HAC	2.04	0.95
1:X:524:CYS:SG	4:X:616:HEC:CB	2.55	0.94
1:X:120:THR:HG21	1:X:226:HIS:O	1.68	0.94
1:X:225:CYS:SG	4:X:607:HEC:HAC	2.13	0.89
1:X:186:VAL:HG22	1:X:189:ASP:HA	1.55	0.85
4:X:616:HEC:O2D	6:X:1046:HOH:O	1.94	0.85
1:X:359:GLN:HE22	1:X:362:ALA:H	1.21	0.84
1:X:344:GLN:OE1	1:X:348:ARG:NH2	2.10	0.84
1:X:337:CYS:SG	4:X:610:HEC:CBB	2.67	0.82
1:X:84:ASN:O	6:X:1230:HOH:O	1.99	0.80
4:X:602:HEC:HMC1	4:X:602:HEC:HBC3	1.63	0.80
1:X:253:LEU:HD21	4:X:608:HEC:HBD2	1.64	0.79
1:X:268:TRP:HE1	1:X:382:GLN:HE21	1.30	0.78
1:X:524:CYS:SG	4:X:616:HEC:C3C	2.71	0.78
1:X:293:CYS:SG	4:X:608:HEC:CB	2.73	0.77
1:X:293:CYS:SG	4:X:608:HEC:HAC	2.23	0.77
1:X:524:CYS:SG	4:X:616:HEC:HBC3	2.26	0.76
1:X:310:CYS:SG	4:X:609:HEC:CAC	2.73	0.76
1:X:120:THR:CG2	1:X:226:HIS:O	2.34	0.76
1:X:37:GLU:OE2	6:X:1114:HOH:O	2.03	0.76
1:X:115:GLU:O	1:X:118:THR:HG22	1.86	0.75
1:X:173:CYS:SG	4:X:605:HEC:CBB	2.77	0.73
1:X:340:CYS:SG	4:X:610:HEC:C3C	2.77	0.72
1:X:225:CYS:SG	4:X:607:HEC:C3C	2.77	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:293:CYS:SG	4:X:608:HEC:C3C	2.79	0.70
4:X:606:HEC:CBC	4:X:606:HEC:HMC1	2.22	0.69
1:X:181:PRO:HB3	1:X:192:VAL:O	1.93	0.68
1:X:482:CYS:SG	4:X:614:HEC:C3C	2.81	0.68
1:X:482:CYS:SG	4:X:614:HEC:CBC	2.82	0.68
1:X:53:CYS:SG	4:X:601:HEC:C3C	2.82	0.68
1:X:14:ASP:CB	1:X:37:GLU:HG3	2.24	0.67
1:X:386:LYS:NZ	4:X:608:HEC:O2A	2.22	0.67
1:X:426:ASP:HB2	1:X:528:LYS:NZ	2.11	0.66
1:X:37:GLU:CD	6:X:1114:HOH:O	2.34	0.66
1:X:490:ARG:NH2	6:X:1261:HOH:O	2.28	0.66
1:X:405:LYS:HB2	6:X:1142:HOH:O	1.96	0.65
1:X:521:CYS:SG	4:X:616:HEC:C3B	2.84	0.65
4:X:605:HEC:HMB1	4:X:605:HEC:HBB3	1.79	0.64
1:X:173:CYS:SG	4:X:605:HEC:C3B	2.84	0.63
1:X:85:CYS:SG	4:X:602:HEC:C3B	2.87	0.63
1:X:337:CYS:SG	4:X:610:HEC:C3B	2.86	0.62
4:X:615:HEC:CGA	6:X:1231:HOH:O	2.47	0.62
4:X:612:HEC:O1D	5:X:804:GOL:O2	2.17	0.62
4:X:614:HEC:HMC1	4:X:614:HEC:HBC3	1.80	0.62
1:X:359:GLN:NE2	1:X:362:ALA:H	1.93	0.62
1:X:524:CYS:SG	4:X:616:HEC:HAC	2.31	0.60
4:X:602:HEC:HMC1	4:X:602:HEC:CBC	2.30	0.60
1:X:101:GLN:O	1:X:102:ALA:HB2	2.02	0.60
1:X:104:GLU:HB3	1:X:107:ARG:HG3	1.83	0.60
1:X:36:HIS:HE1	4:X:601:HEC:NB	1.99	0.59
1:X:152:CYS:SG	4:X:604:HEC:C3C	2.91	0.59
1:X:198:ALA:O	1:X:202:SER:HB2	2.03	0.58
1:X:201:GLU:O	1:X:205:ASN:HB2	2.03	0.58
4:X:601:HEC:C3A	4:X:607:HEC:HBB2	2.34	0.58
1:X:14:ASP:HB3	1:X:37:GLU:HG3	1.85	0.58
1:X:349:LYS:HE3	1:X:513:GLN:NE2	2.18	0.58
1:X:88:CYS:HG	4:X:602:HEC:HAC	1.65	0.57
1:X:261:ASN:N	6:X:1190:HOH:O	2.37	0.57
1:X:458:ASP:O	1:X:461:THR:HG23	2.04	0.57
1:X:50:CYS:HG	4:X:601:HEC:CAB	2.14	0.57
1:X:152:CYS:HG	4:X:604:HEC:CAC	2.17	0.57
1:X:337:CYS:HG	4:X:610:HEC:HAB	1.67	0.57
1:X:437:LYS:HE3	4:X:615:HEC:O1D	2.04	0.57
1:X:207:HIS:O	1:X:211:ARG:HG3	2.05	0.57
4:X:610:HEC:HBD2	4:X:610:HEC:HMD1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:335:THR:HB	4:X:609:HEC:HMA2	1.88	0.56
1:X:437:LYS:HZ1	4:X:615:HEC:CGA	2.04	0.56
4:X:606:HEC:HBB3	4:X:606:HEC:HMB1	1.87	0.56
1:X:421:MET:HE3	4:X:616:HEC:HAA2	1.87	0.56
4:X:613:HEC:HMB1	4:X:613:HEC:HBB3	1.87	0.55
1:X:421:MET:CE	4:X:616:HEC:HAA2	2.37	0.55
1:X:434:PRO:HG3	4:X:615:HEC:HBA1	1.89	0.55
1:X:359:GLN:HE22	1:X:362:ALA:N	2.00	0.55
1:X:43:LEU:HD12	4:X:601:HEC:HMC1	1.89	0.54
1:X:486:PRO:HD2	1:X:489:GLU:HG3	1.89	0.54
1:X:400:LYS:O	1:X:402:GLU:N	2.40	0.54
1:X:117:ALA:HA	1:X:120:THR:HG22	1.89	0.54
4:X:606:HEC:HBC3	4:X:606:HEC:HMC1	1.88	0.53
1:X:120:THR:HG23	6:X:976:HOH:O	2.08	0.53
1:X:426:ASP:HB2	1:X:528:LYS:HZ2	1.73	0.53
4:X:615:HEC:O1A	6:X:1231:HOH:O	2.19	0.53
1:X:437:LYS:CE	4:X:615:HEC:O1A	2.56	0.53
1:X:340:CYS:SG	4:X:610:HEC:CBC	2.93	0.53
4:X:608:HEC:HMB1	4:X:608:HEC:HBB3	1.89	0.52
1:X:348:ARG:NH1	6:X:1010:HOH:O	2.29	0.52
1:X:120:THR:CG2	6:X:976:HOH:O	2.57	0.52
1:X:456:HIS:O	1:X:461:THR:HG21	2.08	0.51
4:X:614:HEC:O1D	5:X:803:GOL:C2	2.55	0.51
1:X:140:ARG:HD3	6:X:1148:HOH:O	2.11	0.51
1:X:143:VAL:HG21	1:X:147:GLU:HG2	1.92	0.50
1:X:40:THR:HG22	4:X:601:HEC:HBB2	1.93	0.50
1:X:150:LYS:O	6:X:1194:HOH:O	2.19	0.50
1:X:509:HIS:CE1	1:X:516:PRO:HD2	2.47	0.50
1:X:88:CYS:SG	4:X:602:HEC:C3C	2.95	0.50
4:X:614:HEC:O2D	5:X:803:GOL:H2	2.12	0.49
1:X:79:GLU:HG3	6:X:1161:HOH:O	2.12	0.49
1:X:143:VAL:CG1	1:X:147:GLU:HB3	2.42	0.49
1:X:329:HIS:HE1	4:X:612:HEC:C4A	2.26	0.49
1:X:101:GLN:O	1:X:102:ALA:CB	2.61	0.49
1:X:396:ILE:HG22	1:X:400:LYS:HE2	1.94	0.49
1:X:174:VAL:HG12	1:X:174:VAL:O	2.11	0.49
4:X:606:HEC:HBC2	4:X:606:HEC:HMC1	1.92	0.49
1:X:491:THR:H	1:X:494:GLN:HE21	1.61	0.49
1:X:329:HIS:HE1	4:X:612:HEC:NA	2.07	0.48
1:X:482:CYS:HG	4:X:614:HEC:HAC	1.74	0.48
1:X:456:HIS:O	1:X:461:THR:CG2	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:293:CYS:SG	4:X:608:HEC:HBC3	2.52	0.48
4:X:615:HEC:HMB1	4:X:615:HEC:HBB3	1.96	0.48
1:X:14:ASP:CG	1:X:37:GLU:HG3	2.33	0.47
1:X:203:CYS:SG	4:X:606:HEC:C3B	2.98	0.47
1:X:509:HIS:HE1	1:X:516:PRO:HD2	1.80	0.47
4:X:609:HEC:HBC2	4:X:609:HEC:HMC1	1.97	0.46
4:X:616:HEC:HMB1	4:X:616:HEC:HBB3	1.97	0.46
1:X:444:GLU:HG3	1:X:445:GLU:N	2.30	0.46
1:X:143:VAL:HG11	1:X:147:GLU:HB3	1.97	0.46
1:X:143:VAL:HG22	1:X:144:LYS:H	1.81	0.46
1:X:345:ALA:O	1:X:351:CYS:HB2	2.16	0.45
4:X:614:HEC:O1A	5:X:803:GOL:C3	2.61	0.45
1:X:247:GLN:HB3	4:X:608:HEC:CHB	2.46	0.45
1:X:221:LEU:HD21	4:X:601:HEC:HBB3	1.97	0.45
1:X:133:HIS:HB3	4:X:604:HEC:HBC3	1.97	0.45
1:X:369:ILE:HG23	6:X:1004:HOH:O	2.17	0.45
1:X:185:PRO:HA	1:X:186:VAL:HB	1.98	0.45
1:X:426:ASP:HB2	1:X:528:LYS:HZ1	1.78	0.45
1:X:203:CYS:HB2	4:X:607:HEC:HBC2	1.99	0.45
1:X:133:HIS:HB3	4:X:604:HEC:CBC	2.47	0.44
1:X:346:ASN:ND2	1:X:356:ALA:HA	2.33	0.44
1:X:203:CYS:SG	4:X:606:HEC:CBB	2.96	0.43
4:X:610:HEC:HBC3	4:X:610:HEC:HMC1	2.01	0.43
1:X:283:HIS:HB3	4:X:608:HEC:HBC2	2.00	0.43
4:X:610:HEC:HMC1	4:X:610:HEC:CBC	2.48	0.43
1:X:454:HIS:CD2	4:X:610:HEC:HMA3	2.53	0.43
1:X:512:MET:O	1:X:513:GLN:HB2	2.18	0.43
1:X:53:CYS:CB	4:X:601:HEC:C3C	2.97	0.43
1:X:85:CYS:SG	4:X:602:HEC:CBB	3.02	0.43
1:X:268:TRP:HB3	1:X:377:PRO:O	2.19	0.43
1:X:199:SER:O	1:X:203:CYS:SG	2.76	0.43
1:X:524:CYS:HG	4:X:616:HEC:CAC	2.22	0.43
1:X:45:LYS:C	1:X:47:ALA:H	2.22	0.42
1:X:360:LYS:NZ	6:X:1043:HOH:O	2.21	0.42
1:X:43:LEU:CD1	4:X:601:HEC:HMC1	2.48	0.42
1:X:468:HIS:HD1	5:X:803:GOL:C1	2.32	0.42
4:X:602:HEC:HMB1	4:X:602:HEC:HBB3	2.01	0.41
1:X:17:VAL:HG22	1:X:33:VAL:HG22	2.02	0.41
1:X:261:ASN:HD22	2:X:900:NAG:C7	2.34	0.41
1:X:491:THR:H	1:X:494:GLN:NE2	2.17	0.41
1:X:88:CYS:HG	4:X:602:HEC:CAC	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:50:CYS:HB2	1:X:61:LEU:HD21	2.01	0.41
1:X:40:THR:CG2	4:X:601:HEC:HBB2	2.50	0.41
1:X:37:GLU:HG2	6:X:1114:HOH:O	2.21	0.41
4:X:608:HEC:HBC3	4:X:608:HEC:HMC1	2.01	0.41
1:X:320:ASN:HD22	1:X:320:ASN:HA	1.64	0.41
1:X:504:GLN:CB	4:X:614:HEC:HMB2	2.50	0.41
4:X:610:HEC:HHB	4:X:610:HEC:HMA1	1.85	0.41
1:X:461:THR:O	4:X:611:HEC:HMD2	2.21	0.41
1:X:33:VAL:HG12	1:X:33:VAL:O	2.21	0.41
1:X:337:CYS:SG	4:X:610:HEC:HBB3	2.58	0.41
1:X:368:CYS:HA	4:X:612:HEC:CHC	2.51	0.40
1:X:225:CYS:HG	4:X:607:HEC:HAC	1.83	0.40
1:X:310:CYS:SG	4:X:609:HEC:C3C	3.09	0.40
1:X:88:CYS:SG	4:X:602:HEC:CBC	3.01	0.40

All (3) 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	Interatomic distance (Å)	Clash overlap (Å)
1:X:401:ASP:O	6:X:1234:HOH:O[3_546]	1.75	0.45
4:X:613:HEC:O2A	6:X:1304:HOH:O[3_556]	2.14	0.06
1:X:437:LYS:NZ	4:X:615:HEC:O2D[2_565]	2.15	0.05

## 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	X	510/560 (91%)	484 (95%)	21 (4%)	5 (1%)	19 13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	102	ALA
1	X	160	GLN
1	X	150	LYS
1	X	161	LYS
1	X	185	PRO

### 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	X	410/450 (91%)	382 (93%)	28 (7%)	20	16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	18	ILE
1	X	26	LYS
1	X	43	LEU
1	X	48	LYS
1	X	72	THR
1	X	93	VAL
1	X	120	THR
1	X	146	ASP
1	X	190	ARG
1	X	202	SER
1	X	217	SER
1	X	245	ARG
1	X	254	VAL
1	X	291	VAL
1	X	299	THR
1	X	320	ASN
1	X	359	GLN
1	X	405	LYS
1	X	415	LYS
1	X	421	MET
1	X	458	ASP
1	X	461	THR

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Mol	Chain	Res	Type
1	X	468	HIS
1	X	472	PRO
1	X	478	LYS
1	X	488	GLN
1	X	489	GLU
1	X	522	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	80	GLN
1	X	231	GLN
1	X	320	ASN
1	X	330	GLN
1	X	346	ASN
1	X	359	GLN
1	X	382	GLN
1	X	494	GLN
1	X	513	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

2 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
2	NAG	X	900	1,2	14,14,15	0.74	1 (7%)	15,19,21	3.11	6 (40%)
2	NAA	X	901	2	14,14,15	0.88	1 (7%)	15,19,21	1.20	1 (6%)

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	NAG	X	900	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAA	X	901	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	900	NAG	C3-C2	2.15	1.57	1.52
2	X	901	NAA	C8-C7	2.81	1.56	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	900	NAG	C3-C4-C5	-4.78	101.87	110.20
2	X	900	NAG	O4-C4-C3	2.40	115.74	110.34
2	X	900	NAG	O4-C4-C5	2.77	116.59	109.24
2	X	900	NAG	C3-C2-N2	2.82	117.31	110.56
2	X	901	NAA	C3-C4-C5	2.87	115.21	110.20
2	X	900	NAG	C1-O5-C5	5.84	119.66	112.25
2	X	900	NAG	O3-C3-C2	7.23	123.43	109.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	900	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	900	NAG	1	0

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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$
4	HEC	X	601	1	24,50,50	1.88	5 (20%)	19,82,82	3.62	11 (57%)
4	HEC	X	602	1	24,50,50	2.53	8 (33%)	19,82,82	2.61	8 (42%)
4	HEC	X	603	1	24,50,50	2.18	4 (16%)	19,82,82	3.04	7 (36%)
4	HEC	X	604	1	24,50,50	2.11	4 (16%)	19,82,82	3.01	7 (36%)
4	HEC	X	605	1	24,50,50	2.05	4 (16%)	19,82,82	2.77	7 (36%)
4	HEC	X	606	1	24,50,50	2.34	6 (25%)	19,82,82	2.81	9 (47%)
4	HEC	X	607	1	24,50,50	2.16	4 (16%)	19,82,82	2.87	10 (52%)
4	HEC	X	608	1	24,50,50	2.20	6 (25%)	19,82,82	3.97	12 (63%)
4	HEC	X	609	1	24,50,50	1.98	4 (16%)	19,82,82	2.79	9 (47%)
4	HEC	X	610	1	24,50,50	2.20	8 (33%)	19,82,82	3.12	12 (63%)
4	HEC	X	611	1	24,50,50	1.55	4 (16%)	19,82,82	3.94	10 (52%)
4	HEC	X	612	1	24,50,50	1.81	5 (20%)	19,82,82	4.10	10 (52%)
4	HEC	X	613	1	24,50,50	2.37	8 (33%)	19,82,82	3.41	8 (42%)
4	HEC	X	614	1,5	24,50,50	3.09	12 (50%)	19,82,82	3.70	10 (52%)
4	HEC	X	615	1	24,50,50	1.81	7 (29%)	19,82,82	3.99	8 (42%)
4	HEC	X	616	1,3	24,50,50	2.38	8 (33%)	19,82,82	3.36	9 (47%)
5	GOL	X	801	-	5,5,5	0.44	0	5,5,5	0.33	0
5	GOL	X	802	-	5,5,5	0.30	0	5,5,5	0.37	0
5	GOL	X	803	4	5,5,5	0.60	0	5,5,5	0.50	0
5	GOL	X	804	-	5,5,5	0.38	0	5,5,5	0.55	0
5	GOL	X	805	-	5,5,5	0.63	0	5,5,5	1.93	2 (40%)

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	HEC	X	601	1	-	0/6/54/54	0/0/8/8
4	HEC	X	602	1	-	0/6/54/54	0/0/8/8
4	HEC	X	603	1	-	0/6/54/54	0/0/8/8
4	HEC	X	604	1	-	0/6/54/54	0/0/8/8
4	HEC	X	605	1	-	0/6/54/54	0/0/8/8
4	HEC	X	606	1	-	0/6/54/54	0/0/8/8
4	HEC	X	607	1	-	0/6/54/54	0/0/8/8
4	HEC	X	608	1	-	0/6/54/54	0/0/8/8
4	HEC	X	609	1	-	0/6/54/54	0/0/8/8
4	HEC	X	610	1	-	0/6/54/54	0/0/8/8
4	HEC	X	611	1	-	0/6/54/54	0/0/8/8
4	HEC	X	612	1	-	0/6/54/54	0/0/8/8
4	HEC	X	613	1	-	0/6/54/54	0/0/8/8
4	HEC	X	614	1,5	-	0/6/54/54	0/0/8/8
4	HEC	X	615	1	-	0/6/54/54	0/0/8/8
4	HEC	X	616	1,3	-	0/6/54/54	0/0/8/8
5	GOL	X	801	-	-	0/4/4/4	0/0/0/0
5	GOL	X	802	-	-	0/4/4/4	0/0/0/0
5	GOL	X	803	4	-	0/4/4/4	0/0/0/0
5	GOL	X	804	-	-	0/4/4/4	0/0/0/0
5	GOL	X	805	-	-	0/4/4/4	0/0/0/0

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	607	HEC	C3B-C2B	-6.89	1.33	1.40
4	X	602	HEC	C3B-C2B	-6.65	1.33	1.40
4	X	608	HEC	C3B-C2B	-6.37	1.34	1.40
4	X	614	HEC	C3C-C2C	-6.26	1.34	1.40
4	X	613	HEC	C3B-C2B	-6.03	1.34	1.40
4	X	606	HEC	C3C-C2C	-6.01	1.34	1.40
4	X	616	HEC	C3B-C2B	-5.96	1.34	1.40
4	X	604	HEC	C3B-C2B	-5.82	1.34	1.40
4	X	614	HEC	C3B-C2B	-5.55	1.35	1.40
4	X	603	HEC	C3B-C2B	-5.53	1.35	1.40
4	X	606	HEC	C3B-C2B	-5.43	1.35	1.40
4	X	602	HEC	C3C-C2C	-5.41	1.35	1.40
4	X	610	HEC	C3C-C2C	-5.15	1.35	1.40
4	X	605	HEC	C3C-C2C	-4.98	1.35	1.40
4	X	609	HEC	C3B-C2B	-4.98	1.35	1.40
4	X	601	HEC	C3B-C2B	-4.97	1.35	1.40
4	X	603	HEC	C3C-C2C	-4.89	1.35	1.40
4	X	616	HEC	C3C-C2C	-4.62	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	610	HEC	C3B-C2B	-4.47	1.36	1.40
4	X	604	HEC	C3C-C2C	-4.45	1.36	1.40
4	X	609	HEC	C3C-C2C	-3.79	1.36	1.40
4	X	605	HEC	C3B-C2B	-3.77	1.36	1.40
4	X	612	HEC	C3C-C2C	-3.38	1.37	1.40
4	X	607	HEC	C3C-C2C	-3.10	1.37	1.40
4	X	608	HEC	C4C-NC	-2.99	1.32	1.36
4	X	612	HEC	C3B-C2B	-2.54	1.38	1.40
4	X	601	HEC	C3C-C2C	-2.31	1.38	1.40
4	X	611	HEC	C1D-CHD	-2.31	1.33	1.39
4	X	602	HEC	C1B-CHB	-2.08	1.34	1.39
4	X	602	HEC	C1C-CHC	-2.05	1.34	1.39
4	X	606	HEC	C2A-C3A	-2.01	1.31	1.37
4	X	615	HEC	CAA-C2A	2.01	1.56	1.52
4	X	616	HEC	CAD-C3D	2.04	1.55	1.52
4	X	604	HEC	CMD-C2D	2.05	1.55	1.51
4	X	606	HEC	CMC-C2C	2.06	1.56	1.51
4	X	608	HEC	C3B-C4B	2.06	1.47	1.42
4	X	613	HEC	CAA-C2A	2.07	1.56	1.52
4	X	602	HEC	CMD-C2D	2.10	1.56	1.51
4	X	610	HEC	C3B-C4B	2.11	1.47	1.42
4	X	609	HEC	CBB-CAB	2.14	1.58	1.49
4	X	615	HEC	C3C-C4C	2.15	1.47	1.42
4	X	611	HEC	CBB-CAB	2.16	1.58	1.49
4	X	603	HEC	CMB-C2B	2.18	1.56	1.51
4	X	610	HEC	CAA-C2A	2.18	1.56	1.52
4	X	606	HEC	CMD-C2D	2.22	1.56	1.51
4	X	601	HEC	C4B-NB	2.25	1.39	1.36
4	X	602	HEC	CAA-C2A	2.26	1.56	1.52
4	X	610	HEC	CMC-C2C	2.26	1.56	1.51
4	X	601	HEC	CAD-C3D	2.30	1.55	1.52
4	X	616	HEC	CMB-C2B	2.31	1.56	1.51
4	X	613	HEC	C4B-NB	2.32	1.39	1.36
4	X	614	HEC	CMB-C2B	2.35	1.56	1.51
4	X	607	HEC	C1A-NA	2.41	1.39	1.36
4	X	616	HEC	CMD-C2D	2.43	1.56	1.51
4	X	616	HEC	C3C-C4C	2.50	1.48	1.42
4	X	614	HEC	CBD-CAD	2.59	1.71	1.53
4	X	615	HEC	CBB-CAB	2.63	1.60	1.49
4	X	610	HEC	CAD-C3D	2.65	1.56	1.52
4	X	614	HEC	CAA-C2A	2.66	1.57	1.52
4	X	612	HEC	C3C-C4C	2.66	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	615	HEC	CAD-C3D	2.68	1.56	1.52
4	X	614	HEC	CBB-CAB	2.70	1.60	1.49
4	X	614	HEC	CMD-C2D	2.70	1.57	1.51
4	X	608	HEC	C3C-C4C	2.72	1.49	1.42
4	X	602	HEC	C1A-NA	2.78	1.40	1.36
4	X	613	HEC	CMA-C3A	2.81	1.57	1.51
4	X	612	HEC	C3B-C4B	2.83	1.49	1.42
4	X	613	HEC	C3D-C2D	2.85	1.46	1.37
4	X	615	HEC	CMB-C2B	2.89	1.57	1.51
4	X	616	HEC	C4A-NA	2.95	1.40	1.36
4	X	605	HEC	CAA-C2A	2.95	1.57	1.52
4	X	610	HEC	C3D-C2D	3.47	1.47	1.37
4	X	608	HEC	CMA-C3A	3.48	1.59	1.51
4	X	610	HEC	C1A-NA	3.48	1.41	1.36
4	X	615	HEC	C3B-C4B	3.63	1.51	1.42
4	X	613	HEC	CAD-C3D	3.65	1.58	1.52
4	X	614	HEC	C1A-NA	3.71	1.41	1.36
4	X	611	HEC	C3B-C4B	3.71	1.51	1.42
4	X	613	HEC	CMC-C2C	3.72	1.59	1.51
4	X	614	HEC	C4C-NC	4.07	1.42	1.36
4	X	614	HEC	C4A-NA	4.13	1.42	1.36
4	X	611	HEC	C3D-C2D	4.24	1.50	1.37
4	X	615	HEC	C3D-C2D	4.27	1.50	1.37
4	X	612	HEC	C3D-C2D	4.70	1.51	1.37
4	X	604	HEC	C3D-C2D	4.81	1.51	1.37
4	X	613	HEC	C1A-NA	4.87	1.43	1.36
4	X	601	HEC	C3D-C2D	4.94	1.52	1.37
4	X	608	HEC	C3D-C2D	4.99	1.52	1.37
4	X	607	HEC	C3D-C2D	5.04	1.52	1.37
4	X	614	HEC	C3D-C2D	5.22	1.53	1.37
4	X	605	HEC	C3D-C2D	5.28	1.53	1.37
4	X	602	HEC	C3D-C2D	5.36	1.53	1.37
4	X	609	HEC	C3D-C2D	5.53	1.54	1.37
4	X	603	HEC	C3D-C2D	5.54	1.54	1.37
4	X	616	HEC	C3D-C2D	5.72	1.54	1.37
4	X	606	HEC	C3D-C2D	5.77	1.54	1.37
4	X	614	HEC	CAD-C3D	6.27	1.62	1.52

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	601	HEC	CBB-CAB-C3B	-9.16	107.00	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	611	HEC	CMC-C2C-C1C	-8.59	114.15	128.36
4	X	612	HEC	CAD-CBD-CGD	-8.34	97.45	112.75
4	X	608	HEC	CMC-C2C-C1C	-8.33	114.58	128.36
4	X	611	HEC	CBC-CAC-C3C	-8.22	109.07	127.35
4	X	608	HEC	CBC-CAC-C3C	-8.12	109.30	127.35
4	X	612	HEC	CBB-CAB-C3B	-8.07	109.42	127.35
4	X	615	HEC	CBB-CAB-C3B	-8.04	109.49	127.35
4	X	603	HEC	CBB-CAB-C3B	-7.95	109.69	127.35
4	X	613	HEC	CBB-CAB-C3B	-7.88	109.84	127.35
4	X	607	HEC	CBB-CAB-C3B	-7.83	109.95	127.35
4	X	616	HEC	CMC-C2C-C1C	-7.75	115.54	128.36
4	X	615	HEC	CBC-CAC-C3C	-7.66	110.33	127.35
4	X	616	HEC	CBD-CAD-C3D	-7.56	98.98	112.53
4	X	604	HEC	CBB-CAB-C3B	-7.26	111.22	127.35
4	X	608	HEC	CAD-CBD-CGD	-7.00	99.91	112.75
4	X	615	HEC	CMC-C2C-C1C	-6.92	116.92	128.36
4	X	612	HEC	CAA-C2A-C1A	-6.88	119.53	127.01
4	X	602	HEC	CBB-CAB-C3B	-6.88	112.06	127.35
4	X	615	HEC	CBD-CAD-C3D	-6.87	100.22	112.53
4	X	613	HEC	CMB-C2B-C1B	-6.55	117.53	128.36
4	X	611	HEC	CBB-CAB-C3B	-6.51	112.89	127.35
4	X	613	HEC	CBC-CAC-C3C	-6.17	113.64	127.35
4	X	605	HEC	CBB-CAB-C3B	-6.10	113.80	127.35
4	X	604	HEC	CBA-CAA-C2A	-6.08	101.63	112.53
4	X	609	HEC	CMC-C2C-C1C	-6.08	118.30	128.36
4	X	601	HEC	CMC-C2C-C1C	-6.02	118.41	128.36
4	X	606	HEC	CBC-CAC-C3C	-5.94	114.16	127.35
4	X	603	HEC	CBD-CAD-C3D	-5.91	101.94	112.53
4	X	612	HEC	CMC-C2C-C1C	-5.83	118.72	128.36
4	X	601	HEC	CBC-CAC-C3C	-5.79	114.49	127.35
4	X	613	HEC	CBD-CAD-C3D	-5.78	102.17	112.53
4	X	610	HEC	CMB-C2B-C1B	-5.62	119.06	128.36
4	X	606	HEC	CBB-CAB-C3B	-5.54	115.05	127.35
4	X	609	HEC	CBB-CAB-C3B	-5.51	115.12	127.35
4	X	614	HEC	CBB-CAB-C3B	-5.46	115.22	127.35
4	X	608	HEC	CBB-CAB-C3B	-5.38	115.40	127.35
4	X	612	HEC	CAA-CBA-CGA	-5.35	102.94	112.75
4	X	614	HEC	CAA-C2A-C1A	-5.26	121.30	127.01
4	X	615	HEC	CMB-C2B-C1B	-5.21	119.74	128.36
4	X	610	HEC	CAD-CBD-CGD	-5.10	103.40	112.75
4	X	611	HEC	CBA-CAA-C2A	-5.03	103.52	112.53
4	X	612	HEC	CBD-CAD-C3D	-4.98	103.60	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	610	HEC	CMD-C2D-C1D	-4.91	120.24	128.36
4	X	602	HEC	CBC-CAC-C3C	-4.73	116.83	127.35
4	X	604	HEC	CBC-CAC-C3C	-4.70	116.90	127.35
4	X	609	HEC	CBC-CAC-C3C	-4.69	116.94	127.35
4	X	603	HEC	CBA-CAA-C2A	-4.67	104.15	112.53
4	X	603	HEC	CBC-CAC-C3C	-4.65	117.03	127.35
4	X	616	HEC	CBB-CAB-C3B	-4.58	117.17	127.35
4	X	611	HEC	C4C-C3C-C2C	-4.52	101.47	106.35
4	X	611	HEC	CAA-C2A-C1A	-4.49	122.13	127.01
4	X	615	HEC	CAD-CBD-CGD	-4.43	104.63	112.75
4	X	601	HEC	CBD-CAD-C3D	-4.31	104.81	112.53
4	X	604	HEC	CMC-C2C-C1C	-4.30	121.25	128.36
4	X	605	HEC	CMB-C2B-C1B	-4.19	121.43	128.36
4	X	601	HEC	CAA-CBA-CGA	-4.13	105.17	112.75
4	X	607	HEC	CBD-CAD-C3D	-4.09	105.20	112.53
4	X	605	HEC	CBC-CAC-C3C	-4.07	118.30	127.35
4	X	605	HEC	CMC-C2C-C1C	-4.06	121.65	128.36
4	X	614	HEC	CBC-CAC-C3C	-3.98	118.51	127.35
4	X	606	HEC	CAA-CBA-CGA	-3.88	105.63	112.75
4	X	614	HEC	CMB-C2B-C1B	-3.88	121.95	128.36
4	X	608	HEC	CAA-C2A-C1A	-3.79	122.89	127.01
4	X	615	HEC	CBA-CAA-C2A	-3.73	105.85	112.53
4	X	614	HEC	CMC-C2C-C1C	-3.69	122.25	128.36
4	X	610	HEC	CBB-CAB-C3B	-3.51	119.55	127.35
4	X	608	HEC	CAA-CBA-CGA	-3.47	106.39	112.75
4	X	607	HEC	CBC-CAC-C3C	-3.46	119.66	127.35
4	X	610	HEC	CAA-CBA-CGA	-3.46	106.40	112.75
4	X	607	HEC	CAD-CBD-CGD	-3.46	106.40	112.75
4	X	603	HEC	CMC-C2C-C1C	-3.46	122.64	128.36
4	X	612	HEC	CBC-CAC-C3C	-3.43	119.73	127.35
4	X	611	HEC	CBD-CAD-C3D	-3.43	106.38	112.53
4	X	607	HEC	CMC-C2C-C1C	-3.42	122.70	128.36
4	X	604	HEC	CAA-CBA-CGA	-3.41	106.49	112.75
4	X	607	HEC	CAA-C2A-C1A	-3.36	123.36	127.01
4	X	601	HEC	CAA-C2A-C1A	-3.35	123.37	127.01
4	X	611	HEC	CMB-C2B-C1B	-3.33	122.85	128.36
4	X	610	HEC	CBA-CAA-C2A	-3.33	106.57	112.53
4	X	602	HEC	CMB-C2B-C1B	-3.32	122.86	128.36
4	X	601	HEC	CMB-C2B-C1B	-3.23	123.02	128.36
5	X	805	GOL	C3-C2-C1	-3.18	98.64	111.12
4	X	606	HEC	CAD-C3D-C4D	-3.15	123.58	127.01
4	X	606	HEC	CMC-C2C-C1C	-3.10	123.24	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	615	HEC	CAA-CBA-CGA	-3.07	107.12	112.75
4	X	613	HEC	CMC-C2C-C1C	-3.05	123.32	128.36
4	X	607	HEC	CBA-CAA-C2A	-3.02	107.11	112.53
4	X	606	HEC	CBD-CAD-C3D	-3.01	107.13	112.53
4	X	609	HEC	CMD-C2D-C1D	-2.94	123.50	128.36
4	X	610	HEC	CAD-C3D-C4D	-2.89	123.86	127.01
4	X	606	HEC	CMB-C2B-C1B	-2.86	123.64	128.36
4	X	609	HEC	CAD-CBD-CGD	-2.82	107.58	112.75
4	X	611	HEC	CAA-CBA-CGA	-2.79	107.63	112.75
4	X	616	HEC	CBC-CAC-C3C	-2.78	121.17	127.35
4	X	616	HEC	CAA-C2A-C1A	-2.72	124.06	127.01
4	X	612	HEC	CMB-C2B-C1B	-2.69	123.91	128.36
4	X	604	HEC	CBD-CAD-C3D	-2.67	107.75	112.53
4	X	614	HEC	CMD-C2D-C1D	-2.65	123.98	128.36
5	X	805	GOL	O1-C1-C2	-2.65	97.33	110.18
4	X	609	HEC	CAA-C2A-C1A	-2.57	124.22	127.01
4	X	605	HEC	CAD-CBD-CGD	-2.52	108.13	112.75
4	X	610	HEC	CMC-C2C-C1C	-2.45	124.32	128.36
4	X	602	HEC	CAA-C2A-C1A	-2.41	124.39	127.01
4	X	607	HEC	CMD-C2D-C1D	-2.39	124.42	128.36
4	X	604	HEC	CAA-C2A-C1A	-2.39	124.42	127.01
4	X	601	HEC	CBA-CAA-C2A	-2.33	108.35	112.53
4	X	606	HEC	CAA-C2A-C1A	-2.31	124.50	127.01
4	X	609	HEC	CMB-C2B-C1B	-2.31	124.54	128.36
4	X	605	HEC	C3B-C4B-NB	-2.29	106.63	110.94
4	X	603	HEC	CMB-C2B-C1B	-2.27	124.61	128.36
4	X	614	HEC	CAA-CBA-CGA	-2.25	108.62	112.75
4	X	610	HEC	C3B-C4B-NB	-2.23	106.73	110.94
4	X	608	HEC	CAD-C3D-C2D	-2.22	122.66	129.00
4	X	607	HEC	C3B-C4B-NB	-2.14	106.90	110.94
4	X	610	HEC	CAA-C2A-C3A	-2.14	122.88	129.00
4	X	608	HEC	C3C-C4C-NC	-2.12	106.95	110.94
4	X	601	HEC	C3B-C4B-NB	-2.08	107.01	110.94
4	X	613	HEC	CAD-CBD-CGD	-2.06	108.98	112.75
4	X	614	HEC	C3B-C4B-NB	-2.05	107.08	110.94
4	X	616	HEC	C3C-C4C-NC	-2.01	107.14	110.94
4	X	616	HEC	CBA-CAA-C2A	-2.01	108.93	112.53
4	X	603	HEC	C4B-C3B-C2B	2.13	108.65	106.35
4	X	611	HEC	CMA-C3A-C2A	2.14	129.71	125.24
4	X	608	HEC	CMA-C3A-C2A	2.27	129.97	125.24
4	X	607	HEC	CMD-C2D-C3D	2.29	130.03	125.24
4	X	602	HEC	C4B-C3B-C2B	2.38	108.92	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	602	HEC	CBA-CAA-C2A	2.41	116.85	112.53
4	X	613	HEC	CMD-C2D-C3D	2.54	130.56	125.24
4	X	609	HEC	CMD-C2D-C3D	2.72	130.92	125.24
4	X	616	HEC	CMA-C3A-C2A	2.79	131.07	125.24
4	X	602	HEC	CAA-CBA-CGA	2.87	118.01	112.75
4	X	612	HEC	CMD-C2D-C1D	2.88	133.13	128.36
4	X	602	HEC	CAD-C3D-C4D	2.92	130.18	127.01
4	X	612	HEC	CMA-C3A-C2A	3.00	131.52	125.24
4	X	614	HEC	CBD-CAD-C3D	3.16	118.19	112.53
4	X	601	HEC	CAD-C3D-C4D	3.16	130.44	127.01
4	X	601	HEC	CAD-CBD-CGD	3.20	118.62	112.75
4	X	608	HEC	CAD-C3D-C4D	3.22	130.50	127.01
4	X	613	HEC	C4C-C3C-C2C	3.25	109.86	106.35
4	X	609	HEC	CAA-CBA-CGA	3.41	118.99	112.75
4	X	608	HEC	CBA-CAA-C2A	3.42	118.66	112.53
4	X	606	HEC	CBA-CAA-C2A	3.42	118.67	112.53
4	X	610	HEC	CAA-C2A-C1A	3.75	131.08	127.01
4	X	608	HEC	CBD-CAD-C3D	4.32	120.28	112.53
4	X	610	HEC	CMD-C2D-C3D	4.91	135.50	125.24
4	X	605	HEC	CBA-CAA-C2A	5.34	122.09	112.53
4	X	616	HEC	CAD-CBD-CGD	6.31	124.31	112.75
4	X	614	HEC	CAD-CBD-CGD	10.85	132.64	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 115 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	601	HEC	14	0
4	X	602	HEC	12	0
4	X	603	HEC	2	0
4	X	604	HEC	6	0
4	X	605	HEC	3	0
4	X	606	HEC	7	0
4	X	607	HEC	6	0
4	X	608	HEC	11	0
4	X	609	HEC	4	0
4	X	610	HEC	13	0
4	X	611	HEC	1	0
4	X	612	HEC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	613	HEC	1	1
4	X	614	HEC	10	0
4	X	615	HEC	7	1
4	X	616	HEC	12	0
5	X	803	GOL	5	0
5	X	804	GOL	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	X	516/560 (92%)	0.41	39 (7%) 17 23	28, 55, 82, 91	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	530	SER	8.6
1	X	159	ALA	5.4
1	X	529	ASN	4.3
1	X	119	VAL	3.8
1	X	58	GLU	3.8
1	X	253	LEU	3.7
1	X	22	ALA	3.0
1	X	182	LEU	3.0
1	X	298	GLN	3.0
1	X	113	GLY	3.0
1	X	59	GLY	2.9
1	X	180	GLU	2.9
1	X	152	CYS	2.9
1	X	23	VAL	2.7
1	X	251	THR	2.5
1	X	276	VAL	2.5
1	X	156	TYR	2.5
1	X	221	LEU	2.5
1	X	215	THR	2.5
1	X	160	GLN	2.5
1	X	34	PHE	2.4
1	X	424	LYS	2.4
1	X	252	LEU	2.4
1	X	24	PHE	2.4
1	X	479	CYS	2.3
1	X	36	HIS	2.3
1	X	116	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	X	361	THR	2.2
1	X	93	VAL	2.2
1	X	158	GLU	2.2
1	X	37	GLU	2.2
1	X	53	CYS	2.2
1	X	191	VAL	2.1
1	X	260	ALA	2.1
1	X	465	GLY	2.1
1	X	44	GLU	2.1
1	X	259	THR	2.1
1	X	143	VAL	2.1
1	X	112	PRO	2.1

## 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
2	NAG	X	900	14/15	0.81	0.26	-	75,79,86,86	0
2	NAA	X	901	14/15	0.86	0.37	-	89,91,94,94	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(Å <sup>2</sup> )	Q<0.9
5	GOL	X	804	6/6	0.85	0.37	3.22	53,61,66,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	HEC	X	612	43/43	0.97	0.21	1.29	30,38,56,65	0
4	HEC	X	611	43/43	0.96	0.15	0.78	28,33,52,58	0
5	GOL	X	803	6/6	0.91	0.17	0.74	28,54,59,60	0
4	HEC	X	601	43/43	0.94	0.19	0.61	52,59,63,65	0
4	HEC	X	604	43/43	0.97	0.16	0.59	38,48,54,57	0
4	HEC	X	606	43/43	0.94	0.15	0.49	45,49,65,71	0
4	HEC	X	602	43/43	0.93	0.18	0.48	45,51,75,80	0
4	HEC	X	615	43/43	0.96	0.15	0.40	25,31,49,56	0
4	HEC	X	608	43/43	0.96	0.14	0.28	27,37,52,61	0
4	HEC	X	605	43/43	0.90	0.17	0.28	48,58,73,78	0
4	HEC	X	614	43/43	0.93	0.14	0.21	20,31,41,50	0
4	HEC	X	607	43/43	0.95	0.14	0.03	49,55,65,72	0
4	HEC	X	613	43/43	0.97	0.14	0.01	28,31,43,53	0
4	HEC	X	603	43/43	0.93	0.15	-0.28	58,73,75,77	0
4	HEC	X	609	43/43	0.95	0.12	-0.32	40,50,61,67	0
4	HEC	X	616	43/43	0.94	0.12	-0.34	29,38,50,64	0
4	HEC	X	610	43/43	0.97	0.10	-0.43	20,26,41,47	0
3	ZN	X	703	1/1	0.84	0.07	-2.01	69,69,69,69	0
3	ZN	X	701	1/1	0.99	0.08	-	42,42,42,42	0
5	GOL	X	805	6/6	0.88	0.17	-	57,62,66,73	0
3	ZN	X	702	1/1	0.85	0.11	-	72,72,72,72	0
5	GOL	X	802	6/6	0.81	0.17	-	62,69,71,73	0
5	GOL	X	801	6/6	0.85	0.29	-	86,88,89,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.