



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:54 am GMT

PDB ID : 3UFK  
Title : Crystal structure of UndA complexed with Iron Nitrilotriacetate  
Authors : Edwards, M.J.; Clarke, T.A.  
Deposited on : 2011-11-01  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

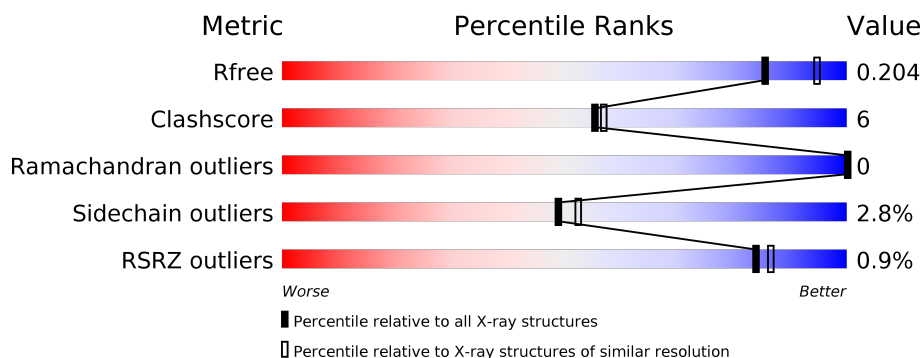
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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	A	874	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; right: 0; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 83%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 83%; width: 17%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 0; left: 99%; width: 2%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 0; left: 100%; width: 0; height: 0; border-left: 5px solid transparent; border-right: 5px solid transparent; border-bottom: 8px solid grey;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>83%</span> <span>8%</span> <span>8%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	925	-	-	X	X
8	GOL	A	927	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	928	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7516 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 UndA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	800	Total	C	N	O	S	0	3	0
			5962	3699	1030	1198	35			

There are 58 discrepancies between the modelled and reference sequences:

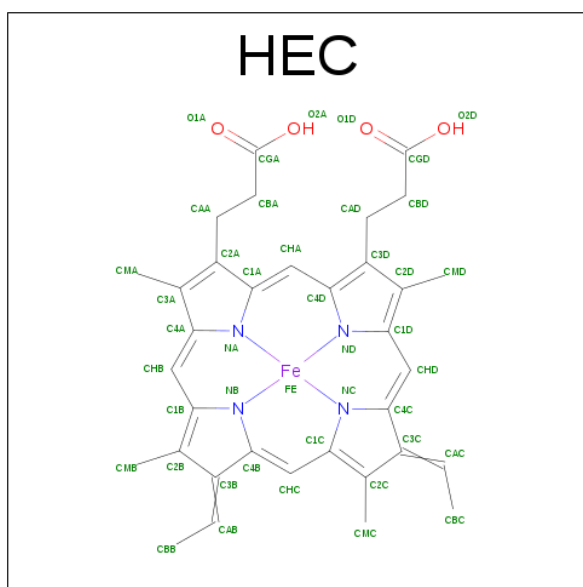
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP F8UWD6
A	1	SER	-	EXPRESSION TAG	UNP F8UWD6
A	2	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	3	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	4	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	5	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	6	SER	-	EXPRESSION TAG	UNP F8UWD6
A	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	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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

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

- 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		

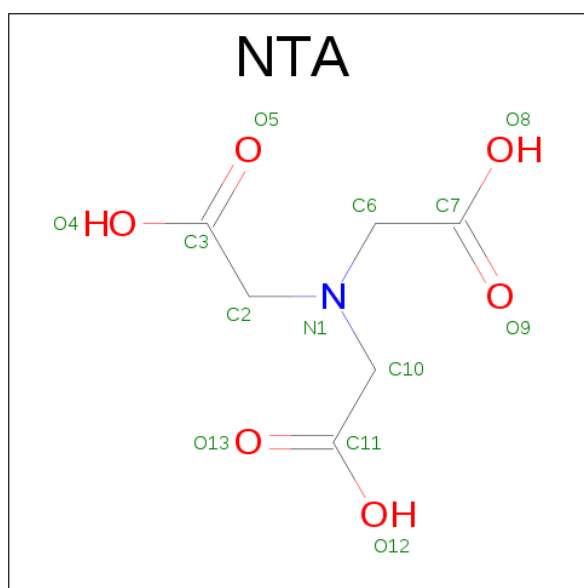
- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Fe	0	0
			4	4		

- Molecule 6 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		

- Molecule 7 is NITRILOTRIACETIC ACID (three-letter code: NTA) (formula: C<sub>6</sub>H<sub>9</sub>NO<sub>6</sub>).



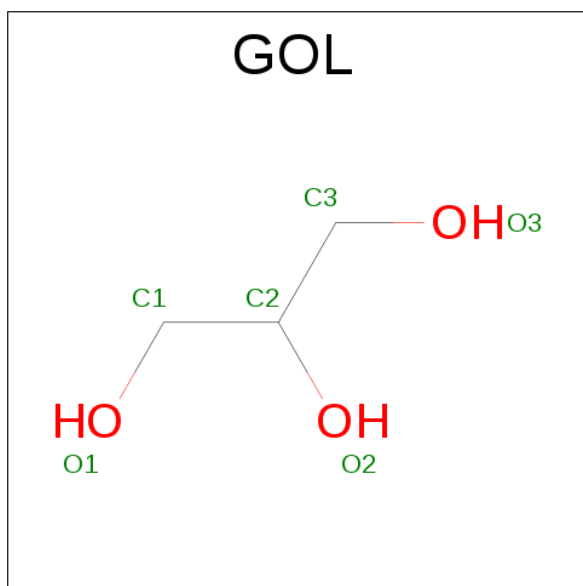
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			13	6	1	6		
7	A	1	Total	C	N	O	0	0
			13	6	1	6		
7	A	1	Total	C	N	O	0	0
			13	6	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			13	6	1	6		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 9 is water.

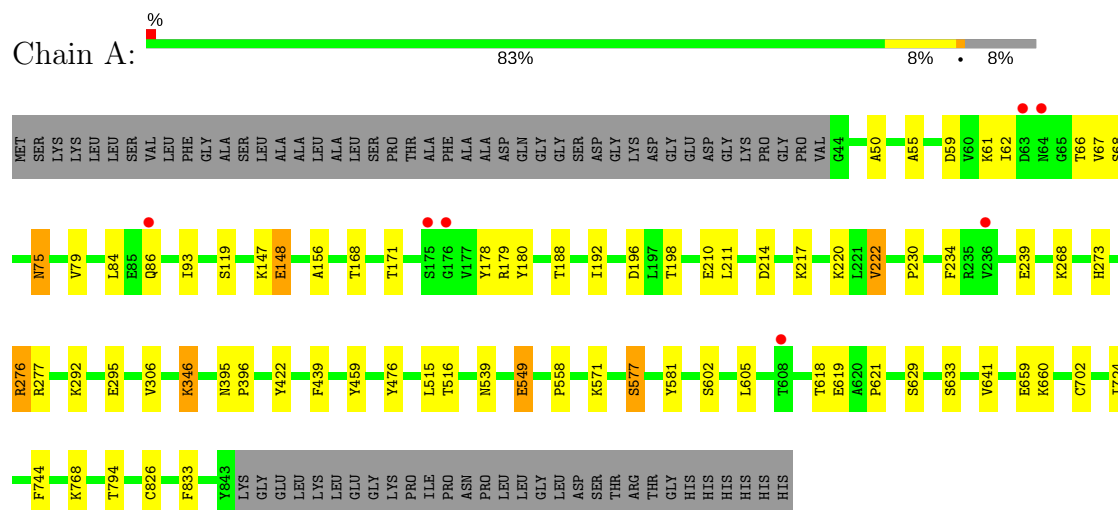
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	996	Total	O	0	0
			996	996		



### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: UndA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.50Å 105.87Å 151.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.61 – 2.10 61.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.61-2.10) 99.3 (61.61-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.05 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.155 , 0.205 0.156 , 0.204	Depositor DCC
$R_{free}$ test set	3323 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CA, O, FE, HEC, NTA

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	0/6096	0.66	0/8295

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	619	GLU	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5962	0	5730	59	0
2	A	473	0	331	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	4	0	0	0	0
6	A	2	0	0	0	0
7	A	52	0	24	3	0
8	A	24	0	32	5	0
9	A	996	0	0	14	0
All	All	7516	0	6117	73	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (73) 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:A:826:CYS:SG	2:A:911:HEC:CAC	2.23	1.25
1:A:558:PRO:HB3	9:A:1178:HOH:O	1.66	0.95
1:A:826:CYS:SG	2:A:911:HEC:CBC	2.64	0.85
1:A:68:SER:OG	1:A:179:ARG:NH1	2.12	0.82
1:A:768:LYS:HG3	9:A:1664:HOH:O	1.81	0.79
1:A:602[B]:SER:OG	1:A:621:PRO:HG2	1.85	0.77
1:A:422:TYR:O	8:A:925:GOL:C3	2.34	0.76
1:A:549:GLU:OE2	9:A:1609:HOH:O	2.03	0.75
1:A:422:TYR:O	8:A:925:GOL:H31	1.87	0.74
1:A:62:ILE:HG12	1:A:67:VAL:HG22	1.68	0.74
2:A:907:HEC:HBB3	2:A:907:HEC:HMB1	1.71	0.70
1:A:659:GLU:OE1	7:A:924:NTA:H21	1.95	0.66
1:A:826:CYS:SG	2:A:911:HEC:HBC3	2.34	0.66
2:A:911:HEC:HBC3	2:A:911:HEC:HMC1	1.76	0.66
1:A:826:CYS:SG	2:A:911:HEC:C3C	2.85	0.63
1:A:702:CYS:SG	2:A:908:HEC:C3C	2.85	0.63
1:A:702:CYS:SG	2:A:908:HEC:CBC	2.89	0.61
1:A:59:ASP:O	1:A:179:ARG:NH2	2.34	0.61
1:A:292:LYS:HE2	9:A:1824:HOH:O	2.00	0.60
1:A:210:GLU:OE1	1:A:276:ARG:HD3	2.03	0.58
2:A:903:HEC:HMB1	2:A:903:HEC:HBB3	1.87	0.57
1:A:55:ALA:HB3	1:A:222:VAL:HG21	1.87	0.56
1:A:75:ASN:HD22	1:A:75:ASN:C	2.09	0.56
1:A:826:CYS:SG	2:A:911:HEC:HAC	2.40	0.55
1:A:422:TYR:HA	8:A:925:GOL:H32	1.89	0.54
1:A:744:PHE:CE1	2:A:906:HEC:HBC2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:918:NTA:H62	9:A:1009:HOH:O	2.08	0.54
1:A:439:PHE:HA	2:A:905:HEC:HMC2	1.90	0.53
1:A:602[B]:SER:OG	1:A:621:PRO:CG	2.57	0.52
1:A:84:LEU:HB3	1:A:178:TYR:CE1	2.47	0.50
2:A:905:HEC:HBC3	2:A:905:HEC:HMC1	1.93	0.50
1:A:273:HIS:HB2	1:A:277:ARG:HD2	1.93	0.50
1:A:724:ILE:HG21	2:A:909:HEC:HMD2	1.94	0.49
2:A:904:HEC:HMC1	2:A:904:HEC:HBC3	1.94	0.49
1:A:459:TYR:CE1	1:A:605:LEU:HD11	2.48	0.48
1:A:516:THR:HA	1:A:539:ASN:O	2.14	0.48
1:A:50:ALA:O	1:A:220:LYS:HE3	2.14	0.48
1:A:422:TYR:O	8:A:925:GOL:H32	2.10	0.48
1:A:422:TYR:CA	8:A:925:GOL:H32	2.43	0.48
1:A:93:ILE:HG12	1:A:211:LEU:HD12	1.96	0.48
1:A:395:ASN:HB2	1:A:396:PRO:HD2	1.96	0.47
1:A:476:TYR:CE2	1:A:629:SER:HB3	2.48	0.47
1:A:306:VAL:HG11	2:A:903:HEC:HMD2	1.96	0.47
1:A:295:GLU:OE2	9:A:1522:HOH:O	2.20	0.47
1:A:239:GLU:HB2	9:A:1800:HOH:O	2.14	0.47
1:A:346:LYS:NZ	9:A:1989:HOH:O	2.48	0.47
1:A:214:ASP:OD2	1:A:220:LYS:NZ	2.37	0.46
2:A:905:HEC:HBB3	2:A:905:HEC:HMB1	1.98	0.46
1:A:558:PRO:CB	9:A:1178:HOH:O	2.41	0.46
1:A:156:ALA:HB1	1:A:292:LYS:HB2	1.97	0.46
1:A:75:ASN:ND2	1:A:75:ASN:C	2.69	0.46
1:A:75:ASN:ND2	1:A:79:VAL:H	2.15	0.45
2:A:910:HEC:HBC3	2:A:910:HEC:HMC1	1.99	0.45
2:A:907:HEC:HBB3	2:A:907:HEC:CMB	2.45	0.44
1:A:62:ILE:HA	1:A:66:THR:O	2.18	0.44
1:A:68:SER:HA	1:A:180:TYR:O	2.18	0.44
1:A:276:ARG:HG2	1:A:276:ARG:O	2.16	0.43
1:A:833:PHE:CE2	2:A:911:HEC:HMD3	2.53	0.43
1:A:196:ASP:OD2	1:A:198:THR:HG23	2.18	0.43
2:A:901:HEC:O1D	9:A:1068:HOH:O	2.21	0.43
1:A:577:SER:HB2	9:A:1644:HOH:O	2.18	0.42
1:A:633:SER:HB3	1:A:641:VAL:HG23	2.01	0.42
2:A:901:HEC:HMB1	2:A:901:HEC:HBB3	2.00	0.42
1:A:168:THR:O	1:A:168:THR:HG22	2.19	0.42
1:A:192:ILE:HD12	9:A:1576:HOH:O	2.19	0.42
1:A:171:THR:HG23	9:A:1496:HOH:O	2.20	0.41
1:A:230:PRO:HB3	1:A:234:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:911:HEC:CBC	2:A:911:HEC:HMC1	2.47	0.41
1:A:61:LYS:HE2	1:A:179:ARG:NH1	2.35	0.41
2:A:910:HEC:HMA3	2:A:910:HEC:HBA1	2.03	0.41
1:A:660:LYS:HE3	7:A:924:NTA:O12	2.20	0.41
2:A:911:HEC:HMB1	2:A:911:HEC:HBB3	2.03	0.40
1:A:148:GLU:HB3	9:A:1656:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	801/874 (92%)	777 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	647/700 (92%)	629 (97%)	18 (3%)	49	52

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	86	GLN
1	A	119	SER
1	A	147	LYS
1	A	148	GLU
1	A	188	THR
1	A	217	LYS
1	A	222	VAL
1	A	268	LYS
1	A	276	ARG
1	A	346	LYS
1	A	515	LEU
1	A	549	GLU
1	A	571	LYS
1	A	577	SER
1	A	581	TYR
1	A	618	THR
1	A	794	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN

### 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](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	28,50,50	2.30	9 (32%)	16,82,82	2.33	5 (31%)
2	HEC	A	902	1,3	28,50,50	2.24	5 (17%)	16,82,82	1.76	4 (25%)
2	HEC	A	903	1	28,50,50	2.10	5 (17%)	16,82,82	2.34	4 (25%)
2	HEC	A	904	1	28,50,50	2.20	7 (25%)	16,82,82	2.15	7 (43%)
2	HEC	A	905	1	28,50,50	2.12	5 (17%)	16,82,82	2.34	6 (37%)
2	HEC	A	906	1	28,50,50	2.22	7 (25%)	16,82,82	2.34	5 (31%)
2	HEC	A	907	1	28,50,50	2.38	6 (21%)	16,82,82	1.83	2 (12%)
2	HEC	A	908	1,4	28,50,50	2.40	8 (28%)	16,82,82	1.86	4 (25%)
2	HEC	A	909	1	28,50,50	2.04	4 (14%)	16,82,82	2.09	4 (25%)
2	HEC	A	910	1	28,50,50	2.19	6 (21%)	16,82,82	2.14	5 (31%)
2	HEC	A	911	1	28,50,50	2.26	7 (25%)	16,82,82	2.15	5 (31%)
7	NTA	A	918	5	3,12,12	0.38	0	6,15,15	3.86	3 (50%)
7	NTA	A	919	5	3,12,12	0.31	0	6,15,15	3.95	4 (66%)
7	NTA	A	923	5	3,12,12	0.81	0	6,15,15	3.99	4 (66%)
7	NTA	A	924	5	3,12,12	0.55	0	6,15,15	3.84	3 (50%)
8	GOL	A	925	-	5,5,5	0.45	0	5,5,5	0.68	0
8	GOL	A	926	-	5,5,5	0.51	0	5,5,5	0.37	0
8	GOL	A	927	-	5,5,5	0.38	0	5,5,5	0.49	0
8	GOL	A	928	-	5,5,5	0.53	0	5,5,5	0.68	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	-	0/6/54/54	0/0/8/8
2	HEC	A	902	1,3	-	0/6/54/54	0/0/8/8
2	HEC	A	903	1	-	0/6/54/54	0/0/8/8
2	HEC	A	904	1	-	0/6/54/54	0/0/8/8
2	HEC	A	905	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	906	1	-	0/6/54/54	0/0/8/8
2	HEC	A	907	1	-	0/6/54/54	0/0/8/8
2	HEC	A	908	1,4	-	0/6/54/54	0/0/8/8
2	HEC	A	909	1	-	0/6/54/54	0/0/8/8
2	HEC	A	910	1	-	0/6/54/54	0/0/8/8
2	HEC	A	911	1	-	0/6/54/54	0/0/8/8
7	NTA	A	918	5	-	0/6/12/12	0/0/0/0
7	NTA	A	919	5	-	0/6/12/12	0/0/0/0
7	NTA	A	923	5	-	0/6/12/12	0/0/0/0
7	NTA	A	924	5	-	0/6/12/12	0/0/0/0
8	GOL	A	925	-	-	0/4/4/4	0/0/0/0
8	GOL	A	926	-	-	0/4/4/4	0/0/0/0
8	GOL	A	927	-	-	0/4/4/4	0/0/0/0
8	GOL	A	928	-	-	0/4/4/4	0/0/0/0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	907	HEC	C3B-C2B	-7.31	1.33	1.40
2	A	908	HEC	C3C-C2C	-6.84	1.33	1.40
2	A	903	HEC	C3B-C2B	-6.69	1.33	1.40
2	A	906	HEC	C3C-C2C	-6.13	1.34	1.40
2	A	902	HEC	C3C-C2C	-5.99	1.34	1.40
2	A	904	HEC	C3C-C2C	-5.94	1.34	1.40
2	A	911	HEC	C3B-C2B	-5.89	1.34	1.40
2	A	910	HEC	C3C-C2C	-5.81	1.34	1.40
2	A	901	HEC	C3B-C2B	-5.81	1.34	1.40
2	A	907	HEC	C3C-C2C	-5.70	1.34	1.40
2	A	908	HEC	C3B-C2B	-5.65	1.34	1.40
2	A	905	HEC	C3B-C2B	-5.44	1.35	1.40
2	A	910	HEC	C3B-C2B	-5.40	1.35	1.40
2	A	911	HEC	C3C-C2C	-5.38	1.35	1.40
2	A	909	HEC	C3B-C2B	-5.35	1.35	1.40
2	A	904	HEC	C3B-C2B	-5.16	1.35	1.40
2	A	902	HEC	C3B-C2B	-5.05	1.35	1.40
2	A	901	HEC	C3C-C2C	-4.97	1.35	1.40
2	A	905	HEC	C3C-C2C	-4.89	1.35	1.40
2	A	909	HEC	C3C-C2C	-4.42	1.36	1.40
2	A	906	HEC	C3B-C2B	-4.24	1.36	1.40
2	A	903	HEC	C3C-C2C	-4.00	1.36	1.40
2	A	903	HEC	CMB-C2B	2.01	1.55	1.51
2	A	903	HEC	CAA-C2A	2.01	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	904	HEC	CMA-C3A	2.03	1.55	1.51
2	A	905	HEC	CMA-C3A	2.03	1.55	1.51
2	A	901	HEC	CAD-C3D	2.06	1.55	1.52
2	A	904	HEC	CAD-C3D	2.07	1.55	1.52
2	A	911	HEC	CMD-C2D	2.09	1.55	1.51
2	A	910	HEC	C3B-C4B	2.10	1.46	1.43
2	A	907	HEC	CMD-C2D	2.11	1.55	1.51
2	A	910	HEC	C3C-C4C	2.12	1.47	1.43
2	A	911	HEC	CAD-C3D	2.13	1.55	1.52
2	A	911	HEC	CMA-C3A	2.15	1.56	1.51
2	A	908	HEC	CMC-C2C	2.17	1.56	1.51
2	A	901	HEC	CMB-C2B	2.20	1.56	1.51
2	A	907	HEC	CAA-C2A	2.21	1.56	1.52
2	A	911	HEC	C4A-NA	2.21	1.39	1.36
2	A	910	HEC	C4D-ND	2.22	1.40	1.36
2	A	907	HEC	C1D-ND	2.25	1.40	1.36
2	A	902	HEC	C4C-NC	2.26	1.39	1.36
2	A	904	HEC	CAA-C2A	2.28	1.56	1.52
2	A	901	HEC	CMD-C2D	2.32	1.56	1.51
2	A	902	HEC	CAD-C3D	2.33	1.56	1.52
2	A	906	HEC	CMC-C2C	2.34	1.56	1.51
2	A	901	HEC	C1B-NB	2.48	1.41	1.36
2	A	906	HEC	C4B-NB	2.48	1.39	1.36
2	A	908	HEC	C1A-NA	2.62	1.39	1.36
2	A	904	HEC	CMB-C2B	2.66	1.57	1.51
2	A	906	HEC	CMD-C2D	2.74	1.57	1.51
2	A	905	HEC	CMB-C2B	2.78	1.57	1.51
2	A	901	HEC	C1D-ND	2.78	1.42	1.36
2	A	908	HEC	CAA-C2A	2.80	1.57	1.52
2	A	908	HEC	CMB-C2B	2.87	1.57	1.51
2	A	909	HEC	C1A-NA	2.94	1.40	1.36
2	A	901	HEC	C4B-NB	3.22	1.40	1.36
2	A	906	HEC	C4A-NA	3.42	1.40	1.36
2	A	908	HEC	CAD-C3D	3.54	1.58	1.52
2	A	908	HEC	C3D-C2D	4.10	1.49	1.37
2	A	903	HEC	C3D-C2D	4.51	1.51	1.37
2	A	906	HEC	C3D-C2D	4.52	1.51	1.37
2	A	909	HEC	C3D-C2D	4.70	1.51	1.37
2	A	901	HEC	C3D-C2D	4.81	1.51	1.37
2	A	904	HEC	C3D-C2D	4.84	1.52	1.37
2	A	902	HEC	C3D-C2D	4.93	1.52	1.37
2	A	907	HEC	C3D-C2D	5.01	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	905	HEC	C3D-C2D	5.06	1.52	1.37
2	A	910	HEC	C3D-C2D	5.10	1.52	1.37
2	A	911	HEC	C3D-C2D	5.84	1.55	1.37

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	903	HEC	CMC-C2C-C1C	-6.44	118.56	128.46
2	A	905	HEC	CMC-C2C-C1C	-5.51	120.00	128.46
2	A	911	HEC	CMC-C2C-C1C	-5.28	120.35	128.46
2	A	905	HEC	CAD-CBD-CGD	-5.06	104.02	112.66
2	A	907	HEC	CMC-C2C-C1C	-4.93	120.88	128.46
2	A	901	HEC	CMC-C2C-C1C	-4.74	121.17	128.46
2	A	906	HEC	CMB-C2B-C1B	-4.65	121.32	128.46
2	A	901	HEC	CAA-CBA-CGA	-4.55	104.89	112.66
2	A	909	HEC	CBA-CAA-C2A	-4.50	103.89	112.47
2	A	910	HEC	CMC-C2C-C1C	-4.41	121.69	128.46
2	A	906	HEC	CAA-CBA-CGA	-4.33	105.27	112.66
2	A	910	HEC	CBD-CAD-C3D	-4.29	104.28	112.48
2	A	903	HEC	CAD-CBD-CGD	-4.27	105.36	112.66
2	A	906	HEC	CMC-C2C-C1C	-4.05	122.24	128.46
2	A	911	HEC	CBA-CAA-C2A	-3.86	105.11	112.47
2	A	902	HEC	CMC-C2C-C1C	-3.79	122.64	128.46
2	A	906	HEC	CBD-CAD-C3D	-3.78	105.26	112.48
2	A	901	HEC	CBD-CAD-C3D	-3.73	105.35	112.48
2	A	908	HEC	CMB-C2B-C1B	-3.61	122.92	128.46
2	A	909	HEC	CMC-C2C-C1C	-3.60	122.94	128.46
2	A	904	HEC	CBA-CAA-C2A	-3.58	105.63	112.47
2	A	904	HEC	C1D-C2D-C3D	-3.52	104.55	107.00
2	A	902	HEC	CMB-C2B-C1B	-3.30	123.39	128.46
2	A	904	HEC	CMC-C2C-C1C	-3.27	123.44	128.46
2	A	904	HEC	CMB-C2B-C1B	-3.18	123.58	128.46
2	A	908	HEC	CMC-C2C-C1C	-3.18	123.58	128.46
2	A	903	HEC	CMB-C2B-C1B	-3.13	123.66	128.46
2	A	909	HEC	CBD-CAD-C3D	-3.05	106.65	112.48
2	A	901	HEC	CBA-CAA-C2A	-3.03	106.69	112.47
2	A	904	HEC	CBD-CAD-C3D	-2.95	106.84	112.48
2	A	910	HEC	CAA-CBA-CGA	-2.94	107.63	112.66
2	A	901	HEC	C1D-C2D-C3D	-2.87	105.00	107.00
2	A	906	HEC	C1D-C2D-C3D	-2.59	105.20	107.00
2	A	907	HEC	C1D-C2D-C3D	-2.58	105.20	107.00
2	A	905	HEC	CBA-CAA-C2A	-2.57	107.57	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	HEC	CAD-CBD-CGD	-2.53	108.33	112.66
2	A	910	HEC	CMB-C2B-C1B	-2.52	124.60	128.46
2	A	903	HEC	C1D-C2D-C3D	-2.50	105.26	107.00
2	A	909	HEC	CMB-C2B-C1B	-2.49	124.63	128.46
2	A	911	HEC	CMD-C2D-C1D	-2.46	124.68	128.46
2	A	904	HEC	CAD-CBD-CGD	-2.42	108.52	112.66
2	A	911	HEC	C1D-C2D-C3D	-2.35	105.36	107.00
2	A	902	HEC	CBA-CAA-C2A	-2.33	108.03	112.47
2	A	905	HEC	CMB-C2B-C1B	-2.26	124.99	128.46
2	A	905	HEC	CBD-CAD-C3D	-2.23	108.22	112.48
2	A	910	HEC	C1D-C2D-C3D	-2.21	105.46	107.00
2	A	905	HEC	C1D-C2D-C3D	-2.14	105.51	107.00
2	A	908	HEC	CMA-C3A-C2A	2.12	128.93	124.94
2	A	904	HEC	C4B-C3B-C2B	2.23	108.76	106.35
7	A	919	NTA	C7-C6-N1	2.65	117.26	113.48
2	A	911	HEC	CMD-C2D-C3D	2.66	129.96	124.94
2	A	908	HEC	CAD-CBD-CGD	3.07	117.92	112.66
7	A	923	NTA	C10-N1-C6	3.26	116.33	110.73
7	A	919	NTA	C2-N1-C10	3.33	116.45	110.73
7	A	924	NTA	C2-N1-C10	4.06	117.71	110.73
7	A	918	NTA	C10-N1-C6	4.31	118.13	110.73
7	A	923	NTA	C2-N1-C10	4.48	118.42	110.73
7	A	924	NTA	C10-N1-C6	4.67	118.75	110.73
7	A	919	NTA	C2-N1-C6	4.71	118.83	110.73
7	A	923	NTA	C3-C2-N1	4.80	120.32	113.48
7	A	918	NTA	C2-N1-C6	5.23	119.72	110.73
7	A	923	NTA	C2-N1-C6	6.33	121.60	110.73
7	A	924	NTA	C2-N1-C6	6.38	121.69	110.73
7	A	918	NTA	C2-N1-C10	6.52	121.93	110.73
7	A	919	NTA	C10-N1-C6	7.05	122.85	110.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEC	2	0
2	A	903	HEC	2	0
2	A	904	HEC	1	0
2	A	905	HEC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	906	HEC	1	0
2	A	907	HEC	2	0
2	A	908	HEC	2	0
2	A	909	HEC	1	0
2	A	910	HEC	2	0
2	A	911	HEC	9	0
7	A	918	NTA	1	0
7	A	924	NTA	2	0
8	A	925	GOL	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	800/874 (91%)	-0.41	7 (0%) 84 86	8, 22, 46, 59	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	THR	6.1
1	A	175	SER	2.7
1	A	63	ASP	2.5
1	A	236	VAL	2.4
1	A	176	GLY	2.2
1	A	64	ASN	2.1
1	A	86	GLN	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GOL	A	925	6/6	0.86	0.27	14.80	38,46,48,52	0
8	GOL	A	928	6/6	0.84	0.22	11.23	22,52,54,55	0
8	GOL	A	927	6/6	0.89	0.14	3.05	32,46,48,54	0
3	CA	A	912	1/1	0.99	0.10	1.11	23,23,23,23	0
2	HEC	A	911	43/43	0.98	0.10	0.94	20,31,51,56	0
2	HEC	A	904	43/43	0.99	0.10	0.67	7,15,19,23	0
2	HEC	A	907	43/43	0.99	0.09	0.55	6,11,15,17	0
2	HEC	A	910	43/43	0.98	0.10	0.50	14,24,45,54	0
2	HEC	A	908	43/43	0.99	0.10	0.49	3,7,15,19	0
2	HEC	A	909	43/43	0.99	0.09	0.37	7,13,19,23	0
2	HEC	A	902	43/43	0.98	0.09	0.15	13,20,26,32	0
2	HEC	A	901	43/43	0.99	0.09	0.10	7,13,29,35	0
2	HEC	A	906	43/43	0.99	0.09	-0.04	4,11,15,17	0
2	HEC	A	903	43/43	0.99	0.09	-0.13	8,15,23,27	0
2	HEC	A	905	43/43	0.98	0.09	-0.22	18,24,29,33	0
4	MG	A	914	1/1	0.98	0.07	-1.54	17,17,17,17	0
4	MG	A	913	1/1	1.00	0.07	-2.77	10,10,10,10	0
7	NTA	A	924	13/13	0.90	0.20	-	41,46,53,54	0
5	FE	A	915	1/1	0.97	0.04	-	44,44,44,44	0
7	NTA	A	918	13/13	0.87	0.32	-	28,59,64,66	0
5	FE	A	920	1/1	0.99	0.04	-	31,31,31,31	0
6	O	A	922	1/1	0.99	0.09	-	31,31,31,31	0
8	GOL	A	926	6/6	0.88	0.15	-	47,51,53,56	0
7	NTA	A	919	13/13	0.91	0.16	-	35,45,55,57	0
5	FE	A	916	1/1	1.00	0.05	-	40,40,40,40	0
5	FE	A	921	1/1	1.00	0.05	-	28,28,28,28	0
7	NTA	A	923	13/13	0.94	0.09	-	20,29,36,36	0
6	O	A	917	1/1	0.98	0.14	-	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.