Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:37 PM GMT

PDB ID	:	3UFH
Title	:	Crystal structure of UndA with Iron Citrate bound
Authors	:	Edwards, M.J.; Clarke, T.A.
Deposited on	:	2011-11-01
Resolution	:	2.23 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

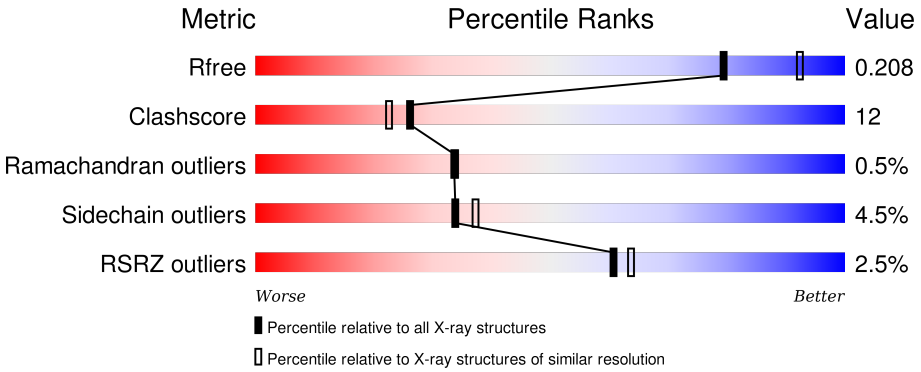
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.23 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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. 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 <=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	2% 77% 12% • 8%

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
6	FLC	A	918	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	FLC	A	919	-	-	-	X
8	GOL	A	922	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7309 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
			Total	C	N	O	S			
1	A	800	5956	3695	1030	1196	35	0	1	0

There are 58 discrepancies between the modelled and reference sequences:

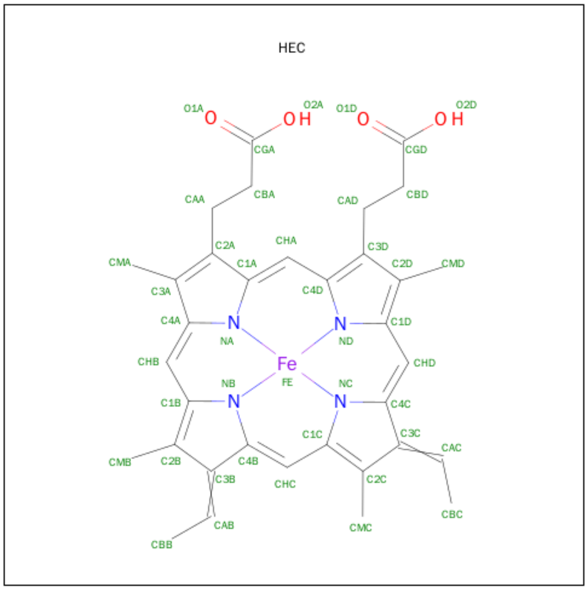
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP F8UWD6
A	1	SER	-	EXPRESSION TAG	UNP F8UWD6
A	2	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	3	LYS	-	EXPRESSION TAG	UNP F8UWD6
A	4	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	5	LEU	-	EXPRESSION TAG	UNP F8UWD6
A	6	SER	-	EXPRESSION TAG	UNP F8UWD6
A	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

Continued on next page...

Continued from previous page...

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	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

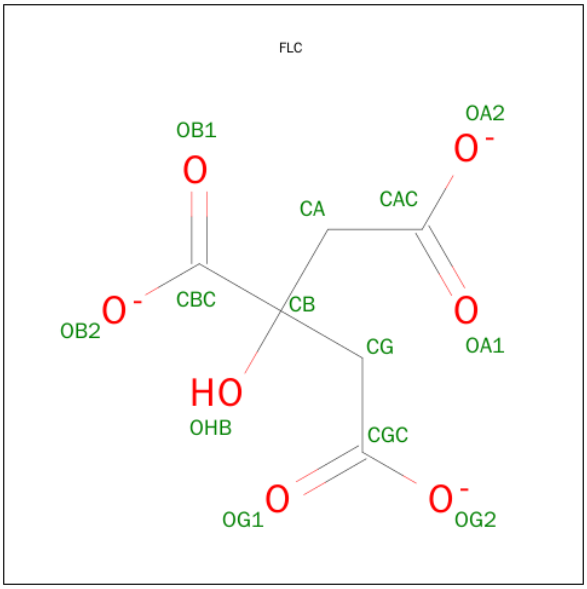
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Fe 3 3	0	0

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

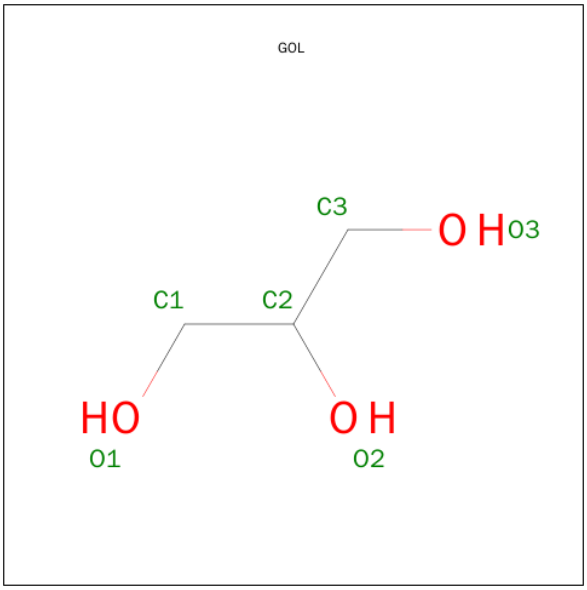


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 6 7	0	0
6	A	1	Total C O 13 6 7	0	0
6	A	1	Total C O 13 6 7	0	0

- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 1 1	0	0

- 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 6 3 3	0	0

- Molecule 9 is water.

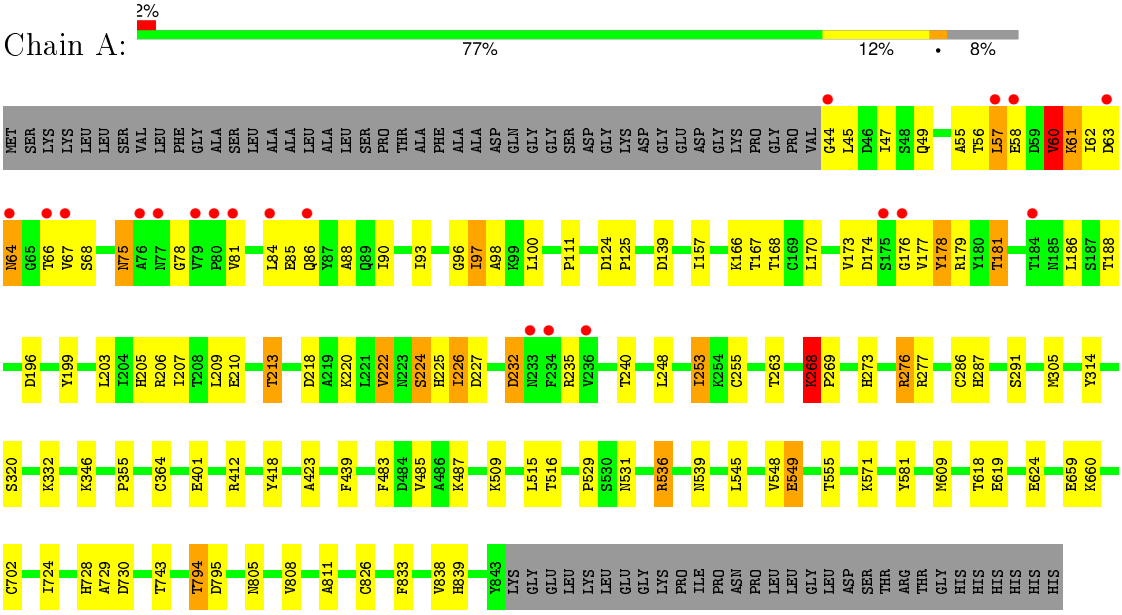
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	828	Total O 828 828	0	0

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: UndA

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.88Å 106.53Å 151.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.63 – 2.23 61.63 – 2.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.63-2.23) 98.9 (61.63-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.163 , 0.211 0.161 , 0.208	Depositor DCC
R_{free} test set	2800 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 55135 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7309	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, MG, CA, O, FE, HEC, FLC

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	0.75	0/6084	0.70	4/8279 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	536	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	536	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	536	ARG	CB-CG-CD	5.35	125.50	111.60
1	A	139	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5956	0	5724	136	0
2	A	473	0	335	51	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
6	A	39	0	12	0	0
7	A	1	0	0	0	0
8	A	6	0	8	0	0
9	A	828	0	0	12	0
All	All	7309	0	6079	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (150) 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:286:CYS:SG	2:A:907:HEC:HAC	1.54	1.47
1:A:826:CYS:SG	2:A:901:HEC:CAC	2.21	1.29
1:A:62:ILE:HG22	1:A:68:SER:H	1.12	1.11
1:A:62:ILE:HG21	1:A:67:VAL:HA	1.35	1.06
1:A:167:THR:HA	1:A:170:LEU:HD12	1.39	1.03
1:A:62:ILE:CG2	1:A:67:VAL:HA	1.88	1.03
1:A:364:CYS:SG	2:A:908:HEC:HAC	1.96	1.02
1:A:702:CYS:SG	2:A:905:HEC:HAC	1.98	1.00
1:A:62:ILE:CG2	1:A:68:SER:H	1.73	1.00
1:A:60:VAL:HA	1:A:61:LYS:HD3	1.45	0.96
1:A:255:CYS:SG	2:A:906:HEC:HAC	2.05	0.94
1:A:210:GLU:OE1	1:A:276:ARG:HD2	1.70	0.91
1:A:62:ILE:HG21	1:A:67:VAL:CA	2.02	0.90
1:A:509:LYS:HE3	1:A:624:GLU:OE2	1.74	0.88
1:A:826:CYS:SG	2:A:901:HEC:HAC	2.13	0.87
1:A:62:ILE:HG22	1:A:68:SER:N	1.89	0.86
1:A:47:ILE:HD12	1:A:81:VAL:HG11	1.56	0.86
1:A:838:VAL:HG11	2:A:911:HEC:C3A	2.07	0.85
1:A:57:LEU:HD13	1:A:209:LEU:HB2	1.61	0.82
1:A:60:VAL:HG12	1:A:61:LYS:H	1.47	0.77
1:A:47:ILE:HD12	1:A:81:VAL:CG1	2.14	0.76
1:A:660:LYS:HE2	9:A:1399:HOH:O	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:CG2	1:A:68:SER:N	2.46	0.73
1:A:364:CYS:SG	2:A:908:HEC:C3C	2.76	0.73
1:A:62:ILE:HG21	1:A:67:VAL:HG13	1.69	0.72
1:A:255:CYS:SG	2:A:906:HEC:C3C	2.77	0.72
1:A:255:CYS:SG	2:A:906:HEC:CBC	2.77	0.72
1:A:702:CYS:SG	2:A:905:HEC:CBC	2.78	0.70
1:A:286:CYS:SG	2:A:907:HEC:C3C	2.79	0.70
1:A:58:GLU:O	1:A:226:ILE:HD13	1.91	0.69
1:A:529:PRO:O	1:A:536:ARG:HD3	1.94	0.68
1:A:838:VAL:HG13	2:A:911:HEC:HAA1	1.76	0.68
1:A:838:VAL:CG1	2:A:911:HEC:C2A	2.72	0.66
1:A:483:PHE:CE2	1:A:485:VAL:HG22	2.30	0.66
1:A:55:ALA:HB3	1:A:222:VAL:HG21	1.77	0.66
2:A:911:HEC:HMA3	2:A:911:HEC:HBA1	1.78	0.66
1:A:60:VAL:CA	1:A:61:LYS:HD3	2.24	0.66
1:A:176:GLY:O	1:A:178:TYR:CD2	2.49	0.65
1:A:60:VAL:HG12	1:A:179:ARG:HH22	1.62	0.65
1:A:62:ILE:HG21	1:A:67:VAL:CG1	2.26	0.64
1:A:702:CYS:SG	2:A:905:HEC:C3C	2.87	0.63
1:A:364:CYS:SG	2:A:908:HEC:CBC	2.84	0.63
1:A:232:ASP:HB3	1:A:235:ARG:HG2	1.81	0.62
1:A:826:CYS:SG	2:A:901:HEC:C3C	2.88	0.62
2:A:908:HEC:HBB3	2:A:908:HEC:HMB1	1.82	0.60
1:A:224:SER:HB3	9:A:1808:HOH:O	2.01	0.59
1:A:60:VAL:HG12	1:A:61:LYS:N	2.17	0.59
2:A:911:HEC:CMA	2:A:911:HEC:HBA1	2.32	0.59
1:A:62:ILE:CG2	1:A:67:VAL:CA	2.69	0.59
1:A:439:PHE:HA	2:A:910:HEC:HMC2	1.85	0.58
1:A:176:GLY:O	1:A:178:TYR:CE2	2.57	0.58
1:A:90:ILE:HD13	1:A:93:ILE:HD11	1.85	0.58
1:A:84:LEU:HB3	1:A:178:TYR:CE1	2.40	0.57
2:A:910:HEC:HBC3	2:A:910:HEC:HMC1	1.86	0.57
1:A:60:VAL:HA	1:A:61:LYS:CD	2.27	0.56
1:A:618:THR:HG22	9:A:1653:HOH:O	2.05	0.56
1:A:826:CYS:SG	2:A:901:HEC:CBC	2.93	0.56
1:A:555:THR:HG21	9:A:1809:HOH:O	2.05	0.56
1:A:100:LEU:HD11	1:A:111:PRO:HB2	1.87	0.56
1:A:97:ILE:HA	1:A:206:ARG:O	2.05	0.56
1:A:186:LEU:HD13	1:A:199:TYR:CD1	2.41	0.56
1:A:838:VAL:CG1	2:A:911:HEC:C3A	2.81	0.56
1:A:808:VAL:CG1	1:A:811:ALA:HB3	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:904:HEC:HMB1	2:A:904:HEC:HBB3	1.87	0.56
1:A:286:CYS:CB	2:A:907:HEC:HAC	2.35	0.55
1:A:838:VAL:HG11	2:A:911:HEC:CMA	2.37	0.55
2:A:901:HEC:HBC3	2:A:901:HEC:HMC1	1.87	0.55
2:A:909:HEC:HMC1	2:A:909:HEC:HBC3	1.89	0.55
1:A:205:HIS:O	1:A:227:ASP:HA	2.07	0.54
1:A:232:ASP:N	9:A:1784:HOH:O	2.41	0.54
2:A:908:HEC:HMC1	2:A:908:HEC:HBC3	1.90	0.53
1:A:248:LEU:HG	1:A:253:ILE:CD1	2.38	0.53
1:A:174:ASP:HB3	1:A:177:VAL:HB	1.92	0.52
1:A:305:MET:HG3	1:A:314:TYR:CZ	2.45	0.52
1:A:176:GLY:O	1:A:178:TYR:HD2	1.91	0.52
1:A:808:VAL:CG1	1:A:811:ALA:CB	2.88	0.52
1:A:60:VAL:CG1	1:A:179:ARG:HH22	2.22	0.52
1:A:808:VAL:HG13	1:A:811:ALA:HB2	1.91	0.52
1:A:483:PHE:CD2	1:A:485:VAL:HG22	2.45	0.52
1:A:68:SER:HB3	1:A:181:THR:HG23	1.90	0.51
1:A:838:VAL:HG11	2:A:911:HEC:C2A	2.40	0.51
1:A:62:ILE:CB	1:A:67:VAL:HA	2.40	0.51
1:A:203:LEU:O	1:A:205:HIS:ND1	2.40	0.51
1:A:286:CYS:CB	2:A:907:HEC:CAC	2.89	0.51
1:A:833:PHE:CE1	2:A:901:HEC:HBD1	2.46	0.50
1:A:62:ILE:HB	1:A:66:THR:O	2.11	0.50
1:A:178:TYR:N	1:A:178:TYR:CD2	2.79	0.50
1:A:84:LEU:HB3	1:A:178:TYR:CZ	2.46	0.50
1:A:743:THR:HB	2:A:906:HEC:HBD1	1.92	0.49
1:A:60:VAL:HA	1:A:61:LYS:HZ2	1.78	0.49
1:A:364:CYS:CB	2:A:908:HEC:C3C	2.91	0.49
1:A:838:VAL:HG11	2:A:911:HEC:HMA2	1.94	0.49
1:A:609:MET:CE	1:A:609:MET:HA	2.43	0.49
1:A:49:GLN:NE2	9:A:1520:HOH:O	2.28	0.48
1:A:839:HIS:CD2	2:A:911:HEC:ND	2.81	0.48
1:A:57:LEU:HD21	1:A:225:HIS:HA	1.95	0.48
2:A:905:HEC:HBC3	2:A:905:HEC:HMC1	1.94	0.48
1:A:268:LYS:N	1:A:269:PRO:CD	2.77	0.47
1:A:186:LEU:HD13	1:A:199:TYR:HD1	1.79	0.47
1:A:60:VAL:HG13	1:A:61:LYS:NZ	2.30	0.47
1:A:124:ASP:C	1:A:124:ASP:OD1	2.51	0.47
2:A:911:HEC:HBB3	2:A:911:HEC:HMB1	1.96	0.47
1:A:100:LEU:CD1	1:A:111:PRO:HB2	2.44	0.47
1:A:531:ASN:HA	1:A:536:ARG:HG3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:O	1:A:548:VAL:HG23	2.16	0.46
1:A:401:GLU:CD	1:A:401:GLU:H	2.18	0.46
2:A:906:HEC:HBD1	9:A:1722:HOH:O	2.14	0.46
1:A:44:GLY:HA2	1:A:45:LEU:HA	1.69	0.46
1:A:62:ILE:HG21	1:A:67:VAL:CB	2.46	0.45
1:A:724:ILE:HG23	1:A:728:HIS:CE1	2.51	0.45
1:A:255:CYS:HG	2:A:906:HEC:HAC	1.77	0.45
1:A:332:LYS:HE2	9:A:1248:HOH:O	2.16	0.44
1:A:286:CYS:CB	2:A:907:HEC:C3C	2.94	0.44
1:A:571:LYS:HD2	9:A:1820:HOH:O	2.17	0.44
1:A:235:ARG:O	1:A:235:ARG:HG3	2.17	0.44
2:A:903:HEC:HBC3	2:A:903:HEC:HMC1	2.00	0.43
1:A:287:HIS:HE1	2:A:907:HEC:NA	2.12	0.43
1:A:255:CYS:HG	2:A:906:HEC:CAC	2.23	0.43
1:A:170:LEU:HA	1:A:179:ARG:O	2.18	0.43
1:A:273:HIS:HB2	1:A:277:ARG:HD2	2.00	0.43
1:A:57:LEU:O	1:A:57:LEU:HG	2.19	0.43
1:A:418:TYR:CE1	1:A:423:ALA:HA	2.53	0.43
1:A:88:ALA:C	9:A:1677:HOH:O	2.57	0.43
1:A:355:PRO:HD3	2:A:903:HEC:HMD3	2.00	0.42
1:A:173:VAL:CG1	1:A:173:VAL:O	2.67	0.42
1:A:196:ASP:C	1:A:196:ASP:OD2	2.58	0.42
2:A:905:HEC:HBA2	2:A:905:HEC:CMA	2.49	0.42
1:A:60:VAL:C	1:A:61:LYS:HD3	2.39	0.42
1:A:516:THR:HA	1:A:539:ASN:O	2.20	0.42
1:A:57:LEU:HD22	1:A:224:SER:HB2	2.02	0.42
1:A:549:GLU:H	1:A:549:GLU:CD	2.21	0.42
1:A:659:GLU:HG2	1:A:660:LYS:HG3	2.01	0.42
1:A:332:LYS:HE2	9:A:1472:HOH:O	2.19	0.42
1:A:794:THR:HG22	1:A:795:ASP:N	2.34	0.42
2:A:901:HEC:HMB1	2:A:901:HEC:HBB3	2.02	0.42
1:A:213:THR:OG1	1:A:220:LYS:HE2	2.19	0.42
1:A:805:ASN:OD1	2:A:901:HEC:HMC2	2.20	0.41
1:A:57:LEU:HD21	1:A:225:HIS:CA	2.50	0.41
1:A:487:LYS:HE3	9:A:1736:HOH:O	2.19	0.41
1:A:97:ILE:HG13	1:A:98:ALA:N	2.34	0.41
1:A:724:ILE:HG13	2:A:902:HEC:HMD2	2.03	0.41
1:A:124:ASP:HA	1:A:125:PRO:HD3	1.93	0.41
1:A:96:GLY:O	1:A:207:ILE:HA	2.20	0.41
1:A:808:VAL:HG13	1:A:811:ALA:CB	2.50	0.41
1:A:63:ASP:O	1:A:64:ASN:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:NH1	2:A:910:HEC:HMA2	2.37	0.40
1:A:157:ILE:O	1:A:291:SER:HA	2.22	0.40
1:A:75:ASN:HB3	1:A:78:GLY:H	1.86	0.40
1:A:729:ALA:O	1:A:730[B]:ASP:HB2	2.22	0.40
1:A:167:THR:O	1:A:170:LEU:N	2.39	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	799/874 (91%)	755 (94%)	40 (5%)	4 (0%)	34 34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	168	THR
1	A	218	ASP
1	A	268	LYS

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	645/700 (92%)	616 (96%)	29 (4%)	34 37

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	57	LEU
1	A	61	LYS
1	A	64	ASN
1	A	75	ASN
1	A	85	GLU
1	A	86	GLN
1	A	97	ILE
1	A	166	LYS
1	A	178	TYR
1	A	181	THR
1	A	188	THR
1	A	213	THR
1	A	222	VAL
1	A	224	SER
1	A	226	ILE
1	A	232	ASP
1	A	240	THR
1	A	253	ILE
1	A	263	THR
1	A	268	LYS
1	A	276	ARG
1	A	320	SER
1	A	346	LYS
1	A	515	LEU
1	A	549	GLU
1	A	581	TYR
1	A	619	GLU
1	A	794	THR

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 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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	24,50,50	2.24	4 (16%)	19,82,82	3.00	10 (52%)
2	HEC	A	902	1	24,50,50	2.32	6 (25%)	19,82,82	2.90	6 (31%)
2	HEC	A	903	1	24,50,50	2.31	6 (25%)	19,82,82	2.90	6 (31%)
2	HEC	A	904	1	24,50,50	2.39	7 (29%)	19,82,82	2.71	6 (31%)
2	HEC	A	905	1,3	24,50,50	2.67	9 (37%)	19,82,82	3.04	8 (42%)
2	HEC	A	906	1	24,50,50	2.27	6 (25%)	19,82,82	2.17	7 (36%)
2	HEC	A	907	1,4	24,50,50	2.20	5 (20%)	19,82,82	2.85	7 (36%)
2	HEC	A	908	1	24,50,50	2.19	6 (25%)	19,82,82	2.58	6 (31%)
2	HEC	A	909	1	24,50,50	2.39	3 (12%)	19,82,82	2.85	7 (36%)
2	HEC	A	910	1	24,50,50	2.28	3 (12%)	19,82,82	2.67	6 (31%)
2	HEC	A	911	1	24,50,50	2.33	6 (25%)	19,82,82	2.73	6 (31%)
6	FLC	A	918	5	3,12,12	0.19	0	3,17,17	1.36	0
6	FLC	A	919	5	3,12,12	0.36	0	3,17,17	1.21	0
6	FLC	A	920	5	3,12,12	0.65	0	3,17,17	1.38	0
8	GOL	A	922	-	5,5,5	0.56	0	5,5,5	0.74	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	-	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	1,3	-	0/6/54/54	0/0/8/8
2	HEC	A	906	1	-	0/6/54/54	0/0/8/8
2	HEC	A	907	1,4	-	0/6/54/54	0/0/8/8
2	HEC	A	908	1	-	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
6	FLC	A	918	5	-	0/6/16/16	0/0/0/0
6	FLC	A	919	5	-	0/6/16/16	0/0/0/0
6	FLC	A	920	5	-	0/6/16/16	0/0/0/0
8	GOL	A	922	-	-	0/4/4/4	0/0/0/0

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	905	HEC	C3B-C2B	-7.31	1.33	1.40
2	A	909	HEC	C3B-C2B	-6.84	1.33	1.40
2	A	903	HEC	C3C-C2C	-6.63	1.33	1.40
2	A	904	HEC	C3B-C2B	-6.12	1.34	1.40
2	A	909	HEC	C3C-C2C	-5.99	1.34	1.40
2	A	905	HEC	C3C-C2C	-5.99	1.34	1.40
2	A	910	HEC	C3C-C2C	-5.96	1.34	1.40
2	A	911	HEC	C3C-C2C	-5.94	1.34	1.40
2	A	910	HEC	C3B-C2B	-5.84	1.34	1.40
2	A	902	HEC	C3C-C2C	-5.71	1.34	1.40
2	A	908	HEC	C3B-C2B	-5.71	1.34	1.40
2	A	906	HEC	C3B-C2B	-5.71	1.34	1.40
2	A	902	HEC	C3B-C2B	-5.70	1.34	1.40
2	A	901	HEC	C3B-C2B	-5.46	1.35	1.40
2	A	907	HEC	C3B-C2B	-5.43	1.35	1.40
2	A	911	HEC	C3B-C2B	-5.32	1.35	1.40
2	A	904	HEC	C3C-C2C	-5.23	1.35	1.40
2	A	908	HEC	C3C-C2C	-5.18	1.35	1.40
2	A	903	HEC	C3B-C2B	-5.17	1.35	1.40
2	A	907	HEC	C3C-C2C	-5.16	1.35	1.40
2	A	901	HEC	C3C-C2C	-5.10	1.35	1.40
2	A	906	HEC	C3C-C2C	-4.87	1.35	1.40
2	A	911	HEC	CMB-C2B	2.01	1.56	1.51
2	A	906	HEC	CMB-C2B	2.04	1.56	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	HEC	CMC-C2C	2.05	1.56	1.51
2	A	901	HEC	CMA-C3A	2.06	1.56	1.51
2	A	907	HEC	CMA-C3A	2.10	1.56	1.51
2	A	908	HEC	CMB-C2B	2.11	1.56	1.51
2	A	911	HEC	C4B-NB	2.13	1.39	1.36
2	A	903	HEC	CAA-C2A	2.14	1.56	1.52
2	A	908	HEC	CMC-C2C	2.16	1.56	1.51
2	A	904	HEC	CMC-C2C	2.20	1.56	1.51
2	A	904	HEC	C4B-NB	2.23	1.39	1.36
2	A	906	HEC	C4A-NA	2.27	1.39	1.36
2	A	903	HEC	C4B-NB	2.29	1.39	1.36
2	A	907	HEC	CAD-C3D	2.31	1.56	1.52
2	A	908	HEC	CAA-C2A	2.39	1.56	1.52
2	A	911	HEC	CAD-C3D	2.45	1.56	1.52
2	A	902	HEC	C4C-NC	2.45	1.40	1.36
2	A	903	HEC	CMC-C2C	2.49	1.57	1.51
2	A	902	HEC	C4A-NA	2.53	1.40	1.36
2	A	905	HEC	CMC-C2C	2.56	1.57	1.51
2	A	904	HEC	CBC-CAC	2.63	1.60	1.49
2	A	906	HEC	C4B-NB	2.65	1.40	1.36
2	A	905	HEC	CMB-C2B	2.65	1.57	1.51
2	A	905	HEC	CAA-C2A	2.83	1.57	1.52
2	A	905	HEC	CAD-C3D	2.85	1.56	1.52
2	A	905	HEC	CMA-C3A	2.86	1.57	1.51
2	A	904	HEC	CMA-C3A	2.94	1.58	1.51
2	A	905	HEC	C1A-NA	3.22	1.41	1.36
2	A	905	HEC	C3D-C2D	4.24	1.50	1.37
2	A	908	HEC	C3D-C2D	4.40	1.50	1.37
2	A	903	HEC	C3D-C2D	4.54	1.51	1.37
2	A	902	HEC	C3D-C2D	4.63	1.51	1.37
2	A	909	HEC	C3D-C2D	4.80	1.51	1.37
2	A	907	HEC	C3D-C2D	4.89	1.52	1.37
2	A	904	HEC	C3D-C2D	4.92	1.52	1.37
2	A	906	HEC	C3D-C2D	5.07	1.52	1.37
2	A	911	HEC	C3D-C2D	5.14	1.52	1.37
2	A	910	HEC	C3D-C2D	5.17	1.53	1.37
2	A	901	HEC	C3D-C2D	5.44	1.53	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	HEC	CBB-CAB-C3B	-7.98	109.61	127.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	909	HEC	CBB-CAB-C3B	-7.47	110.74	127.35
2	A	907	HEC	CBB-CAB-C3B	-7.17	111.41	127.35
2	A	905	HEC	CBC-CAC-C3C	-7.10	111.58	127.35
2	A	910	HEC	CBC-CAC-C3C	-7.09	111.59	127.35
2	A	904	HEC	CBB-CAB-C3B	-7.06	111.67	127.35
2	A	905	HEC	CBB-CAB-C3B	-6.81	112.21	127.35
2	A	903	HEC	CBC-CAC-C3C	-6.73	112.40	127.35
2	A	902	HEC	CBB-CAB-C3B	-6.63	112.63	127.35
2	A	904	HEC	CBC-CAC-C3C	-6.57	112.74	127.35
2	A	903	HEC	CBB-CAB-C3B	-6.54	112.82	127.35
2	A	902	HEC	CBA-CAA-C2A	-6.40	101.05	112.53
2	A	911	HEC	CBC-CAC-C3C	-6.16	113.66	127.35
2	A	909	HEC	CBC-CAC-C3C	-6.16	113.67	127.35
2	A	907	HEC	CBC-CAC-C3C	-6.09	113.82	127.35
2	A	911	HEC	CBB-CAB-C3B	-6.02	113.97	127.35
2	A	910	HEC	CBB-CAB-C3B	-5.86	114.32	127.35
2	A	901	HEC	CBC-CAC-C3C	-5.85	114.36	127.35
2	A	908	HEC	CBC-CAC-C3C	-5.71	114.66	127.35
2	A	908	HEC	CAD-CBD-CGD	-5.42	102.82	112.75
2	A	908	HEC	CBB-CAB-C3B	-5.40	115.35	127.35
2	A	902	HEC	CBC-CAC-C3C	-5.18	115.84	127.35
2	A	906	HEC	CBC-CAC-C3C	-4.90	116.47	127.35
2	A	911	HEC	CMC-C2C-C1C	-4.88	120.28	128.36
2	A	909	HEC	CMC-C2C-C1C	-4.53	120.87	128.36
2	A	905	HEC	CAA-C2A-C1A	-4.43	122.20	127.01
2	A	907	HEC	CAA-C2A-C1A	-4.34	122.30	127.01
2	A	911	HEC	CBD-CAD-C3D	-4.29	104.85	112.53
2	A	906	HEC	CBB-CAB-C3B	-4.24	117.92	127.35
2	A	903	HEC	CBD-CAD-C3D	-4.16	105.08	112.53
2	A	904	HEC	CMC-C2C-C1C	-4.14	121.51	128.36
2	A	901	HEC	CBA-CAA-C2A	-4.06	105.25	112.53
2	A	906	HEC	CMC-C2C-C1C	-4.03	121.69	128.36
2	A	902	HEC	CBD-CAD-C3D	-3.96	105.42	112.53
2	A	903	HEC	CMC-C2C-C1C	-3.90	121.91	128.36
2	A	903	HEC	CAA-CBA-CGA	-3.89	105.61	112.75
2	A	909	HEC	CBD-CAD-C3D	-3.79	105.74	112.53
2	A	903	HEC	CMB-C2B-C1B	-3.70	122.24	128.36
2	A	901	HEC	CMC-C2C-C1C	-3.64	122.34	128.36
2	A	910	HEC	CMC-C2C-C1C	-3.57	122.46	128.36
2	A	910	HEC	CAD-CBD-CGD	-3.55	106.24	112.75
2	A	908	HEC	CMC-C2C-C1C	-3.32	122.88	128.36
2	A	907	HEC	CMC-C2C-C1C	-3.32	122.88	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	905	HEC	CBA-CAA-C2A	-3.08	107.01	112.53
2	A	901	HEC	CAA-CBA-CGA	-3.02	107.22	112.75
2	A	910	HEC	CMB-C2B-C1B	-2.98	123.43	128.36
2	A	905	HEC	CMC-C2C-C1C	-2.94	123.49	128.36
2	A	901	HEC	CAA-C2A-C1A	-2.89	123.87	127.01
2	A	906	HEC	CAA-CBA-CGA	-2.80	107.61	112.75
2	A	902	HEC	CMB-C2B-C1B	-2.75	123.81	128.36
2	A	901	HEC	CMB-C2B-C1B	-2.73	123.84	128.36
2	A	907	HEC	CBD-CAD-C3D	-2.72	107.65	112.53
2	A	908	HEC	CMB-C2B-C1B	-2.47	124.28	128.36
2	A	909	HEC	CBA-CAA-C2A	-2.44	108.16	112.53
2	A	911	HEC	CAA-C2A-C1A	-2.42	124.39	127.01
2	A	902	HEC	CMC-C2C-C1C	-2.41	124.38	128.36
2	A	909	HEC	CAD-CBD-CGD	-2.37	108.41	112.75
2	A	906	HEC	CMB-C2B-C1B	-2.33	124.51	128.36
2	A	901	HEC	CBD-CAD-C3D	-2.30	108.40	112.53
2	A	909	HEC	CMB-C2B-C1B	-2.27	124.61	128.36
2	A	906	HEC	CBA-CAA-C2A	-2.23	108.52	112.53
2	A	904	HEC	CAA-C2A-C1A	-2.23	124.58	127.01
2	A	904	HEC	CBA-CAA-C2A	-2.21	108.56	112.53
2	A	910	HEC	CBD-CAD-C3D	-2.21	108.56	112.53
2	A	907	HEC	CBA-CAA-C2A	-2.19	108.59	112.53
2	A	905	HEC	CAD-C3D-C2D	-2.06	123.13	129.00
2	A	901	HEC	CMD-C2D-C1D	-2.02	125.03	128.36
2	A	911	HEC	CAD-C3D-C4D	2.13	129.32	127.01
2	A	904	HEC	CAD-C3D-C4D	2.15	129.34	127.01
2	A	901	HEC	CMD-C2D-C3D	2.16	129.75	125.24
2	A	906	HEC	CAD-C3D-C4D	2.20	129.40	127.01
2	A	907	HEC	CAD-C3D-C4D	2.24	129.44	127.01
2	A	908	HEC	CAD-C3D-C4D	2.25	129.45	127.01
2	A	905	HEC	C4B-C3B-C2B	2.88	109.46	106.35
2	A	905	HEC	CAD-C3D-C4D	4.17	131.53	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEC	8	0
2	A	902	HEC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	HEC	2	0
2	A	904	HEC	1	0
2	A	905	HEC	5	0
2	A	906	HEC	7	0
2	A	907	HEC	6	0
2	A	908	HEC	6	0
2	A	909	HEC	1	0
2	A	910	HEC	3	0
2	A	911	HEC	11	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^{th} 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%)	-0.22	20 (2%) 61 64	11, 31, 67, 88	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	VAL	4.7
1	A	175	SER	4.3
1	A	57	LEU	3.8
1	A	63	ASP	3.5
1	A	44	GLY	3.2
1	A	64	ASN	3.1
1	A	58	GLU	3.1
1	A	81	VAL	2.9
1	A	233	ASN	2.5
1	A	67	VAL	2.5
1	A	66	THR	2.4
1	A	236	VAL	2.4
1	A	176	GLY	2.3
1	A	84	LEU	2.3
1	A	184	THR	2.2
1	A	77	ASN	2.2
1	A	76	ALA	2.2
1	A	234	PHE	2.2
1	A	86	GLN	2.0
1	A	80	PRO	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 (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^{th} 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^2)	Q<0.9
6	FLC	A	918	13/13	0.93	0.17	8.30	39,40,50,50	0
8	GOL	A	922	6/6	0.94	0.14	4.25	26,32,42,43	0
6	FLC	A	919	13/13	0.91	0.14	3.95	39,40,48,48	0
2	HEC	A	906	43/43	0.99	0.12	1.18	14,22,42,46	0
2	HEC	A	905	43/43	0.99	0.12	0.97	4,11,18,27	0
2	HEC	A	901	43/43	0.97	0.12	0.55	25,42,54,64	0
2	HEC	A	909	43/43	0.99	0.12	0.54	13,21,27,41	0
2	HEC	A	910	43/43	0.98	0.11	0.43	23,32,40,43	0
2	HEC	A	911	43/43	0.98	0.11	0.24	18,33,61,69	0
2	HEC	A	903	43/43	0.99	0.11	0.19	11,17,23,24	0
2	HEC	A	902	43/43	0.99	0.10	0.14	11,21,28,34	0
2	HEC	A	908	43/43	0.99	0.10	0.05	15,21,34,39	0
2	HEC	A	904	43/43	0.99	0.11	-0.06	8,15,21,24	0
2	HEC	A	907	43/43	0.98	0.11	-0.18	21,31,39,43	0
3	MG	A	914	1/1	1.00	0.10	-1.54	17,17,17,17	0
3	MG	A	912	1/1	0.97	0.05	-4.36	23,23,23,23	0
4	CA	A	913	1/1	0.99	0.08	-6.43	33,33,33,33	0
6	FLC	A	920	13/13	0.86	0.18	-	55,65,67,70	0
7	O	A	921	1/1	0.97	0.31	-	61,61,61,61	0
5	FE	A	915	1/1	0.98	0.07	-	53,53,53,53	0
5	FE	A	917	1/1	0.96	0.06	-	44,44,44,44	0
5	FE	A	916	1/1	0.99	0.05	-	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.