Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 12:46 PM EDT

PDB ID	:	3KMV
Title	:	Crystal structure of CBM42A from Clostridium thermocellum
Authors	:	Santos-Silva, T.; Alves, V.D.; Prates, J.A.M.; Fontes, C.M.G.A.; Romao, M.J.
Deposited on	:	2009-11-11
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

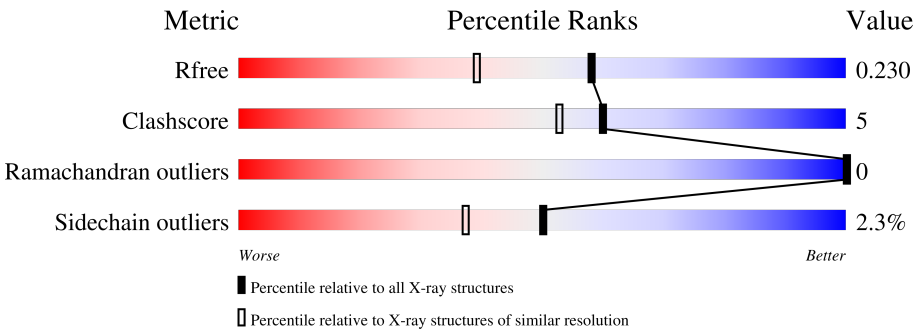
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Mol	Chain	Length	Quality of chain
1	A	157	77% 8% • 13%
1	B	157	76% 10% • 12%
1	C	157	78% 8% •• 13%
1	D	157	78% 9% • 12%
1	E	157	73% 12% • • 11%
1	F	157	78% 8% • 13%
1	G	157	79% 8% • 12%

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Mol	Chain	Length	Quality of chain
1	H	157	80% 8% • 11%

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	GOL	H	158	-	-	X	-
3	FMT	F	159	-	-	X	-
5	ACT	G	158	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10306 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 Alpha-L-arabinofuranosidase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	136	1163	748	188	225	2	0	9	0
1	B	138	1185	760	191	232	2	0	10	0
1	C	137	1154	739	190	223	2	0	5	0
1	D	138	1172	752	190	227	3	0	7	0
1	E	140	1194	766	194	231	3	0	8	0
1	F	137	1148	735	186	225	2	0	5	0
1	G	138	1171	751	190	228	2	0	7	0
1	H	139	1151	737	187	225	2	0	2	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A3DBC8
A	2	ALA	-	expression tag	UNP A3DBC8
A	3	SER	-	expression tag	UNP A3DBC8
A	150	LEU	-	expression tag	UNP A3DBC8
A	151	GLU	-	expression tag	UNP A3DBC8
A	152	HIS	-	expression tag	UNP A3DBC8
A	153	HIS	-	expression tag	UNP A3DBC8
A	154	HIS	-	expression tag	UNP A3DBC8
A	155	HIS	-	expression tag	UNP A3DBC8
A	156	HIS	-	expression tag	UNP A3DBC8
A	157	HIS	-	expression tag	UNP A3DBC8
B	1	MET	-	expression tag	UNP A3DBC8
B	2	ALA	-	expression tag	UNP A3DBC8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	SER	-	expression tag	UNP A3DBC8
B	150	LEU	-	expression tag	UNP A3DBC8
B	151	GLU	-	expression tag	UNP A3DBC8
B	152	HIS	-	expression tag	UNP A3DBC8
B	153	HIS	-	expression tag	UNP A3DBC8
B	154	HIS	-	expression tag	UNP A3DBC8
B	155	HIS	-	expression tag	UNP A3DBC8
B	156	HIS	-	expression tag	UNP A3DBC8
B	157	HIS	-	expression tag	UNP A3DBC8
C	1	MET	-	expression tag	UNP A3DBC8
C	2	ALA	-	expression tag	UNP A3DBC8
C	3	SER	-	expression tag	UNP A3DBC8
C	150	LEU	-	expression tag	UNP A3DBC8
C	151	GLU	-	expression tag	UNP A3DBC8
C	152	HIS	-	expression tag	UNP A3DBC8
C	153	HIS	-	expression tag	UNP A3DBC8
C	154	HIS	-	expression tag	UNP A3DBC8
C	155	HIS	-	expression tag	UNP A3DBC8
C	156	HIS	-	expression tag	UNP A3DBC8
C	157	HIS	-	expression tag	UNP A3DBC8
D	1	MET	-	expression tag	UNP A3DBC8
D	2	ALA	-	expression tag	UNP A3DBC8
D	3	SER	-	expression tag	UNP A3DBC8
D	150	LEU	-	expression tag	UNP A3DBC8
D	151	GLU	-	expression tag	UNP A3DBC8
D	152	HIS	-	expression tag	UNP A3DBC8
D	153	HIS	-	expression tag	UNP A3DBC8
D	154	HIS	-	expression tag	UNP A3DBC8
D	155	HIS	-	expression tag	UNP A3DBC8
D	156	HIS	-	expression tag	UNP A3DBC8
D	157	HIS	-	expression tag	UNP A3DBC8
E	1	MET	-	expression tag	UNP A3DBC8
E	2	ALA	-	expression tag	UNP A3DBC8
E	3	SER	-	expression tag	UNP A3DBC8
E	150	LEU	-	expression tag	UNP A3DBC8
E	151	GLU	-	expression tag	UNP A3DBC8
E	152	HIS	-	expression tag	UNP A3DBC8
E	153	HIS	-	expression tag	UNP A3DBC8
E	154	HIS	-	expression tag	UNP A3DBC8
E	155	HIS	-	expression tag	UNP A3DBC8
E	156	HIS	-	expression tag	UNP A3DBC8
E	157	HIS	-	expression tag	UNP A3DBC8

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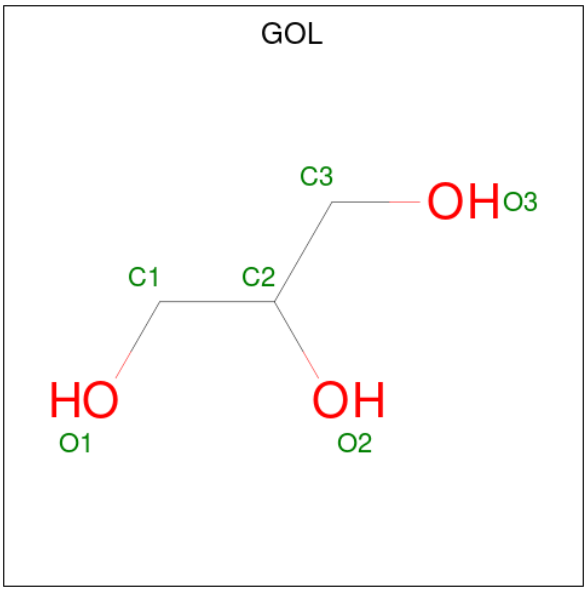
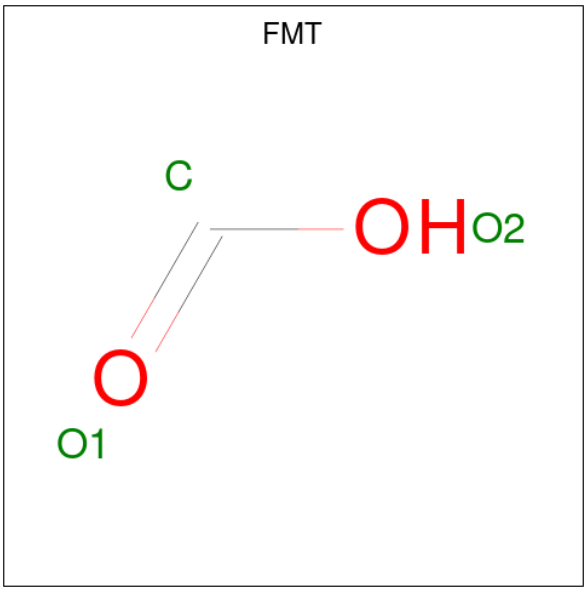
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP A3DBC8
F	2	ALA	-	expression tag	UNP A3DBC8
F	3	SER	-	expression tag	UNP A3DBC8
F	150	LEU	-	expression tag	UNP A3DBC8
F	151	GLU	-	expression tag	UNP A3DBC8
F	152	HIS	-	expression tag	UNP A3DBC8
F	153	HIS	-	expression tag	UNP A3DBC8
F	154	HIS	-	expression tag	UNP A3DBC8
F	155	HIS	-	expression tag	UNP A3DBC8
F	156	HIS	-	expression tag	UNP A3DBC8
F	157	HIS	-	expression tag	UNP A3DBC8
G	1	MET	-	expression tag	UNP A3DBC8
G	2	ALA	-	expression tag	UNP A3DBC8
G	3	SER	-	expression tag	UNP A3DBC8
G	150	LEU	-	expression tag	UNP A3DBC8
G	151	GLU	-	expression tag	UNP A3DBC8
G	152	HIS	-	expression tag	UNP A3DBC8
G	153	HIS	-	expression tag	UNP A3DBC8
G	154	HIS	-	expression tag	UNP A3DBC8
G	155	HIS	-	expression tag	UNP A3DBC8
G	156	HIS	-	expression tag	UNP A3DBC8
G	157	HIS	-	expression tag	UNP A3DBC8
H	1	MET	-	expression tag	UNP A3DBC8
H	2	ALA	-	expression tag	UNP A3DBC8
H	3	SER	-	expression tag	UNP A3DBC8
H	150	LEU	-	expression tag	UNP A3DBC8
H	151	GLU	-	expression tag	UNP A3DBC8
H	152	HIS	-	expression tag	UNP A3DBC8
H	153	HIS	-	expression tag	UNP A3DBC8
H	154	HIS	-	expression tag	UNP A3DBC8
H	155	HIS	-	expression tag	UNP A3DBC8
H	156	HIS	-	expression tag	UNP A3DBC8
H	157	HIS	-	expression tag	UNP A3DBC8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	6	3	3	0	0
2	C	1	6	3	3	0	0
2	D	1	6	3	3	0	0
2	E	1	6	3	3	0	0
2	F	1	6	3	3	0	0
2	H	1	6	3	3	0	0

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	A	1	3	1	2		0	0
			Total	C	O			
3	B	1	3	1	2		0	0
			Total	C	O			
3	B	1	3	1	2		0	0
			Total	C	O			
3	B	1	3	1	2		0	0
			Total	C	O			
3	B	1	3	1	2		0	0
			Total	C	O			
3	C	1	3	1	2		0	0
			Total	C	O			
3	C	1	3	1	2		0	0
			Total	C	O			
3	C	1	3	1	2		0	0
			Total	C	O			
3	C	1	3	1	2		0	0
			Total	C	O			
3	E	1	3	1	2		0	0
			Total	C	O			
3	E	1	3	1	2		0	0

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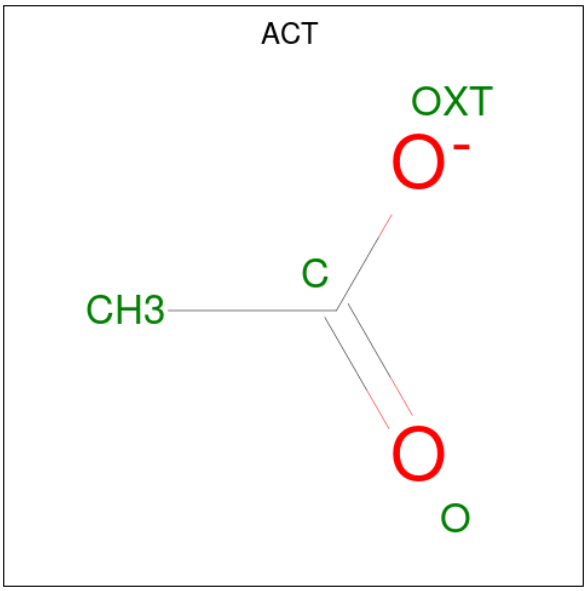
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

- 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
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	G	1	4	2	2	0	0

- Molecule 6 is water.

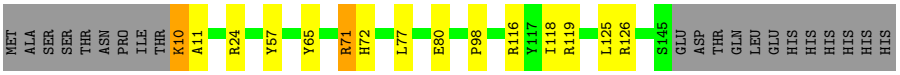
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	137	137	137	0	0
6	B	128	128	128	0	0
6	C	131	131	131	0	0
6	D	104	104	104	0	0
6	E	86	86	86	0	0
6	F	82	82	82	0	0
6	G	108	108	108	0	0
6	H	87	87	87	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Alpha-L-arabinofuranosidase B

Chain A:

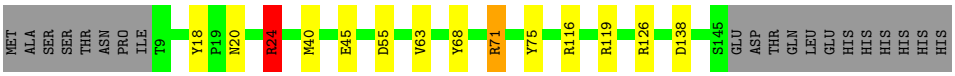


• Molecule 1: Alpha-L-arabinofuranosidase B

Chain B:

• Molecule 1: Alpha-L-arabinofuranosidase B

Chain C:

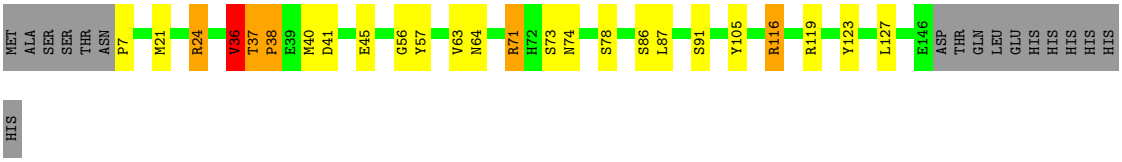


• Molecule 1: Alpha-L-arabinofuranosidase B

Chain D:

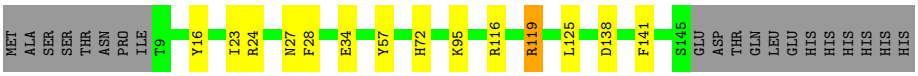
• Molecule 1: Alpha-L-arabinofuranosidase B

Chain E:



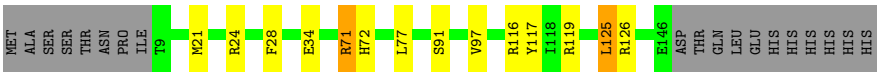
• Molecule 1: Alpha-L-arabinofuranosidase B

Chain F:



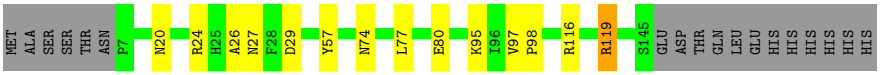
- Molecule 1: Alpha-L-arabinofuranosidase B

Chain G:



- Molecule 1: Alpha-L-arabinofuranosidase B

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	106.37Å 106.37Å 237.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.22 – 1.80 44.15 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.22-1.80) 99.9 (44.15-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.192 0.207 , 0.230	Depositor DCC
R_{free} test set	7239 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10306	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1479e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CA, FMT, ACT

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	1.37	2/1221 (0.2%)	1.14	2/1660 (0.1%)
1	B	1.42	6/1246 (0.5%)	1.14	4/1693 (0.2%)
1	C	1.34	2/1200 (0.2%)	1.13	6/1631 (0.4%)
1	D	1.32	3/1224 (0.2%)	1.09	5/1663 (0.3%)
1	E	1.30	5/1250 (0.4%)	1.11	6/1697 (0.4%)
1	F	1.27	3/1194 (0.3%)	1.06	2/1624 (0.1%)
1	G	1.31	3/1223 (0.2%)	1.12	4/1662 (0.2%)
1	H	1.24	2/1189 (0.2%)	1.07	6/1617 (0.4%)
All	All	1.32	26/9747 (0.3%)	1.11	35/13247 (0.3%)

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	E	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	56	GLY	C-O	9.10	1.38	1.23
1	D	119	ARG	CG-CD	6.85	1.69	1.51
1	E	38	PRO	N-CD	6.48	1.56	1.47
1	D	56	GLY	C-O	6.44	1.33	1.23
1	H	80	GLU	CD-OE2	6.13	1.32	1.25
1	B	108	PHE	CD1-CE1	6.07	1.51	1.39
1	G	117	TYR	CD2-CE2	6.05	1.48	1.39
1	F	119	ARG	CG-CD	6.01	1.67	1.51
1	H	119	ARG	CG-CD	5.93	1.66	1.51
1	D	94	PHE	CE2-CZ	5.83	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	141	PHE	CE2-CZ	5.67	1.48	1.37
1	B	119	ARG	CZ-NH1	5.65	1.40	1.33
1	G	28	PHE	CE2-CZ	5.52	1.47	1.37
1	F	16	TYR	CG-CD2	5.45	1.46	1.39
1	E	105	TYR	CD1-CE1	5.43	1.47	1.39
1	A	57	TYR	CD1-CE1	5.42	1.47	1.39
1	E	78	SER	CB-OG	-5.38	1.35	1.42
1	B	13	PHE	CD1-CE1	5.29	1.49	1.39
1	A	65	TYR	CG-CD1	5.27	1.46	1.39
1	G	97	VAL	CB-CG1	5.19	1.63	1.52
1	B	80	GLU	CD-OE1	5.17	1.31	1.25
1	E	36	VAL	CA-CB	-5.12	1.44	1.54
1	C	18	TYR	CD2-CE2	5.12	1.47	1.39
1	B	80	GLU	CG-CD	5.11	1.59	1.51
1	C	68	TYR	CG-CD1	5.08	1.45	1.39
1	B	133	GLU	CD-OE2	5.05	1.31	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	21	MET	CG-SD-CE	-9.84	84.45	100.20
1	E	116	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	G	21	MET	CG-SD-CE	-8.73	86.23	100.20
1	H	116	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	F	116	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	A	116	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	E	37	THR	CA-CB-CG2	-7.11	102.45	112.40
1	F	138	ASP	CB-CG-OD1	6.77	124.39	118.30
1	C	24	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	H	116	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	116	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	E	116	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	B	116	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	138	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	76[A]	ASP	CB-CG-OD1	6.23	123.91	118.30
1	D	76[B]	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	71	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	24	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	G	126[A]	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	G	126[B]	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	40	MET	CG-SD-CE	-6.14	90.38	100.20
1	D	138	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	83	ASP	CB-CG-OD1	6.10	123.79	118.30
1	C	116	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	G	116	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	116	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	55	ASP	CB-CG-OD1	5.29	123.06	118.30
1	H	77	LEU	CB-CG-CD1	5.28	119.98	111.00
1	D	116	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	E	71[A]	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	71[B]	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	E	57	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	H	119	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	H	29	ASP	CB-CG-OD2	5.06	122.85	118.30
1	H	77	LEU	CB-CG-CD2	-5.03	102.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	36	VAL	Mainchain

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	1163	0	1124	9	0
1	B	1185	0	1143	7	0
1	C	1154	0	1103	9	0
1	D	1172	0	1125	8	0
1	E	1194	0	1151	31	0
1	F	1148	0	1091	6	0
1	G	1171	0	1123	7	0
1	H	1151	0	1090	10	1
2	A	6	0	8	1	0
2	C	6	0	8	1	0
2	D	6	0	8	1	0
2	E	6	0	8	3	0
2	F	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	6	0	8	5	0
3	A	12	0	4	1	0
3	B	12	0	4	1	0
3	C	12	0	4	0	0
3	E	6	0	2	0	0
3	F	3	0	1	2	0
3	G	9	0	3	0	0
3	H	3	0	1	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	G	4	0	3	2	0
6	A	137	0	0	3	1
6	B	128	0	0	2	0
6	C	131	0	0	3	0
6	D	104	0	0	1	0
6	E	86	0	0	1	0
6	F	82	0	0	0	0
6	G	108	0	0	0	0
6	H	87	0	0	0	0
All	All	10306	0	9020	85	1

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 5.

All (85) 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:C:20[A]:ASN:OD1	6:C:821:HOH:O	1.88	0.89
1:D:8:ILE:HG22	1:D:9:THR:HG23	1.54	0.89
1:A:126[B]:ARG:HD2	6:A:847:HOH:O	1.78	0.83
1:B:35:ASN:O	1:B:37[A]:THR:HG23	1.89	0.73
1:D:21:MET:HE3	1:D:123:TYR:HE1	1.53	0.72
1:E:40[A]:MET:CE	1:E:64:ASN:HD22	2.03	0.71
1:A:77[B]:LEU:HD12	1:A:125:LEU:HD13	1.74	0.69
1:H:74:ASN:HA	2:H:158:GOL:H11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:ASN:N	2:H:158:GOL:H11	2.07	0.69
1:H:74:ASN:CA	2:H:158:GOL:H11	2.24	0.67
1:G:72:HIS:CE1	5:G:158:ACT:H1	2.30	0.67
1:C:40:MET:HE1	1:C:63:VAL:CG1	2.25	0.66
1:B:35:ASN:O	1:B:37[B]:THR:HG22	1.95	0.65
1:A:98:PRO:HA	3:A:159:FMT:H	1.77	0.65
1:E:38:PRO:HG2	1:E:40[A]:MET:CG	2.27	0.64
1:E:40[B]:MET:SD	1:H:98:PRO:HD3	2.38	0.64
1:C:40:MET:HE1	1:C:63:VAL:HG12	1.81	0.63
1:E:71[B]:ARG:HH11	1:E:73:SER:HB3	1.64	0.62
1:E:38:PRO:HD2	1:E:41:ASP:OD2	2.00	0.62
1:F:72:HIS:CE1	2:F:158:GOL:H32	2.35	0.61
1:G:72:HIS:HE1	5:G:158:ACT:H1	1.65	0.60
1:E:40[A]:MET:HG3	1:E:64:ASN:ND2	2.18	0.59
1:E:40[A]:MET:HE2	1:E:64:ASN:HD22	1.66	0.59
1:F:28:PHE:H	3:F:159:FMT:C	2.16	0.57
1:F:57:TYR:CE1	1:F:95:LYS:HB2	2.40	0.57
1:E:74:ASN:HA	2:E:158:GOL:H32	1.87	0.56
1:E:74:ASN:H	2:E:158:GOL:C3	2.19	0.55
1:E:40[B]:MET:HG2	1:H:98:PRO:HG3	1.87	0.55
1:E:38:PRO:HG2	1:E:40[A]:MET:HG2	1.88	0.55
1:E:38:PRO:HG2	1:E:40[A]:MET:HG3	1.90	0.54
1:E:71[B]:ARG:NH2	1:E:91[B]:SER:OG	2.40	0.53
1:A:10:LYS:HG2	1:A:11:ALA:N	2.23	0.53
1:G:77[B]:LEU:HD23	1:G:125:LEU:HD13	1.91	0.52
1:A:72:HIS:CE1	2:A:158:GOL:H32	2.45	0.52
1:E:36:VAL:O	6:E:787:HOH:O	2.19	0.51
1:E:40[A]:MET:HG3	1:E:64:ASN:HD22	1.73	0.51
1:A:77[B]:LEU:HD11	1:A:118:ILE:HD13	1.91	0.51
1:G:71:ARG:HG2	1:G:91[B]:SER:OG	2.10	0.51
1:D:121:TYR:CE1	1:D:126[B]:ARG:NH1	2.78	0.51
1:D:8:ILE:N	6:D:850:HOH:O	2.43	0.51
1:D:72:HIS:CE1	2:D:158:GOL:H11	2.46	0.50
1:A:71:ARG:HD2	1:A:80[A]:GLU:OE1	2.12	0.49
1:F:27:ASN:N	3:F:159:FMT:O2	2.45	0.49
1:E:71[A]:ARG:HH21	1:E:87:LEU:HG	1.78	0.49
1:B:20:ASN:ND2	1:B:34:GLU:OE1	2.46	0.49
1:C:75:TYR:H	2:C:158:GOL:C1	2.26	0.49
1:H:57:TYR:CE1	1:H:95:LYS:HB2	2.48	0.48
1:H:74:ASN:H	2:H:158:GOL:H11	1.75	0.48
1:E:71[A]:ARG:NH2	1:E:87:LEU:HG	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:N	6:A:784:HOH:O	2.46	0.48
1:D:21:MET:HE3	1:D:123:TYR:CE1	2.41	0.47
1:E:71[B]:ARG:CG	1:E:91[B]:SER:OG	2.62	0.47
1:H:74:ASN:H	2:H:158:GOL:C1	2.27	0.47
1:B:116:ARG:HB3	1:B:127:LEU:HG	1.97	0.47
1:B:71:ARG:HG2	1:B:91[B]:SER:OG	2.15	0.47
1:E:71[B]:ARG:NH1	1:E:73:SER:HB3	2.29	0.46
1:C:126[B]:ARG:NH2	6:C:566:HOH:O	2.43	0.46
1:E:74:ASN:CA	2:E:158:GOL:H32	2.46	0.45
1:C:45[B]:GLU:HG3	1:C:63:VAL:HG22	1.98	0.45
1:E:21:MET:HE3	1:E:123:TYR:HE1	1.82	0.45
1:E:45[A]:GLU:HG3	1:E:63:VAL:HG22	1.97	0.45
1:D:21:MET:CE	1:D:123:TYR:HE1	2.25	0.45
1:D:21:MET:CE	1:D:123:TYR:CE1	2.99	0.45
1:E:21:MET:HE3	1:E:123:TYR:CE1	2.52	0.45
1:F:34:GLU:OE1	1:G:34:GLU:OE2	2.34	0.45
1:E:40[A]:MET:HE3	1:E:64:ASN:HB2	1.99	0.45
1:E:38:PRO:HB2	1:E:40[A]:MET:HG2	1.98	0.44
1:F:23:ILE:HG23	1:F:125:LEU:HD11	1.99	0.43
1:B:10[B]:LYS:HG2	6:B:380:HOH:O	2.16	0.43
1:C:24:ARG:C	1:C:24:ARG:HD3	2.39	0.43
1:G:77[B]:LEU:CD2	1:G:125:LEU:HD13	2.49	0.43
1:E:38:PRO:CG	1:E:40[A]:MET:CG	2.97	0.42
1:E:38:PRO:CG	1:E:40[A]:MET:HG2	2.49	0.42
1:E:24:ARG:NH2	1:E:37:THR:O	2.50	0.42
1:G:77[B]:LEU:HD23	1:G:125:LEU:CD1	2.49	0.42
1:A:126[B]:ARG:CD	6:A:847:HOH:O	2.52	0.42
1:H:26:ALA:O	1:H:27:ASN:HB2	2.20	0.42
1:B:130:ILE:HG23	1:B:135:ASP:HB3	2.01	0.41
1:E:21:MET:CE	1:E:123:TYR:CE1	3.03	0.41
1:E:116:ARG:HB3	1:E:127:LEU:HG	2.03	0.41
1:C:126[B]:ARG:NE	6:C:566:HOH:O	2.36	0.40
1:E:7:PRO:HB2	1:E:45[B]:GLU:OE2	2.21	0.40
3:B:158:FMT:C	6:B:564:HOH:O	2.70	0.40
1:C:40:MET:HE2	1:C:40:MET:HB3	1.52	0.40
1:H:97:VAL:HB	1:H:98:PRO:HD2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ASN:OD1	6:A:656:HOH:O[4_555]	2.07	0.13

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	143/157 (91%)	139 (97%)	4 (3%)	0	100	100
1	B	146/157 (93%)	143 (98%)	3 (2%)	0	100	100
1	C	140/157 (89%)	135 (96%)	5 (4%)	0	100	100
1	D	143/157 (91%)	137 (96%)	6 (4%)	0	100	100
1	E	146/157 (93%)	143 (98%)	3 (2%)	0	100	100
1	F	140/157 (89%)	136 (97%)	4 (3%)	0	100	100
1	G	143/157 (91%)	140 (98%)	3 (2%)	0	100	100
1	H	139/157 (88%)	135 (97%)	4 (3%)	0	100	100
All	All	1140/1256 (91%)	1108 (97%)	32 (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	131/142 (92%)	127 (97%)	4 (3%)	40	25
1	B	134/142 (94%)	131 (98%)	3 (2%)	52	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	128/142 (90%)	125 (98%)	3 (2%)	50	37
1	D	131/142 (92%)	129 (98%)	2 (2%)	65	56
1	E	134/142 (94%)	131 (98%)	3 (2%)	52	39
1	F	128/142 (90%)	126 (98%)	2 (2%)	62	54
1	G	131/142 (92%)	127 (97%)	4 (3%)	40	25
1	H	127/142 (89%)	125 (98%)	2 (2%)	62	54
All	All	1044/1136 (92%)	1021 (98%)	23 (2%)	50	39

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	24	ARG
1	A	71	ARG
1	A	119	ARG
1	B	24	ARG
1	B	71	ARG
1	B	119	ARG
1	C	24	ARG
1	C	71	ARG
1	C	119	ARG
1	D	24	ARG
1	D	119	ARG
1	E	24	ARG
1	E	86	SER
1	E	119	ARG
1	F	24	ARG
1	F	119	ARG
1	G	24	ARG
1	G	71	ARG
1	G	119	ARG
1	G	125	LEU
1	H	24	ARG
1	H	119	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	14	GLN

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Mol	Chain	Res	Type
1	E	64	ASN
1	F	109	GLN
1	G	43	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 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	GOL	C	158	-	5,5,5	0.83	0	5,5,5	1.60	1 (20%)
3	FMT	B	161	-	2,2,2	0.60	0	1,1,1	0.03	0
3	FMT	B	160	-	2,2,2	0.92	0	1,1,1	0.14	0
3	FMT	A	162	-	2,2,2	0.57	0	1,1,1	0.45	0
2	GOL	E	158	-	5,5,5	0.63	0	5,5,5	1.57	1 (20%)
3	FMT	A	159	-	2,2,2	0.75	0	1,1,1	0.36	0
3	FMT	G	160	-	2,2,2	0.59	0	1,1,1	0.20	0
3	FMT	A	160	-	2,2,2	0.34	0	1,1,1	0.04	0
3	FMT	G	159	-	2,2,2	0.67	0	1,1,1	0.22	0
3	FMT	C	160	-	2,2,2	0.97	0	1,1,1	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FMT	G	161	-	2,2,2	0.67	0	1,1,1	0.05	0
5	ACT	G	158	-	3,3,3	0.68	0	3,3,3	1.90	2 (66%)
3	FMT	B	159	-	2,2,2	0.41	0	1,1,1	0.36	0
3	FMT	A	161	-	2,2,2	0.62	0	1,1,1	0.24	0
3	FMT	B	158	-	2,2,2	1.34	0	1,1,1	0.30	0
3	FMT	E	159	-	2,2,2	0.79	0	1,1,1	0.07	0
3	FMT	E	160	-	2,2,2	0.61	0	1,1,1	0.21	0
2	GOL	F	158	-	5,5,5	0.38	0	5,5,5	1.53	1 (20%)
2	GOL	A	158	-	5,5,5	0.69	0	5,5,5	0.79	0
2	GOL	H	158	-	5,5,5	0.47	0	5,5,5	1.15	1 (20%)
3	FMT	C	162	-	2,2,2	0.71	0	1,1,1	0.11	0
3	FMT	F	159	-	2,2,2	0.70	0	1,1,1	0.36	0
3	FMT	C	159	-	2,2,2	0.60	0	1,1,1	0.03	0
3	FMT	C	161	-	2,2,2	0.70	0	1,1,1	0.16	0
3	FMT	H	159	-	2,2,2	0.60	0	1,1,1	0.25	0
2	GOL	D	158	-	5,5,5	0.56	0	5,5,5	1.34	1 (20%)

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	GOL	C	158	-	-	4/4/4/4	-
2	GOL	E	158	-	-	3/4/4/4	-
2	GOL	F	158	-	-	3/4/4/4	-
2	GOL	A	158	-	-	0/4/4/4	-
2	GOL	H	158	-	-	1/4/4/4	-
2	GOL	D	158	-	-	2/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	158	GOL	O2-C2-C3	2.46	119.94	109.12
2	F	158	GOL	O1-C1-C2	-2.39	98.75	110.20
5	G	158	ACT	OXT-C-CH3	2.33	124.80	115.18
5	G	158	ACT	O-C-CH3	-2.31	113.33	122.33
2	E	158	GOL	O2-C2-C3	-2.23	99.30	109.12
2	H	158	GOL	O1-C1-C2	-2.16	99.86	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	158	GOL	C3-C2-C1	-2.10	103.53	111.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	158	GOL	O1-C1-C2-C3
2	D	158	GOL	O1-C1-C2-C3
2	E	158	GOL	O2-C2-C3-O3
2	F	158	GOL	O1-C1-C2-C3
2	F	158	GOL	C1-C2-C3-O3
2	C	158	GOL	O2-C2-C3-O3
2	D	158	GOL	O1-C1-C2-O2
2	C	158	GOL	C1-C2-C3-O3
2	E	158	GOL	C1-C2-C3-O3
2	C	158	GOL	O1-C1-C2-O2
2	F	158	GOL	O2-C2-C3-O3
2	E	158	GOL	O1-C1-C2-O2
2	H	158	GOL	O2-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	158	GOL	1	0
2	E	158	GOL	3	0
3	A	159	FMT	1	0
5	G	158	ACT	2	0
3	B	158	FMT	1	0
2	F	158	GOL	1	0
2	A	158	GOL	1	0
2	H	158	GOL	5	0
3	F	159	FMT	2	0
2	D	158	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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.