



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 09:16 pm GMT

PDB ID : 5HCF  
Title : T. cruzi calreticulin globular domain  
Authors : Moreau, C.P.; Gaboriaud, C.  
Deposited on : 2016-01-04  
Resolution : 2.45 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

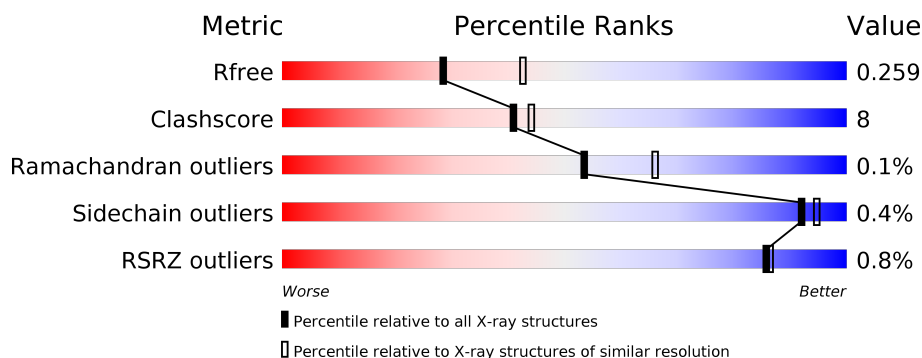
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	111664	1259 (2.48-2.44)
Clashscore	122126	1323 (2.48-2.44)
Ramachandran outliers	120053	1314 (2.48-2.44)
Sidechain outliers	120020	1314 (2.48-2.44)
RSRZ outliers	108989	1238 (2.48-2.44)

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	271	
1	B	271	
1	C	271	
1	D	271	
1	E	271	
1	F	271	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12998 atoms, of which 9 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 Calreticulin, putative, Calreticulin, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	5	0
			2153	1373	363	409	8			
1	B	263	Total	C	N	O	S	0	1	0
			2131	1362	353	408	8			
1	C	262	Total	C	N	O	S	0	4	0
			2145	1368	357	410	10			
1	D	264	Total	C	N	O	S	0	4	0
			2157	1377	358	414	8			
1	E	263	Total	C	N	O	S	0	5	0
			2156	1375	360	411	10			
1	F	262	Total	C	N	O	S	0	5	0
			2151	1371	358	412	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLY	-	linker	UNP Q4CPZ0
A	210	SER	-	linker	UNP Q4CPZ0
A	211	GLY	-	linker	UNP Q4CPZ0
A	368	GLY	-	expression tag	UNP Q4CPZ0
A	369	ASP	-	expression tag	UNP Q4CPZ0
A	370	HIS	-	expression tag	UNP Q4CPZ0
A	371	HIS	-	expression tag	UNP Q4CPZ0
A	372	HIS	-	expression tag	UNP Q4CPZ0
A	373	HIS	-	expression tag	UNP Q4CPZ0
A	374	HIS	-	expression tag	UNP Q4CPZ0
A	375	HIS	-	expression tag	UNP Q4CPZ0
B	209	GLY	-	linker	UNP Q4CPZ0
B	210	SER	-	linker	UNP Q4CPZ0
B	211	GLY	-	linker	UNP Q4CPZ0
B	368	GLY	-	expression tag	UNP Q4CPZ0
B	369	ASP	-	expression tag	UNP Q4CPZ0
B	370	HIS	-	expression tag	UNP Q4CPZ0

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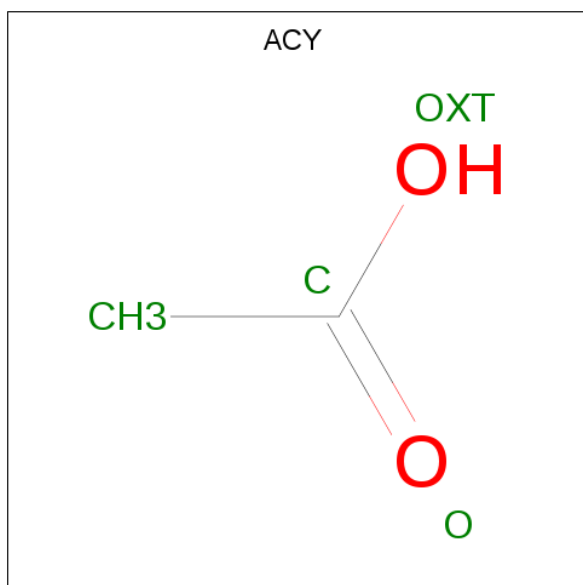
Chain	Residue	Modelled	Actual	Comment	Reference
B	371	HIS	-	expression tag	UNP Q4CPZ0
B	372	HIS	-	expression tag	UNP Q4CPZ0
B	373	HIS	-	expression tag	UNP Q4CPZ0
B	374	HIS	-	expression tag	UNP Q4CPZ0
B	375	HIS	-	expression tag	UNP Q4CPZ0
C	209	GLY	-	linker	UNP Q4CPZ0
C	210	SER	-	linker	UNP Q4CPZ0
C	211	GLY	-	linker	UNP Q4CPZ0
C	368	GLY	-	expression tag	UNP Q4CPZ0
C	369	ASP	-	expression tag	UNP Q4CPZ0
C	370	HIS	-	expression tag	UNP Q4CPZ0
C	371	HIS	-	expression tag	UNP Q4CPZ0
C	372	HIS	-	expression tag	UNP Q4CPZ0
C	373	HIS	-	expression tag	UNP Q4CPZ0
C	374	HIS	-	expression tag	UNP Q4CPZ0
C	375	HIS	-	expression tag	UNP Q4CPZ0
D	209	GLY	-	linker	UNP Q4CPZ0
D	210	SER	-	linker	UNP Q4CPZ0
D	211	GLY	-	linker	UNP Q4CPZ0
D	368	GLY	-	expression tag	UNP Q4CPZ0
D	369	ASP	-	expression tag	UNP Q4CPZ0
D	370	HIS	-	expression tag	UNP Q4CPZ0
D	371	HIS	-	expression tag	UNP Q4CPZ0
D	372	HIS	-	expression tag	UNP Q4CPZ0
D	373	HIS	-	expression tag	UNP Q4CPZ0
D	374	HIS	-	expression tag	UNP Q4CPZ0
D	375	HIS	-	expression tag	UNP Q4CPZ0
E	209	GLY	-	linker	UNP Q4CPZ0
E	210	SER	-	linker	UNP Q4CPZ0
E	211	GLY	-	linker	UNP Q4CPZ0
E	368	GLY	-	expression tag	UNP Q4CPZ0
E	369	ASP	-	expression tag	UNP Q4CPZ0
E	370	HIS	-	expression tag	UNP Q4CPZ0
E	371	HIS	-	expression tag	UNP Q4CPZ0
E	372	HIS	-	expression tag	UNP Q4CPZ0
E	373	HIS	-	expression tag	UNP Q4CPZ0
E	374	HIS	-	expression tag	UNP Q4CPZ0
E	375	HIS	-	expression tag	UNP Q4CPZ0
F	209	GLY	-	linker	UNP Q4CPZ0
F	210	SER	-	linker	UNP Q4CPZ0
F	211	GLY	-	linker	UNP Q4CPZ0
F	368	GLY	-	expression tag	UNP Q4CPZ0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	369	ASP	-	expression tag	UNP Q4CPZ0
F	370	HIS	-	expression tag	UNP Q4CPZ0
F	371	HIS	-	expression tag	UNP Q4CPZ0
F	372	HIS	-	expression tag	UNP Q4CPZ0
F	373	HIS	-	expression tag	UNP Q4CPZ0
F	374	HIS	-	expression tag	UNP Q4CPZ0
F	375	HIS	-	expression tag	UNP Q4CPZ0

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).

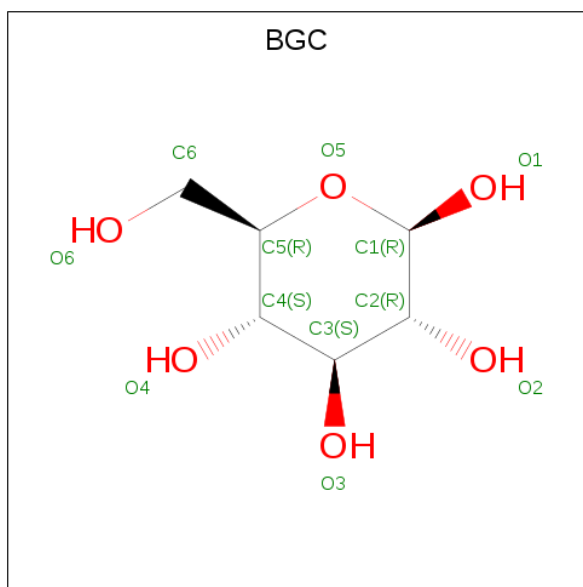


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	C	1	Total	C	O		0	0
			4	2	2			
2	E	1	Total	C	O		0	0
			4	2	2			
2	E	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



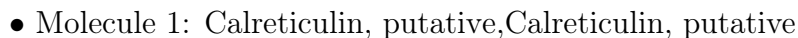
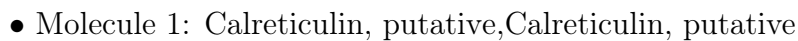
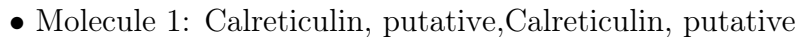
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 6 6	0	0
4	F	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	5	Total O 5 5	0	0
5	C	12	Total O 12 12	0	0
5	D	8	Total O 8 8	0	0
5	E	6	Total O 6 6	0	0
5	F	9	Total O 9 9	0	0

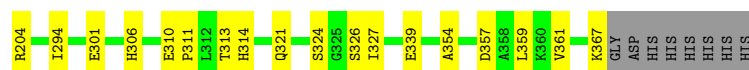
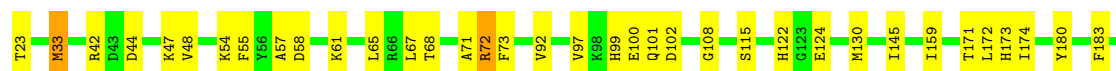
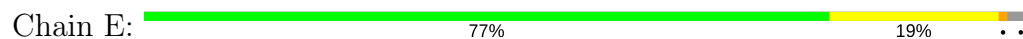


- Molecule 1: Calreticulin, putative, Calreticulin, putative

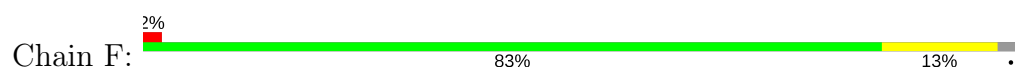




- Molecule 1: Calreticulin, putative, Calreticulin, putative



- Molecule 1: Calreticulin, putative, Calreticulin, putative





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.30Å 79.38Å 85.08Å 95.57° 98.69° 119.86°	Depositor
Resolution (Å)	47.70 – 2.45 47.70 – 2.45	Depositor EDS
% Data completeness (in resolution range)	92.1 (47.70-2.45) 86.9 (47.70-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 2.45Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, $R_{free}$	0.223 , 0.257 0.224 , 0.259	Depositor DCC
$R_{free}$ test set	2985 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.13% 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: ACY, BGC, CL

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	0.26	0/2210	0.43	0/2979
1	B	0.27	0/2188	0.46	0/2951
1	C	0.26	0/2202	0.45	0/2970
1	D	0.27	0/2214	0.47	0/2986
1	E	0.27	0/2213	0.45	0/2984
1	F	0.26	0/2208	0.44	0/2978
All	All	0.27	0/13235	0.45	0/17848

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2153	0	2080	31	0
1	B	2131	0	2067	31	0
1	C	2145	0	2075	32	0
1	D	2157	0	2089	42	0
1	E	2156	0	2088	41	0
1	F	2151	0	2079	26	0
2	A	8	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	3	0	0
2	E	8	3	6	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	12	0	12	4	0
4	F	12	0	12	2	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
5	C	12	0	0	1	0
5	D	8	0	0	1	0
5	E	6	0	0	1	0
5	F	9	0	0	1	0
All	All	12989	9	12517	195	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 8.

All (195) 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:104:LYS:HA	1:A:135[B]:ARG:HH12	1.35	0.90
1:D:47:LYS:HG3	1:D:68:THR:OG1	1.75	0.86
1:A:115:SER:HA	1:A:313:THR:HG21	1.56	0.86
1:E:115:SER:HA	1:E:313:THR:HG21	1.57	0.86
1:D:47:LYS:HG2	1:D:69:GLU:HG3	1.60	0.82
1:B:115:SER:HA	1:B:313:THR:HG21	1.62	0.81
1:A:116:MET:HE1	1:A:121:PHE:HB2	1.68	0.75
1:B:162:PRO:HD3	1:B:184:LEU:HD21	1.69	0.74
1:C:116:MET:HE1	1:C:121:PHE:HB2	1.70	0.74
1:D:193[B]:GLN:HE21	1:E:159:ILE:HG13	1.54	0.73
1:B:42:ARG:NH1	1:B:44:ASP:OD1	2.22	0.73
1:A:104:LYS:HA	1:A:135[B]:ARG:NH1	2.04	0.72
1:B:313:THR:HG23	1:B:314:HIS:ND1	2.06	0.71
1:B:73:PHE:CZ	1:D:294:ILE:HD11	2.26	0.71
1:D:80:PHE:CE1	1:D:315:VAL:HG23	2.27	0.70
1:C:80:PHE:CE1	1:C:315:VAL:HG23	2.26	0.69
1:C:103:LEU:O	1:C:135[B]:ARG:NH1	2.26	0.69
1:E:313:THR:HG23	1:E:314:HIS:ND1	2.08	0.69
1:C:34:GLU:OE2	1:E:367:LYS:HE3	1.92	0.68
1:C:362:MET:O	1:C:363:GLU:HB2	1.93	0.67
1:A:71:ALA:O	1:A:72[B]:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:SER:HB2	1:C:294:ILE:HD13	1.77	0.67
1:E:71:ALA:O	1:E:72:ARG:HD2	1.95	0.67
1:A:313:THR:HG23	1:A:314:HIS:ND1	2.09	0.67
1:E:101:GLN:O	1:E:102:ASP:HB2	1.96	0.65
1:D:96:SER:HB3	1:D:169[B]:VAL:HG22	1.78	0.65
1:C:116:MET:CE	1:C:121:PHE:HB2	2.27	0.65
1:A:116:MET:CE	1:A:121:PHE:HB2	2.27	0.64
1:D:366:GLU:O	1:D:367:LYS:HB2	1.96	0.64
1:D:24:VAL:HG23	1:D:339:GLU:OE1	1.97	0.64
1:F:55:PHE:CZ	1:F:359:LEU:HD13	2.34	0.63
1:B:330:ASP:CG	1:B:347:THR:HG21	2.19	0.62
1:D:47:LYS:HG2	1:D:69:GLU:CG	2.27	0.62
1:A:210:SER:HB2	1:A:294:ILE:HD13	1.82	0.61
1:C:101:GLN:O	1:C:102:ASP:HB2	1.99	0.61
1:D:101:GLN:O	1:D:102:ASP:HB2	2.01	0.61
1:D:169[A]:VAL:HG12	1:D:185:ASP:HA	1.83	0.60
1:C:47:LYS:HG3	1:C:68:THR:OG1	2.02	0.60
1:F:101:GLN:O	1:F:102:ASP:HB2	2.01	0.60
1:B:174:ILE:HG22	1:B:306:HIS:HB2	1.84	0.60
1:E:33:MET:HG3	1:E:33:MET:O	2.01	0.59
1:E:57:ALA:HB1	1:E:354:ALA:HB3	1.84	0.59
1:B:73:PHE:HZ	1:D:294:ILE:HD11	1.68	0.59
1:A:101:GLN:O	1:A:102:ASP:HB2	2.03	0.59
1:B:101:GLN:O	1:B:102:ASP:HB2	2.03	0.58
1:F:23:THR:HG22	1:F:339:GLU:OE1	2.03	0.58
1:D:362:MET:O	1:D:362:MET:HG2	2.03	0.58
1:B:57:ALA:HB1	1:B:354:ALA:HB3	1.85	0.58
1:A:362:MET:O	1:A:362:MET:HG2	2.04	0.58
1:D:42:ARG:NH1	1:D:44:ASP:OD1	2.37	0.57
1:D:193[B]:GLN:NE2	1:E:159:ILE:HA	2.20	0.56
1:E:174:ILE:O	5:E:501:HOH:O	2.17	0.56
1:A:57:ALA:HB1	1:A:354:ALA:HB3	1.88	0.55
1:B:122:HIS:NE2	1:B:124:GLU:HB2	2.22	0.55
1:A:294:ILE:HD11	1:E:73:PHE:CZ	2.42	0.54
1:E:72:ARG:HG2	1:E:72:ARG:HH11	1.72	0.54
1:D:210:SER:HB2	1:D:294:ILE:HD13	1.89	0.54
1:D:67:LEU:N	1:D:67:LEU:HD23	2.22	0.54
1:E:174:ILE:HG22	1:E:306:HIS:HB2	1.90	0.53
1:F:33:MET:CE	1:F:49:GLU:HA	2.39	0.53
1:B:111:LYS:NZ	4:B:401:BGC:H6C1	2.24	0.53
1:D:363:GLU:O	1:D:367:LYS:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:HG22	1:A:306[A]:HIS:HB2	1.90	0.52
1:F:310:GLU:HB3	1:F:311:PRO:HD2	1.92	0.52
1:D:169[A]:VAL:CG1	1:D:185:ASP:HA	2.39	0.52
1:D:193[B]:GLN:NE2	1:E:159:ILE:HG13	2.21	0.52
1:F:122:HIS:NE2	1:F:124:GLU:HB2	2.24	0.52
1:C:57:ALA:HB1	1:C:354:ALA:HB3	1.91	0.52
1:A:24:VAL:HG23	1:A:339:GLU:OE1	2.09	0.52
1:C:122:HIS:NE2	1:C:124:GLU:HB2	2.25	0.51
1:D:66:ARG:NH1	1:D:68:THR:HG22	2.25	0.51
1:D:99:HIS:O	5:D:401:HOH:O	2.19	0.51
1:C:105[B]:CYS:HB3	1:C:136[B]:CYS:SG	2.50	0.51
1:E:47:LYS:HG3	1:E:68:THR:OG1	2.11	0.51
1:F:42:ARG:NH1	1:F:44:ASP:OD1	2.44	0.51
1:D:193[B]:GLN:HE21	1:E:159:ILE:HA	1.74	0.50
1:C:162:PRO:HD3	1:C:184:LEU:HD21	1.93	0.50
1:E:58:ASP:HB3	1:E:61:LYS:HB2	1.93	0.50
1:F:57:ALA:HB1	1:F:354:ALA:HB3	1.93	0.50
1:B:204:ARG:NH2	1:B:301:GLU:OE2	2.42	0.50
1:C:80:PHE:CZ	1:C:315:VAL:HG23	2.47	0.50
1:F:24:VAL:HG23	1:F:339:GLU:OE1	2.12	0.50
1:A:122:HIS:NE2	1:A:124:GLU:HB2	2.27	0.50
1:E:23:THR:N	1:E:339:GLU:OE1	2.45	0.50
1:B:111:LYS:HZ1	4:B:401:BGC:C6	2.25	0.49
1:F:33:MET:HE3	1:F:49:GLU:HA	1.94	0.49
1:E:171:THR:HB	1:E:183:PHE:HB2	1.94	0.49
1:F:210:SER:HB2	1:F:294:ILE:HD13	1.95	0.49
1:A:171:THR:HB	1:A:183:PHE:HB2	1.94	0.49
1:C:362:MET:O	1:C:363:GLU:CB	2.61	0.49
1:A:67:LEU:HD12	1:A:321:GLN:OE1	2.12	0.49
1:D:122:HIS:NE2	1:D:124:GLU:HB2	2.28	0.49
1:F:55:PHE:CE2	1:F:359:LEU:HB2	2.48	0.49
1:F:105[B]:CYS:HA	1:F:136[B]:CYS:HA	1.95	0.48
1:A:42:ARG:NH1	1:A:44:ASP:OD1	2.46	0.48
1:D:23:THR:O	1:D:24:VAL:HB	2.13	0.48
1:E:42:ARG:NH1	1:E:44:ASP:OD1	2.46	0.48
1:F:111:LYS:NZ	4:F:401:BGC:H6C1	2.28	0.48
1:E:54:LYS:HG2	1:E:100:GLU:OE2	2.12	0.48
1:C:105[A]:CYS:HA	1:C:136[A]:CYS:HA	1.96	0.48
1:E:71:ALA:C	1:E:72:ARG:HD2	2.33	0.48
1:C:174:ILE:HG22	1:C:306:HIS:HB2	1.96	0.48
1:E:310:GLU:HB3	1:E:311:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:THR:HB	1:B:183:PHE:HB2	1.95	0.47
1:A:310:GLU:HB3	1:A:311:PRO:HD2	1.95	0.47
1:A:115:SER:CA	1:A:313:THR:HG21	2.38	0.47
1:C:210:SER:HB2	1:C:294:ILE:CD1	2.42	0.47
1:F:294:ILE:N	1:F:294:ILE:HD12	2.30	0.47
1:A:105:CYS:HA	1:A:136:CYS:HA	1.96	0.47
1:E:122:HIS:NE2	1:E:124:GLU:HB2	2.30	0.47
1:D:80:PHE:CZ	1:D:315:VAL:HG23	2.50	0.46
1:C:105[B]:CYS:HA	1:C:136[B]:CYS:HA	1.96	0.46
1:D:174:ILE:HG22	1:D:306:HIS:HB2	1.96	0.46
1:F:117:ASP:OD1	1:F:119:GLU:HB2	2.14	0.46
1:A:113:LEU:HD22	1:A:116:MET:SD	2.55	0.46
1:F:105[A]:CYS:HA	1:F:136[A]:CYS:HA	1.97	0.46
1:D:47:LYS:HG2	1:D:69:GLU:CD	2.36	0.46
1:A:23:THR:HG22	1:A:339:GLU:OE1	2.16	0.46
1:B:330:ASP:OD2	1:B:347:THR:HG21	2.15	0.46
1:B:78:THR:HG22	1:B:315:VAL:CG1	2.46	0.46
1:F:111:LYS:HZ3	4:F:401:BGC:H6C1	1.81	0.45
1:E:65:LEU:O	1:E:327:ILE:HA	2.17	0.45
1:D:105:CYS:HA	1:D:136:CYS:HA	1.98	0.45
1:D:55:PHE:CZ	1:D:359:LEU:HD13	2.51	0.45
1:D:166:LEU:CD2	1:D:359:LEU:HD22	2.47	0.45
1:C:294:ILE:N	1:C:294:ILE:HD12	2.32	0.45
1:D:321:GLN:NE2	1:D:324[B]:SER:HA	2.31	0.45
1:F:96:SER:HB3	1:F:169:VAL:HG22	1.99	0.45
1:C:140:ASN:HB3	1:C:160:ARG:NH1	2.31	0.45
1:B:105:CYS:HA	1:B:136:CYS:HA	1.98	0.45
1:B:162:PRO:CD	1:B:184:LEU:HD21	2.44	0.45
1:B:294:ILE:N	1:B:294:ILE:HD12	2.32	0.45
1:A:294:ILE:N	1:A:294:ILE:HD12	2.32	0.44
1:F:158:ARG:HA	5:F:508:HOH:O	2.17	0.44
1:C:92:VAL:O	1:C:333:ILE:HA	2.17	0.44
1:E:294:ILE:HD12	1:E:294:ILE:N	2.32	0.44
1:B:36:TRP:CE3	1:B:76:LEU:HD13	2.52	0.44
1:C:158:ARG:HA	5:C:509:HOH:O	2.17	0.44
1:C:166:LEU:HD21	1:C:359:LEU:HD22	2.00	0.44
1:D:294:ILE:HD12	1:D:294:ILE:N	2.33	0.44
1:A:67:LEU:N	1:A:67:LEU:HD23	2.32	0.44
1:A:210:SER:HB2	1:A:294:ILE:CD1	2.48	0.44
1:C:194:LEU:HD23	1:C:198:TRP:CZ3	2.53	0.44
1:D:321:GLN:NE2	1:D:324[A]:SER:HA	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:321:GLN:NE2	1:E:324:SER:HA	2.33	0.43
1:B:111:LYS:NZ	4:B:401:BGC:C6	2.81	0.43
1:E:130[B]:MET:HB3	1:E:145:ILE:HB	2.00	0.43
1:F:92:VAL:O	1:F:333:ILE:HA	2.18	0.43
1:C:54:LYS:HA	1:C:54:LYS:HD3	1.70	0.43
1:B:47:LYS:HG3	1:B:68:THR:OG1	2.18	0.43
1:D:171:THR:HB	1:D:183:PHE:HB2	1.99	0.43
1:E:130[A]:MET:HB3	1:E:145:ILE:HB	2.00	0.43
1:F:155:TRP:CE2	1:F:157:LYS:HB2	2.53	0.43
1:A:97:VAL:HG21	1:A:108:GLY:O	2.18	0.43
1:F:105[B]:CYS:SG	1:F:322:VAL:HG21	2.58	0.43
1:B:321:GLN:NE2	1:B:324:SER:HA	2.34	0.43
1:D:103:LEU:HD11	1:D:106:GLY:HA3	2.01	0.43
1:F:54:LYS:HD3	1:F:54:LYS:HA	1.62	0.43
1:C:42:ARG:HG2	1:C:45:PHE:CZ	2.54	0.42
1:D:166:LEU:HD21	1:D:359:LEU:HD22	2.01	0.42
1:E:173:HIS:O	1:E:180:TYR:HA	2.19	0.42
1:E:33:MET:SD	1:E:48:VAL:HG23	2.59	0.42
1:B:111:LYS:HZ2	4:B:401:BGC:H6C1	1.84	0.42
1:C:166:LEU:CD2	1:C:359:LEU:HD22	2.49	0.42
1:D:32:SER:OG	1:D:33:MET:N	2.52	0.42
1:C:321:GLN:NE2	1:C:324:SER:HA	2.35	0.42
1:B:36:TRP:CE3	1:B:76:LEU:CD1	3.02	0.42
1:A:23:THR:HG23	1:A:335:ASP:OD1	2.19	0.42
1:B:103:LEU:HD11	1:B:106:GLY:HA3	2.02	0.42
1:E:204:ARG:NH2	1:E:301:GLU:OE2	2.49	0.42
1:B:134:ASP:OD2	1:B:143:HIS:HE1	2.03	0.42
1:A:144:ILE:HD12	1:A:155:TRP:CE3	2.55	0.41
1:B:210:SER:HB2	1:B:294:ILE:HD13	2.02	0.41
1:D:95:PHE:HE2	1:D:97:VAL:CG2	2.33	0.41
1:E:99:HIS:ND1	1:E:326:SER:OG	2.46	0.41
1:E:357:ASP:O	1:E:361:VAL:HG23	2.20	0.41
1:F:357:ASP:O	1:F:361:VAL:HG23	2.19	0.41
1:C:130[B]:MET:HB3	1:C:145:ILE:HB	2.01	0.41
1:E:55:PHE:CZ	1:E:359:LEU:HD13	2.56	0.41
1:A:103:LEU:HD11	1:A:106:GLY:HA3	2.02	0.41
1:D:92:VAL:O	1:D:333:ILE:HA	2.21	0.41
1:E:67:LEU:HD23	1:E:67:LEU:N	2.35	0.41
1:C:130[A]:MET:HB3	1:C:145:ILE:HB	2.01	0.41
1:C:54:LYS:HD3	1:C:54:LYS:N	2.33	0.41
1:D:310:GLU:HB3	1:D:311:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:TYR:HA	1:B:132:GLY:HA3	2.03	0.41
1:B:57:ALA:HB2	1:B:355:GLU:HB2	2.03	0.41
1:E:115:SER:CA	1:E:313:THR:HG21	2.40	0.41
1:D:57:ALA:HB1	1:D:354:ALA:HB3	2.03	0.41
1:E:72:ARG:HG2	1:E:72:ARG:NH1	2.36	0.41
1:E:47:LYS:CG	1:E:68:THR:OG1	2.69	0.40
1:F:47:LYS:HG3	1:F:68:THR:OG1	2.21	0.40
1:A:65:LEU:O	1:A:327:ILE:HA	2.21	0.40
1:E:92:VAL:HA	1:E:172:LEU:O	2.22	0.40
1:E:97:VAL:HG21	1:E:108:GLY: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	262/271 (97%)	254 (97%)	8 (3%)	0	100	100
1	B	262/271 (97%)	255 (97%)	7 (3%)	0	100	100
1	C	264/271 (97%)	254 (96%)	9 (3%)	1 (0%)	36	45
1	D	266/271 (98%)	257 (97%)	8 (3%)	1 (0%)	36	45
1	E	266/271 (98%)	259 (97%)	7 (3%)	0	100	100
1	F	265/271 (98%)	256 (97%)	9 (3%)	0	100	100
All	All	1585/1626 (98%)	1535 (97%)	48 (3%)	2 (0%)	53	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	24	VAL
1	C	363	GLU



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/239 (98%)	233 (99%)	2 (1%)	81	87
1	B	233/239 (98%)	233 (100%)	0	100	100
1	C	235/239 (98%)	235 (100%)	0	100	100
1	D	236/239 (99%)	234 (99%)	2 (1%)	83	89
1	E	236/239 (99%)	234 (99%)	2 (1%)	83	89
1	F	236/239 (99%)	235 (100%)	1 (0%)	92	95
All	All	1411/1434 (98%)	1404 (100%)	7 (0%)	92	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135[A]	ARG
1	A	135[B]	ARG
1	D	365	MET
1	D	366	GLU
1	E	33	MET
1	E	72	ARG
1	F	54	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	321	GLN
1	B	143	HIS

### 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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	ACY	A	401	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
2	ACY	A	402	-	1,3,3	1.61	0	0,3,3	0.00	-
4	BGC	B	401	-	12,12,12	0.54	0	17,17,17	2.37	5 (29%)
2	ACY	C	401	-	1,3,3	1.53	0	0,3,3	0.00	-
2	ACY	E	401	-	1,3,3	1.39	0	0,3,3	0.00	-
2	ACY	E	402	-	1,3,3	1.45	0	0,3,3	0.00	-
4	BGC	F	401	-	12,12,12	0.54	0	17,17,17	0.76	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	ACY	A	401	-	-	0/0/0/0	0/0/0/0
2	ACY	A	402	-	-	0/0/0/0	0/0/0/0
4	BGC	B	401	-	-	0/2/22/22	0/1/1/1
2	ACY	C	401	-	-	0/0/0/0	0/0/0/0
2	ACY	E	401	-	-	0/0/0/0	0/0/0/0
2	ACY	E	402	-	-	0/0/0/0	0/0/0/0
4	BGC	F	401	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ACY	CH3-C	2.26	1.51	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	BGC	C6-C5-C4	-2.98	105.94	112.99
4	B	401	BGC	O1-C1-C2	-2.91	100.72	109.02
4	B	401	BGC	O1-C1-O5	-2.08	104.17	110.44
4	B	401	BGC	C1-O5-C5	4.91	123.13	113.69
4	B	401	BGC	O5-C5-C4	6.53	121.68	109.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	BGC	4	0
4	F	401	BGC	2	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	261/271 (96%)	-0.06	0 <span>100</span> <span>100</span>	28, 43, 61, 85	0
1	B	263/271 (97%)	-0.07	2 (0%) <span>86</span> <span>86</span>	27, 46, 74, 113	0
1	C	262/271 (96%)	-0.03	0 <span>100</span> <span>100</span>	27, 44, 68, 90	0
1	D	264/271 (97%)	0.08	5 (1%) <span>66</span> <span>63</span>	27, 46, 73, 93	0
1	E	263/271 (97%)	-0.05	0 <span>100</span> <span>100</span>	26, 46, 72, 111	0
1	F	262/271 (96%)	0.13	5 (1%) <span>66</span> <span>63</span>	29, 49, 78, 100	0
All	All	1575/1626 (96%)	0.00	12 (0%) <span>86</span> <span>86</span>	26, 45, 74, 113	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	ILE	4.6
1	F	60	GLU	3.0
1	D	80	PHE	2.9
1	F	82	THR	2.6
1	D	367	LYS	2.4
1	D	84	ILE	2.2
1	F	43	ASP	2.2
1	F	34	GLU	2.1
1	F	121	PHE	2.1
1	B	34	GLU	2.1
1	D	35	HIS	2.0
1	D	53	GLY	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BGC	B	401	12/12	0.82	0.23	93,95,96,97	0
2	ACY	A	402	4/4	0.83	0.14	47,49,57,57	0
2	ACY	E	401	4/4	0.85	0.17	63,65,66,66	0
4	BGC	F	401	12/12	0.87	0.20	80,82,83,83	0
3	CL	C	402	1/1	0.87	0.28	81,81,81,81	0
2	ACY	E	402	4/4	0.88	0.21	47,49,57,57	0
2	ACY	C	401	4/4	0.89	0.14	54,57,58,58	0
2	ACY	A	401	4/4	0.90	0.13	53,54,64,64	0
3	CL	A	403	1/1	0.93	0.30	73,73,73,73	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.