



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:19 PM BST

PDB ID : 4IT4  
Title : Crystal structure of residues 1-211 of CG17282  
Authors : Agyekum, B.; Bouyain, S.  
Deposited on : 2013-01-17  
Resolution : 2.50 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

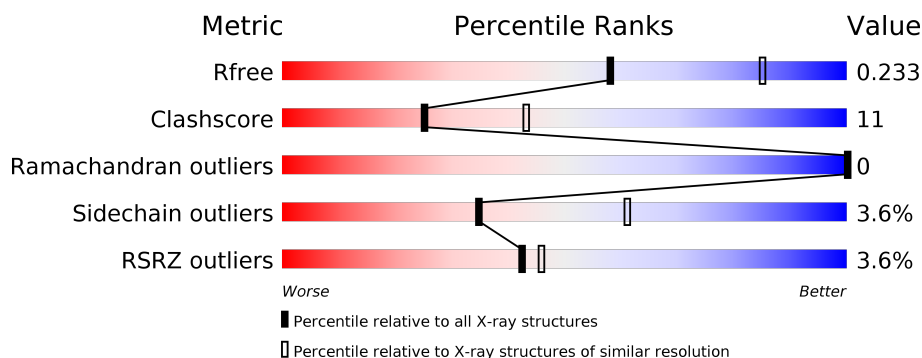
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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  $\leq 5\%$ . 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	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 81%, yellow 13%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>81%</span> <span>13%</span> <span>• •</span> </div> </div>
1	B	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, green 75%, yellow 21%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>75%</span> <span>21%</span> <span>• •</span> </div> </div>
1	C	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 80%, yellow 16%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>80%</span> <span>16%</span> <span>•</span> </div> </div>
1	D	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 19%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>76%</span> <span>19%</span> <span>• •</span> </div> </div>
1	E	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 77%, yellow 15%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>5%</span> <span>77%</span> <span>15%</span> <span>• 5%</span> </div> </div>
1	F	215	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 11%, green 67%, yellow 24%, orange 8%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>11%</span> <span>67%</span> <span>24%</span> <span>• 8%</span> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMT	F	302	-	-	X	-
3	GOL	B	302	-	-	X	-
3	GOL	C	301	-	-	X	-
4	ACY	F	303	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10043 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 CG17282.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1657	1071	269	312	5			
1	B	210	Total	C	N	O	S	0	0	0
			1677	1082	272	318	5			
1	C	206	Total	C	N	O	S	0	0	0
			1649	1067	268	309	5			
1	D	208	Total	C	N	O	S	0	0	0
			1663	1075	270	312	6			
1	E	205	Total	C	N	O	S	0	0	0
			1640	1063	267	305	5			
1	F	198	Total	C	N	O	S	0	0	0
			1584	1028	260	292	4			

There are 24 discrepancies between the modelled and reference sequences:

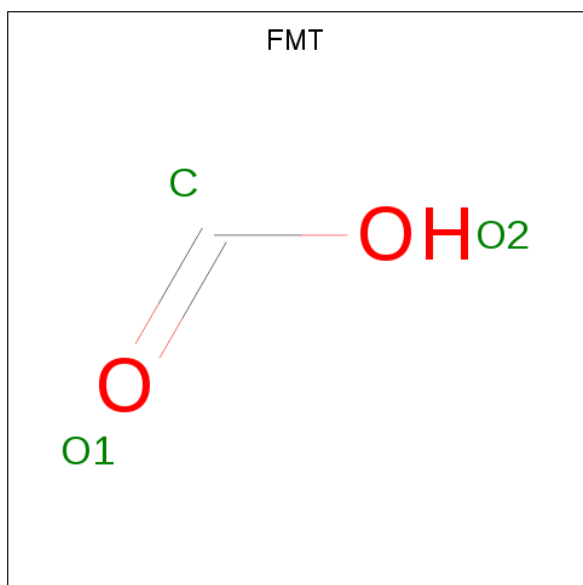
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q9VDE4
A	-2	PRO	-	EXPRESSION TAG	UNP Q9VDE4
A	-1	GLY	-	EXPRESSION TAG	UNP Q9VDE4
A	0	SER	-	EXPRESSION TAG	UNP Q9VDE4
B	-3	GLY	-	EXPRESSION TAG	UNP Q9VDE4
B	-2	PRO	-	EXPRESSION TAG	UNP Q9VDE4
B	-1	GLY	-	EXPRESSION TAG	UNP Q9VDE4
B	0	SER	-	EXPRESSION TAG	UNP Q9VDE4
C	-3	GLY	-	EXPRESSION TAG	UNP Q9VDE4
C	-2	PRO	-	EXPRESSION TAG	UNP Q9VDE4
C	-1	GLY	-	EXPRESSION TAG	UNP Q9VDE4
C	0	SER	-	EXPRESSION TAG	UNP Q9VDE4
D	-3	GLY	-	EXPRESSION TAG	UNP Q9VDE4
D	-2	PRO	-	EXPRESSION TAG	UNP Q9VDE4
D	-1	GLY	-	EXPRESSION TAG	UNP Q9VDE4
D	0	SER	-	EXPRESSION TAG	UNP Q9VDE4
E	-3	GLY	-	EXPRESSION TAG	UNP Q9VDE4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	PRO	-	EXPRESSION TAG	UNP Q9VDE4
E	-1	GLY	-	EXPRESSION TAG	UNP Q9VDE4
E	0	SER	-	EXPRESSION TAG	UNP Q9VDE4
F	-3	GLY	-	EXPRESSION TAG	UNP Q9VDE4
F	-2	PRO	-	EXPRESSION TAG	UNP Q9VDE4
F	-1	GLY	-	EXPRESSION TAG	UNP Q9VDE4
F	0	SER	-	EXPRESSION TAG	UNP Q9VDE4

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



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

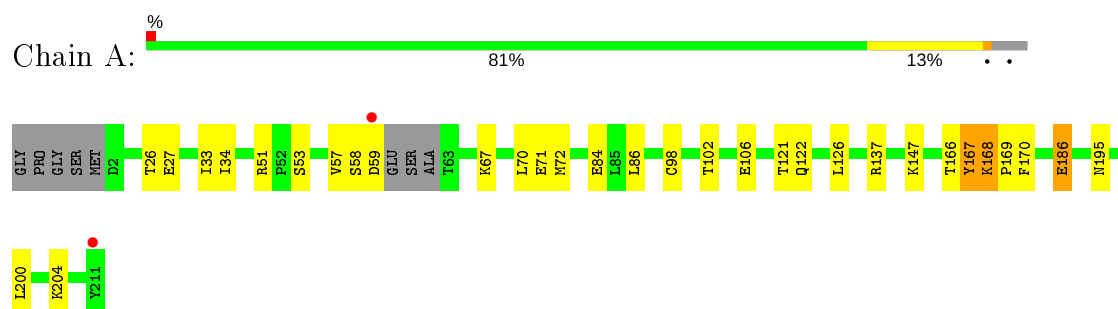
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total	O	0	0
			31	31		
5	B	21	Total	O	0	0
			21	21		
5	C	28	Total	O	0	0
			28	28		
5	D	8	Total	O	0	0
			8	8		
5	E	16	Total	O	0	0
			16	16		
5	F	11	Total	O	0	0
			11	11		

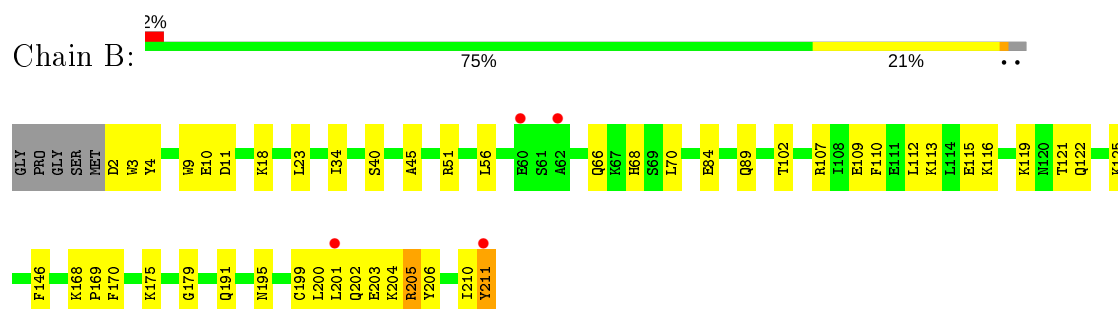
### 3 Residue-property plots [i](#)

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 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.

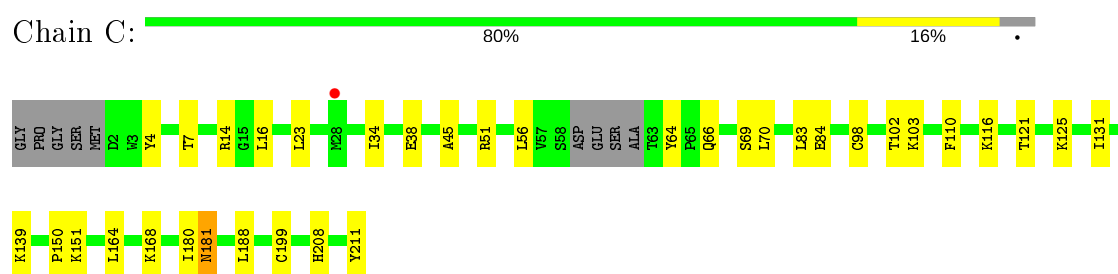
#### • Molecule 1: CG17282



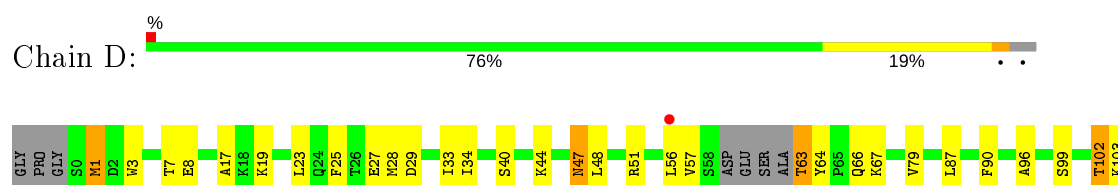
#### • Molecule 1: CG17282



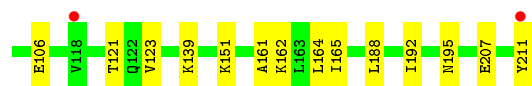
#### • Molecule 1: CG17282



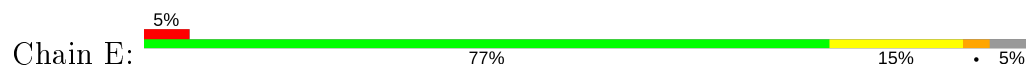
#### • Molecule 1: CG17282



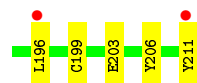
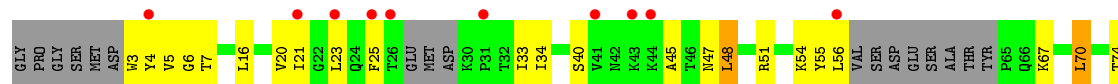




• Molecule 1: CG17282



• Molecule 1: CG17282



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.10 Å 90.19 Å 249.67 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 2.50 49.03 – 2.49	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.65-2.50) 93.3 (49.03-2.49)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.48 Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.197 , 0.230 0.199 , 0.233	Depositor DCC
$R_{free}$ test set	2657 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, ACY

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	0.51	1/1687 (0.1%)	0.49	0/2276
1	B	0.46	0/1708	0.51	0/2306
1	C	0.45	0/1679	0.49	0/2265
1	D	0.32	0/1693	0.49	0/2283
1	E	0.36	0/1670	0.51	0/2253
1	F	0.34	0/1612	0.49	0/2171
All	All	0.41	1/10049 (0.0%)	0.50	0/13554

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	TYR	CD1-CE1	-5.25	1.31	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1657	0	1693	24	0
1	B	1677	0	1710	45	0
1	C	1649	0	1689	26	0
1	D	1663	0	1706	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1640	0	1685	37	0
1	F	1584	0	1636	64	0
2	A	6	0	4	0	0
2	B	3	0	2	0	0
2	D	6	0	4	0	0
2	E	3	0	2	0	0
2	F	6	0	4	4	0
3	B	12	0	14	4	0
3	C	12	0	14	6	0
3	F	6	0	7	2	0
4	F	4	0	3	2	0
5	A	31	0	0	2	0
5	B	21	0	0	1	0
5	C	28	0	0	0	0
5	D	8	0	0	0	0
5	E	16	0	0	0	0
5	F	11	0	0	0	0
All	All	10043	0	10173	215	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 11.

All (215) 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:D:1:MET:HB3	1:D:23:LEU:HD23	1.24	1.19
1:E:100:ILE:HB	1:E:108:ILE:CG2	1.73	1.19
1:F:6:GLY:H	1:F:20:VAL:HG23	1.09	1.15
1:F:139:LYS:NZ	2:F:302:FMT:H	1.63	1.13
1:F:139:LYS:HZ1	2:F:302:FMT:H	1.02	1.12
1:F:67:LYS:HE2	1:F:115:GLU:HG3	1.34	1.09
1:B:205:ARG:O	1:B:205:ARG:HG3	1.44	1.09
1:B:113:LYS:HD3	1:B:115:GLU:OE2	1.54	1.05
1:E:100:ILE:HB	1:E:108:ILE:HG22	1.38	1.05
1:C:151:LYS:HD2	3:C:301:GOL:H2	1.41	1.03
1:F:6:GLY:N	1:F:20:VAL:HG23	1.73	1.01
1:C:38:GLU:OE1	1:C:116:LYS:HE2	1.60	0.99
1:D:1:MET:CB	1:D:23:LEU:HD23	1.94	0.98
1:F:90:PHE:HA	1:F:94:GLU:OE2	1.66	0.94
1:F:67:LYS:HE2	1:F:115:GLU:CG	2.03	0.88
1:F:199:CYS:O	1:F:203:GLU:HG3	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD21	1:C:84:GLU:HG2	1.56	0.87
1:A:102:THR:HB	1:B:211:TYR:HA	1.55	0.86
1:F:33:ILE:HG13	1:F:34:ILE:HG23	1.57	0.86
1:F:4:TYR:O	1:F:4:TYR:CD1	2.30	0.85
1:F:192:ILE:O	1:F:196:LEU:HG	1.77	0.83
1:D:34:ILE:HG13	1:D:121:THR:OG1	1.78	0.83
1:E:48:LEU:HA	1:E:108:ILE:HD13	1.61	0.83
1:F:67:LYS:CE	1:F:115:GLU:HG3	2.10	0.81
1:E:100:ILE:HB	1:E:108:ILE:HG21	1.62	0.81
1:B:201:LEU:HD11	1:D:162:LYS:HG3	1.62	0.79
1:B:113:LYS:CD	1:B:115:GLU:OE2	2.30	0.79
1:B:205:ARG:O	1:B:205:ARG:CG	2.30	0.78
1:B:34:ILE:HG13	1:B:121:THR:OG1	1.84	0.77
1:E:3:TRP:CD1	1:E:3:TRP:N	2.54	0.76
1:F:6:GLY:N	1:F:20:VAL:CG2	2.49	0.76
1:D:33:ILE:HG13	1:D:34:ILE:HG23	1.68	0.76
1:B:119:LYS:HE2	1:B:121:THR:HG21	1.70	0.74
1:F:33:ILE:HD11	1:F:123:VAL:HG21	1.68	0.73
1:D:103:LYS:NZ	1:F:206:TYR:O	2.21	0.73
1:D:57:VAL:CG2	1:D:57:VAL:O	2.36	0.72
1:B:211:TYR:CD2	1:B:211:TYR:N	2.56	0.72
1:F:6:GLY:H	1:F:20:VAL:CG2	1.97	0.72
3:B:302:GOL:O3	1:E:139:LYS:NZ	2.22	0.71
1:B:119:LYS:HE2	1:B:121:THR:CG2	2.20	0.71
1:B:11:ASP:OD1	1:B:11:ASP:C	2.30	0.69
1:D:57:VAL:O	1:D:57:VAL:HG23	1.90	0.69
1:C:103:LYS:NZ	1:E:206:TYR:O	2.25	0.69
1:E:48:LEU:HA	1:E:108:ILE:CD1	2.22	0.69
1:B:211:TYR:H	1:B:211:TYR:HD2	1.38	0.68
1:B:4:TYR:HD2	1:B:23:LEU:HD22	1.59	0.67
1:F:48:LEU:HD21	1:F:56:LEU:HB3	1.74	0.67
1:A:26:THR:HG23	1:A:27:GLU:HG2	1.77	0.67
1:E:70:LEU:HD21	1:E:84:GLU:HG2	1.77	0.67
1:B:205:ARG:HG2	1:B:206:TYR:CD2	2.31	0.66
1:F:4:TYR:O	1:F:20:VAL:HG21	1.95	0.66
1:A:168:LYS:O	1:F:147:LYS:HE3	1.94	0.66
1:B:4:TYR:CD2	1:B:23:LEU:HD22	2.31	0.66
1:F:20:VAL:HG12	1:F:94:GLU:OE1	1.96	0.65
1:A:195:ASN:OD1	1:C:168:LYS:NZ	2.27	0.65
1:E:108:ILE:HG23	1:E:108:ILE:O	1.96	0.65
1:B:170:PHE:HB2	3:B:302:GOL:O1	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LEU:O	1:B:204:LYS:HG2	1.96	0.65
1:F:121:THR:HG21	1:F:126:LEU:HD21	1.78	0.65
1:D:8:GLU:HG3	1:D:19:LYS:HG3	1.79	0.64
1:B:168:LYS:HD3	1:B:169:PRO:HA	1.80	0.64
1:B:107:ARG:NH2	1:B:109:GLU:OE2	2.26	0.63
1:F:20:VAL:HG23	1:F:20:VAL:O	1.98	0.62
1:B:146:PHE:CE2	1:B:202:GLN:OE1	2.52	0.62
1:F:48:LEU:O	1:F:51:ARG:NH1	2.32	0.62
1:B:170:PHE:N	3:B:302:GOL:O1	2.31	0.61
1:C:38:GLU:OE1	1:C:116:LYS:CE	2.41	0.61
1:A:186:GLU:HG3	1:A:186:GLU:O	2.00	0.61
1:C:211:TYR:HB3	1:E:103:LYS:HD2	1.83	0.60
1:E:53:SER:HB3	1:E:57:VAL:HG23	1.83	0.60
1:E:100:ILE:CB	1:E:108:ILE:HG22	2.23	0.60
1:F:193:GLN:HA	1:F:196:LEU:HD12	1.83	0.60
1:F:3:TRP:CE3	1:F:3:TRP:HA	2.36	0.60
1:C:14:ARG:HB2	1:C:16:LEU:HG	1.84	0.59
1:E:56:LEU:HD21	1:E:110:PHE:CD1	2.38	0.59
1:E:29:ASP:O	1:E:92:PRO:HD3	2.03	0.58
1:A:33:ILE:HG13	1:A:34:ILE:HG23	1.86	0.58
1:C:164:LEU:HD11	1:C:188:LEU:HD23	1.86	0.58
1:A:53:SER:HB3	1:A:57:VAL:HG23	1.86	0.58
1:B:205:ARG:HG2	1:B:206:TYR:CE2	2.39	0.58
1:B:68:HIS:ND1	5:B:421:HOH:O	2.32	0.57
1:F:121:THR:CG2	1:F:126:LEU:HD21	2.35	0.57
1:C:150:PRO:HD2	3:C:301:GOL:O3	2.05	0.57
1:F:170:PHE:N	3:F:304:GOL:O3	2.32	0.56
1:D:195:ASN:OD1	1:E:168:LYS:NZ	2.39	0.56
1:E:164:LEU:HD11	1:E:188:LEU:HD23	1.87	0.55
1:F:67:LYS:HE2	1:F:115:GLU:CD	2.27	0.55
1:B:113:LYS:HD3	1:B:115:GLU:CD	2.27	0.55
1:D:56:LEU:HD12	1:D:79:VAL:CG1	2.37	0.55
1:F:139:LYS:HZ3	2:F:302:FMT:H	1.65	0.54
3:C:301:GOL:H12	1:E:211:TYR:CE2	2.42	0.54
1:C:180:ILE:HG13	1:C:181:ASN:N	2.22	0.54
1:B:175:LYS:HD2	1:B:179:GLY:C	2.28	0.54
1:A:72:MET:O	1:A:137:ARG:NH2	2.41	0.54
1:D:34:ILE:HD13	1:D:123:VAL:HG22	1.89	0.54
1:B:119:LYS:HG2	1:B:121:THR:HG23	1.89	0.53
1:B:146:PHE:CZ	1:B:202:GLN:OE1	2.61	0.53
1:F:211:TYR:CD2	4:F:303:ACY:OXT	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:TYR:O	1:F:4:TYR:CG	2.62	0.53
1:F:23:LEU:HD21	1:F:25:PHE:HB2	1.92	0.52
1:E:48:LEU:O	1:E:51:ARG:NH1	2.37	0.52
1:A:122:GLN:HG2	5:A:422:HOH:O	2.09	0.52
1:A:71:GLU:HG2	1:A:137:ARG:HH22	1.75	0.52
1:C:139:LYS:HZ1	3:F:304:GOL:HO1	1.52	0.52
1:E:108:ILE:O	1:E:108:ILE:CG2	2.58	0.52
1:D:34:ILE:HG13	1:D:121:THR:HG1	1.74	0.52
1:B:205:ARG:HH21	1:D:165:ILE:HD11	1.75	0.51
1:D:1:MET:HB3	1:D:23:LEU:CD2	2.17	0.51
1:A:51:ARG:NH2	1:B:211:TYR:O	2.40	0.51
1:F:21:ILE:HD11	1:F:95:THR:HG22	1.93	0.51
1:F:139:LYS:NZ	2:F:302:FMT:C	2.56	0.51
1:F:90:PHE:CD2	1:F:94:GLU:HG2	2.45	0.51
1:D:27:GLU:HG3	1:D:29:ASP:H	1.76	0.51
1:F:157:PHE:HB3	1:F:196:LEU:CD2	2.40	0.50
1:A:167:TYR:O	1:A:169:PRO:O	2.30	0.50
1:D:40:SER:HB3	1:D:67:LYS:HA	1.94	0.50
1:F:33:ILE:CD1	1:F:123:VAL:HG21	2.39	0.50
1:F:157:PHE:HB3	1:F:196:LEU:HD21	1.94	0.50
1:F:45:ALA:HB2	1:F:56:LEU:HG	1.95	0.49
1:C:151:LYS:HE3	3:C:301:GOL:H31	1.93	0.49
1:B:2:ASP:O	1:B:3:TRP:CD1	2.65	0.49
1:B:70:LEU:HD21	1:B:84:GLU:HG2	1.94	0.49
1:A:102:THR:HA	1:B:210:ILE:O	2.13	0.49
1:B:2:ASP:C	1:B:4:TYR:H	2.15	0.49
1:D:1:MET:HB2	1:D:23:LEU:HD23	1.92	0.49
1:D:1:MET:HG3	1:D:3:TRP:CZ2	2.48	0.49
1:D:1:MET:CB	1:D:23:LEU:CD2	2.81	0.49
1:B:2:ASP:O	1:B:4:TYR:N	2.36	0.49
1:F:174:THR:HG22	1:F:176:LYS:H	1.77	0.49
1:D:161:ALA:HB2	1:D:192:ILE:HG21	1.93	0.49
1:E:48:LEU:CD1	1:E:108:ILE:HD11	2.44	0.48
1:E:128:ALA:HB3	1:E:178:ASN:HB3	1.95	0.48
1:A:166:THR:O	1:A:166:THR:HG22	2.14	0.48
1:C:34:ILE:CD1	1:C:121:THR:OG1	2.61	0.48
1:E:136:LEU:HD23	1:E:188:LEU:HD13	1.96	0.48
1:F:40:SER:HB3	1:F:115:GLU:OE2	2.14	0.48
1:F:187:GLU:O	1:F:191:GLN:HG3	2.15	0.47
1:D:64:TYR:CD1	1:D:66:GLN:HG3	2.49	0.47
1:A:57:VAL:HG21	5:A:418:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:TYR:HD2	1:C:23:LEU:HD22	1.78	0.47
1:E:18:LYS:HD2	1:E:90:PHE:CE1	2.48	0.47
1:E:8:GLU:HG3	1:E:19:LYS:HG3	1.96	0.47
1:F:121:THR:HG22	1:F:122:GLN:N	2.29	0.47
1:D:17:ALA:HB3	1:D:99:SER:OG	2.15	0.47
1:F:164:LEU:HD11	1:F:188:LEU:HD23	1.96	0.47
1:A:70:LEU:HD21	1:A:84:GLU:HG2	1.97	0.47
3:C:302:GOL:H11	1:E:151:LYS:HB2	1.97	0.46
1:E:46:THR:O	1:E:108:ILE:HD12	2.15	0.46
1:F:70:LEU:HD21	1:F:84:GLU:HG2	1.98	0.46
1:E:48:LEU:HD12	1:E:108:ILE:CD1	2.45	0.46
1:A:121:THR:HG21	1:A:126:LEU:HD21	1.98	0.45
1:E:93:GLY:C	1:E:113:LYS:HE3	2.37	0.45
1:E:3:TRP:HD1	1:E:3:TRP:N	2.12	0.45
1:F:51:ARG:NH2	1:F:102:THR:HG21	2.32	0.45
1:F:54:LYS:HG2	1:F:55:TYR:CE1	2.52	0.45
1:C:150:PRO:O	1:C:151:LYS:C	2.53	0.45
1:F:48:LEU:HA	1:F:48:LEU:HD13	1.74	0.45
1:C:51:ARG:NH2	1:C:102:THR:HG21	2.32	0.45
1:C:64:TYR:CD1	1:C:66:GLN:HG3	2.52	0.45
1:D:25:PHE:HE1	1:D:28:MET:HG2	1.81	0.45
1:D:102:THR:HB	1:F:211:TYR:C	2.37	0.45
1:B:9:TRP:CG	1:B:10:GLU:N	2.85	0.45
1:B:11:ASP:OD1	1:B:11:ASP:O	2.35	0.44
1:F:16:LEU:HD21	1:F:82:TYR:HB3	2.00	0.44
1:F:7:THR:N	1:F:20:VAL:HG22	2.32	0.44
1:B:122:GLN:OE1	1:B:125:LYS:HE2	2.18	0.44
1:F:3:TRP:HA	1:F:3:TRP:HE3	1.82	0.44
1:B:45:ALA:HB2	1:B:56:LEU:HG	1.99	0.44
1:F:34:ILE:HD13	1:F:123:VAL:HG22	2.00	0.44
1:F:5:VAL:HA	1:F:20:VAL:CG2	2.48	0.44
1:D:47:ASN:ND2	1:D:106:GLU:HG3	2.33	0.44
1:D:51:ARG:HH21	1:F:211:TYR:C	2.21	0.43
1:E:48:LEU:HD13	1:E:108:ILE:HD11	2.00	0.43
1:F:193:GLN:CD	1:F:196:LEU:HD12	2.38	0.43
1:E:33:ILE:O	1:E:33:ILE:HG22	2.18	0.43
1:B:51:ARG:NH2	1:B:102:THR:HG21	2.34	0.43
1:F:102:THR:OG1	1:F:106:GLU:HB3	2.17	0.43
1:E:6:GLY:N	1:E:20:VAL:O	2.47	0.43
1:C:34:ILE:HD12	1:C:121:THR:OG1	2.17	0.43
1:D:48:LEU:HD21	1:D:57:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:THR:HG22	1:F:137:ARG:HD2	2.00	0.43
1:A:53:SER:H	1:A:57:VAL:HG21	1.83	0.43
1:E:48:LEU:CA	1:E:108:ILE:CD1	2.96	0.42
1:A:86:LEU:HD13	1:A:98:CYS:HB3	2.02	0.42
1:F:47:ASN:HB3	1:F:106:GLU:OE2	2.19	0.42
1:D:151:LYS:HD3	4:F:303:ACY:H2	2.01	0.42
1:D:63:THR:O	1:D:63:THR:OG1	2.30	0.42
1:A:147:LYS:HE3	1:C:168:LYS:O	2.20	0.42
1:C:45:ALA:HB2	1:C:56:LEU:HG	2.01	0.42
1:C:4:TYR:O	1:C:7:THR:HG23	2.19	0.42
1:D:90:PHE:CZ	1:D:96:ALA:HB3	2.54	0.42
1:B:199:CYS:O	1:B:203:GLU:HG3	2.20	0.42
1:C:98:CYS:HB2	1:C:110:PHE:CE1	2.55	0.42
3:C:302:GOL:O1	1:E:150:PRO:HD2	2.20	0.42
1:F:180:ILE:HD12	1:F:180:ILE:HA	1.82	0.42
1:B:18:LYS:NZ	1:B:89:GLN:O	2.53	0.42
1:E:56:LEU:HA	1:E:56:LEU:HD12	1.88	0.42
1:B:110:PHE:HE2	1:B:112:LEU:HD11	1.84	0.41
1:E:18:LYS:HD2	1:E:90:PHE:HE1	1.85	0.41
1:A:170:PHE:HD2	1:A:186:GLU:HB2	1.86	0.41
1:F:5:VAL:HA	1:F:20:VAL:HG23	2.02	0.41
1:A:53:SER:O	1:A:57:VAL:CG2	2.69	0.41
1:C:4:TYR:HA	1:C:7:THR:CG2	2.50	0.41
1:B:40:SER:HA	1:B:66:GLN:O	2.21	0.41
1:C:4:TYR:HA	1:C:7:THR:HG21	2.03	0.41
1:A:200:LEU:O	1:A:204:LYS:HG2	2.20	0.41
1:C:131:ILE:HD13	1:C:131:ILE:HA	1.90	0.41
1:A:71:GLU:OE2	1:A:137:ARG:NH1	2.54	0.40
1:B:170:PHE:CB	3:B:302:GOL:O1	2.66	0.40
1:F:157:PHE:CB	1:F:196:LEU:CD2	2.99	0.40
1:F:67:LYS:NZ	1:F:115:GLU:HG3	2.35	0.40
1:F:174:THR:HG22	1:F:176:LYS:HG2	2.03	0.40
1:B:191:GLN:O	1:B:195:ASN:ND2	2.52	0.40
1:D:164:LEU:HD11	1:D:188:LEU:HD23	2.03	0.40
1:D:87:LEU:HD23	1:D:87:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	203/215 (94%)	201 (99%)	2 (1%)	0	100	100
1	B	208/215 (97%)	200 (96%)	8 (4%)	0	100	100
1	C	202/215 (94%)	196 (97%)	6 (3%)	0	100	100
1	D	204/215 (95%)	200 (98%)	4 (2%)	0	100	100
1	E	201/215 (94%)	198 (98%)	3 (2%)	0	100	100
1	F	192/215 (89%)	187 (97%)	5 (3%)	0	100	100
All	All	1210/1290 (94%)	1182 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	181/186 (97%)	175 (97%)	6 (3%)	38	64
1	B	183/186 (98%)	180 (98%)	3 (2%)	62	84
1	C	180/186 (97%)	174 (97%)	6 (3%)	38	64
1	D	182/186 (98%)	173 (95%)	9 (5%)	25	47
1	E	178/186 (96%)	168 (94%)	10 (6%)	21	40
1	F	172/186 (92%)	167 (97%)	5 (3%)	42	69
All	All	1076/1116 (96%)	1037 (96%)	39 (4%)	35	61

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	59	ASP
1	A	67	LYS
1	A	106	GLU
1	A	168	LYS
1	A	186	GLU
1	B	116	LYS
1	B	205	ARG
1	B	211	TYR
1	C	69	SER
1	C	83	LEU
1	C	125	LYS
1	C	181	ASN
1	C	199	CYS
1	C	208	HIS
1	D	1	MET
1	D	7	THR
1	D	44	LYS
1	D	47	ASN
1	D	63	THR
1	D	102	THR
1	D	139	LYS
1	D	207	GLU
1	D	211	TYR
1	E	3	TRP
1	E	18	LYS
1	E	29	ASP
1	E	56	LEU
1	E	94	GLU
1	E	106	GLU
1	E	136	LEU
1	E	139	LYS
1	E	186	GLU
1	E	190	ILE
1	F	48	LEU
1	F	70	LEU
1	F	94	GLU
1	F	139	LYS
1	F	168	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	ASN
1	B	181	ASN
1	C	178	ASN
1	D	183	GLN
1	E	178	ASN
1	E	183	GLN
1	E	208	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	B	303	-	5,5,5	0.80	0	5,5,5	1.20	0
4	ACY	F	303	-	1,3,3	0.69	0	0,3,3	0.00	-
2	FMT	A	302	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	B	302	-	5,5,5	0.80	0	5,5,5	1.20	0
2	FMT	E	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	F	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	D	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A	301	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FMT	B	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	F	302	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	C	301	-	5,5,5	0.80	0	5,5,5	1.20	0
3	GOL	C	302	-	5,5,5	0.80	0	5,5,5	1.20	0
2	FMT	D	302	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	F	304	-	5,5,5	0.79	0	5,5,5	1.20	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
3	GOL	B	303	-	-	3/4/4/4	-
3	GOL	F	304	-	-	1/4/4/4	-
3	GOL	C	301	-	-	4/4/4/4	-
3	GOL	C	302	-	-	2/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	303	GOL	C1-C2-C3-O3
3	C	301	GOL	O1-C1-C2-C3
3	C	301	GOL	C1-C2-C3-O3
3	C	302	GOL	O1-C1-C2-C3
3	C	301	GOL	O1-C1-C2-O2
3	C	301	GOL	O2-C2-C3-O3
3	C	302	GOL	O1-C1-C2-O2
3	B	303	GOL	O2-C2-C3-O3
3	B	303	GOL	O1-C1-C2-O2
3	F	304	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	303	ACY	2	0
3	B	302	GOL	4	0
2	F	302	FMT	4	0
3	C	301	GOL	4	0
3	C	302	GOL	2	0
3	F	304	GOL	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	207/215 (96%)	0.04	2 (0%) 82 84	26, 44, 81, 103	0
1	B	210/215 (97%)	0.05	4 (1%) 66 69	28, 48, 84, 111	0
1	C	206/215 (95%)	-0.05	1 (0%) 91 91	31, 47, 77, 92	0
1	D	208/215 (96%)	0.06	3 (1%) 75 77	30, 53, 84, 103	0
1	E	205/215 (95%)	0.21	10 (4%) 29 31	29, 62, 94, 112	0
1	F	198/215 (92%)	0.68	24 (12%) 4 4	34, 70, 102, 111	0
All	All	1234/1290 (95%)	0.16	44 (3%) 42 46	26, 52, 91, 112	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	211	TYR	7.2
1	E	22	GLY	5.7
1	F	23	LEU	5.7
1	F	90	PHE	5.1
1	E	93	GLY	5.0
1	F	21	ILE	5.0
1	F	95	THR	4.9
1	E	23	LEU	4.6
1	F	118	VAL	4.5
1	F	4	TYR	4.5
1	F	44	LYS	4.0
1	F	91	VAL	3.9
1	E	28	MET	3.9
1	F	123	VAL	3.6
1	A	211	TYR	3.6
1	F	41	VAL	3.6
1	B	211	TYR	3.6
1	F	112	LEU	3.5
1	F	93	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	211	TYR	3.3
1	E	25	PHE	3.3
1	F	43	LYS	3.2
1	F	56	LEU	3.2
1	F	110	PHE	2.9
1	F	114	LEU	2.8
1	F	94	GLU	2.8
1	B	201	LEU	2.6
1	E	116	LYS	2.5
1	E	211	TYR	2.5
1	F	87	LEU	2.5
1	E	56	LEU	2.4
1	B	62	ALA	2.3
1	D	118	VAL	2.3
1	C	28	MET	2.3
1	F	26	THR	2.3
1	F	196	LEU	2.3
1	F	31	PRO	2.3
1	B	60	GLU	2.3
1	F	25	PHE	2.2
1	E	42	ASN	2.1
1	A	59	ASP	2.1
1	F	124	GLU	2.0
1	D	56	LEU	2.0
1	E	175	LYS	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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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	ACY	F	303	4/4	0.70	0.23	57,60,65,71	0
2	FMT	D	302	3/3	0.70	0.27	77,77,79,80	0
2	FMT	F	302	3/3	0.76	0.26	84,84,86,88	0
3	GOL	B	302	6/6	0.76	0.19	81,86,88,89	0
2	FMT	D	301	3/3	0.78	0.25	68,68,70,70	0
3	GOL	F	304	6/6	0.79	0.19	73,79,81,82	0
3	GOL	C	302	6/6	0.80	0.23	53,64,70,84	0
2	FMT	A	302	3/3	0.83	0.25	54,54,66,70	0
2	FMT	E	301	3/3	0.86	0.15	59,59,62,66	0
2	FMT	A	301	3/3	0.87	0.18	59,59,60,61	0
2	FMT	B	301	3/3	0.87	0.35	63,63,67,71	0
3	GOL	C	301	6/6	0.90	0.24	59,68,74,83	0
2	FMT	F	301	3/3	0.91	0.17	59,59,64,65	0
3	GOL	B	303	6/6	0.94	0.24	51,61,64,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.