



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:00 AM GMT

PDB ID : 2P10  
Title : CRYSTAL STRUCTURE OF A PUTATIVE PHOSPHONOPYRUVATE HYDROLASE (MLL9387) FROM MESORHIZOBIUM LOTI MAFF303099 AT 2.15 Å RESOLUTION  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-03-01  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

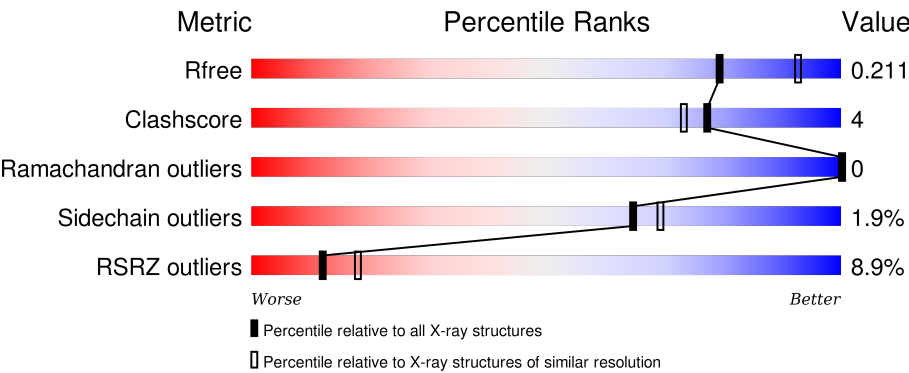
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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 <sub>free</sub>	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	286	<div><div>2%</div><div>87%6%6%</div></div>
1	B	286	<div><div>5%</div><div>86%7%6%</div></div>
1	C	286	<div><div>5%</div><div>89%5%6%</div></div>
1	D	286	<div><div>4%</div><div>88%6%6%</div></div>
1	E	286	<div><div>12%</div><div>84%10%6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	286	

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
4	GOL	B	289	-	-	-	X
4	GOL	B	290	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12944 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 Mll9387 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	Se	0	3	0
			2034	1273	359	387	5	10			
1	B	268	Total	C	N	O	S	Se	0	3	0
			2013	1265	355	378	5	10			
1	C	270	Total	C	N	O	S	Se	0	4	0
			2055	1287	363	388	5	12			
1	D	268	Total	C	N	O	S	Se	0	3	0
			2034	1275	358	386	5	10			
1	E	269	Total	C	N	O	S	Se	0	5	0
			2026	1271	356	382	5	12			
1	F	266	Total	C	N	O	S	Se	0	3	0
			1988	1254	344	373	5	12			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q981G2
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	61	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	83	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	107	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	146	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	154	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	190	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	206	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
A	261	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	0	GLY	-	LEADER SEQUENCE	UNP Q981G2
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	61	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	83	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	107	MSE	MET	MODIFIED RESIDUE	UNP Q981G2

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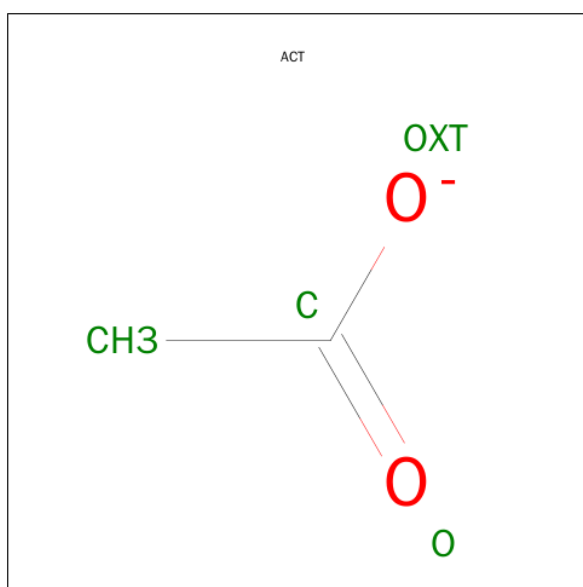
Chain	Residue	Modelled	Actual	Comment	Reference
B	109	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	146	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	154	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	178	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	190	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	206	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
B	261	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	0	GLY	-	LEADER SEQUENCE	UNP Q981G2
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	61	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	83	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	107	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	146	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	154	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	178	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	190	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	206	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
C	261	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	0	GLY	-	LEADER SEQUENCE	UNP Q981G2
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	61	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	83	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	107	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	146	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	154	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	178	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	190	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	206	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
D	261	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	0	GLY	-	LEADER SEQUENCE	UNP Q981G2
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	61	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	83	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	107	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	109	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	146	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	154	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	178	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	190	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
E	206	MSE	MET	MODIFIED RESIDUE	UNP Q981G2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	261	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	0	GLY	-	LEADER SEQUENCE	UNP Q981G2
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	61	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	83	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	107	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	109	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	146	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	154	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	178	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	190	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	206	MSE	MET	MODIFIED RESIDUE	UNP Q981G2
F	261	MSE	MET	MODIFIED RESIDUE	UNP Q981G2

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

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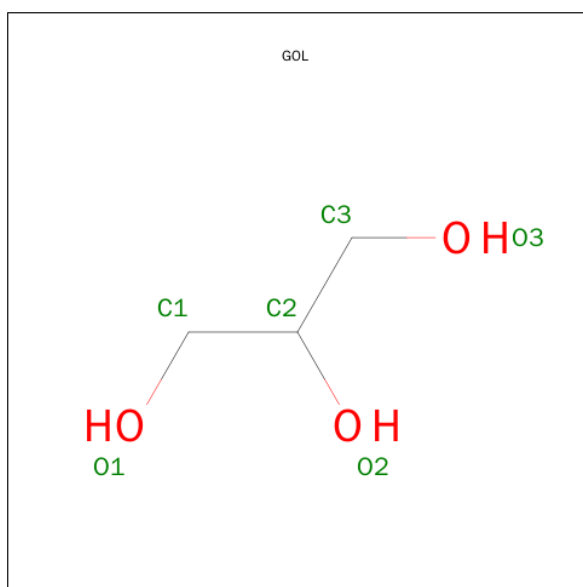
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	2	Total Cl 2 2	0	0
3	D	1	Total Cl 1 1	0	0
3	C	2	Total Cl 2 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

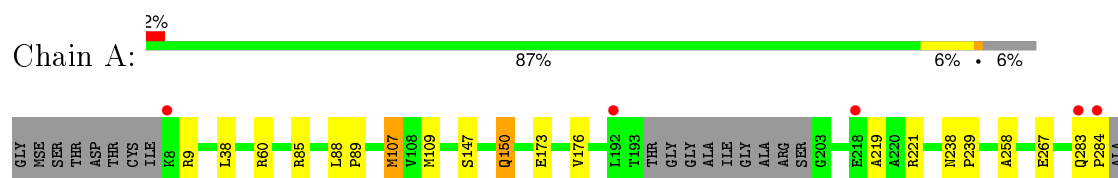
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	118	Total	O	0	0
			118	118		
5	C	174	Total	O	0	0
			174	174		
5	D	131	Total	O	0	0
			131	131		
5	E	59	Total	O	0	0
			59	59		
5	F	54	Total	O	0	0
			54	54		

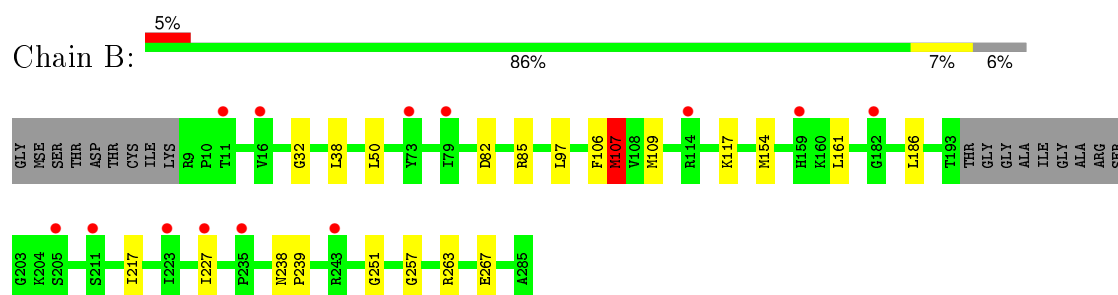
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

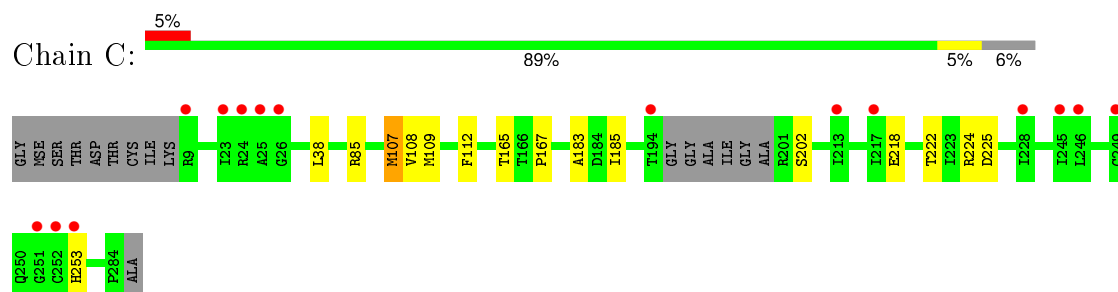
#### • Molecule 1: Mll9387 protein



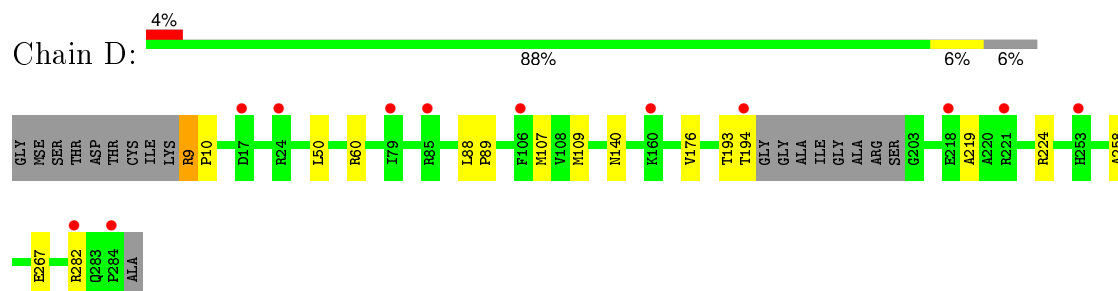
#### • Molecule 1: Mll9387 protein



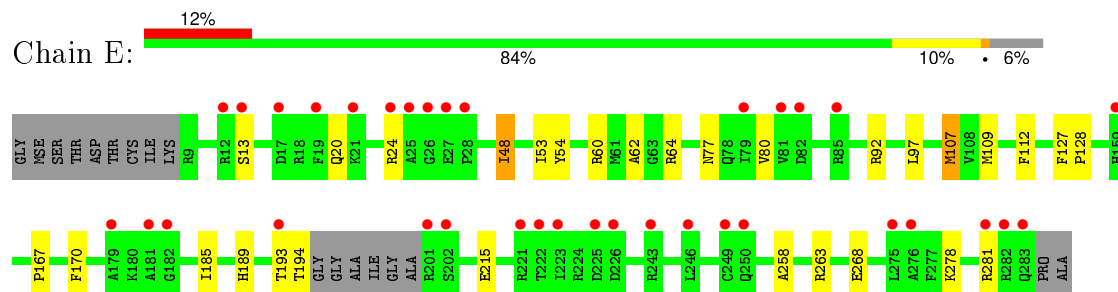
#### • Molecule 1: Mll9387 protein



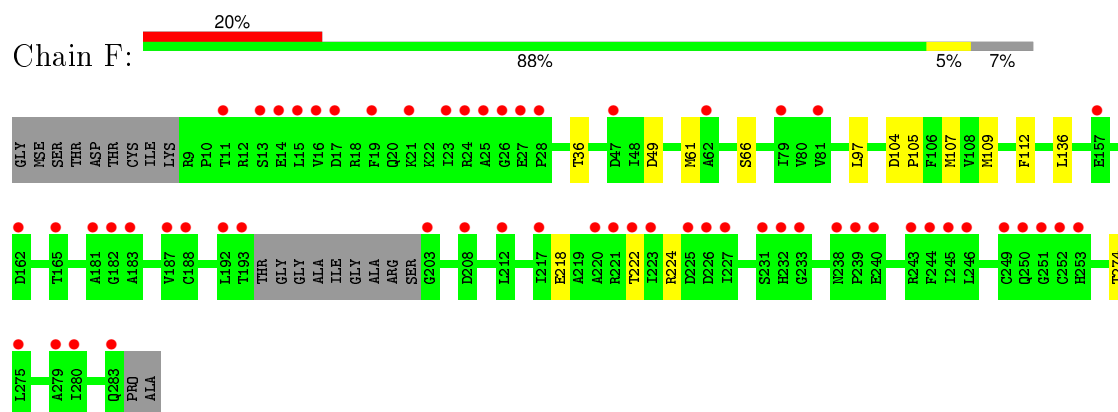
#### • Molecule 1: Mll9387 protein



- Molecule 1: Mll9387 protein



- Molecule 1: Mll9387 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.27Å 180.27Å 185.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.08 – 2.15 45.07 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.08-2.15) 99.3 (45.07-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.162 , 0.204 0.173 , 0.211	Depositor DCC
$R_{free}$ test set	6092 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.2	EDS
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 121409 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, CL, 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	0.60	0/2062	0.69	1/2763 (0.0%)
1	B	0.56	0/2043	0.66	1/2740 (0.0%)
1	C	0.60	0/2088	0.65	0/2799
1	D	0.55	0/2063	0.67	2/2766 (0.1%)
1	E	0.50	0/2058	0.64	0/2755
1	F	0.47	0/2016	0.60	0/2702
All	All	0.55	0/12330	0.65	4/16525 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	MSE	CG-SE-CE	7.17	114.67	98.90
1	D	282	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	107	MSE	CG-SE-CE	6.80	113.85	98.90
1	D	282	ARG	NE-CZ-NH2	-5.70	117.45	120.30

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	2034	0	2033	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2013	0	2011	19	0
1	C	2055	0	2058	11	0
1	D	2034	0	2036	11	0
1	E	2026	0	2019	18	0
1	F	1988	0	1981	18	0
2	A	12	0	9	1	0
2	B	8	0	6	0	0
2	C	16	0	12	0	0
2	D	8	0	6	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	1	0
5	A	176	0	0	1	0
5	B	118	0	0	2	0
5	C	174	0	0	2	0
5	D	131	0	0	2	0
5	E	59	0	0	0	0
5	F	54	0	0	0	0
All	All	12944	0	12209	90	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 4.

All (90) 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:109:MSE:CE	1:D:109:MSE:SE	2.17	1.43
1:E:107[A]:MSE:HE2	1:E:109[A]:MSE:HA	1.20	1.18
1:F:107[A]:MSE:HE2	1:F:109[A]:MSE:HA	1.11	1.10
1:C:107[A]:MSE:HE2	1:C:109[A]:MSE:HA	1.19	1.08
1:A:107:MSE:HE2	1:A:109:MSE:HG3	1.26	1.07
1:E:107[A]:MSE:HE2	1:E:109[A]:MSE:CA	1.86	1.05
1:D:107:MSE:HE2	1:D:109:MSE:HA	1.40	1.02
1:A:107:MSE:HE2	1:A:109:MSE:CG	1.96	0.95
1:F:107[B]:MSE:HG2	1:F:109[B]:MSE:HE1	1.45	0.94
1:F:107[B]:MSE:CG	1:F:109[B]:MSE:CE	2.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107[B]:MSE:HB3	1:F:109[B]:MSE:HE3	1.50	0.93
1:F:107[A]:MSE:HE2	1:F:109[A]:MSE:CA	2.03	0.84
1:F:107[B]:MSE:HB3	1:F:109[B]:MSE:CE	2.08	0.83
1:F:107[B]:MSE:CG	1:F:109[B]:MSE:HE1	2.06	0.82
1:F:107[A]:MSE:CE	1:F:109[A]:MSE:HA	2.04	0.82
1:A:107:MSE:CE	1:A:109:MSE:HG3	2.11	0.78
1:F:107[B]:MSE:HG3	1:F:109[B]:MSE:HE2	1.67	0.76
1:F:107[B]:MSE:CB	1:F:109[B]:MSE:CE	2.67	0.73
1:C:107[A]:MSE:HE2	1:C:109[A]:MSE:CA	2.12	0.71
1:E:60[B]:ARG:HH22	1:E:258:ALA:HB1	1.56	0.71
1:E:107[A]:MSE:CE	1:E:109[A]:MSE:HA	2.06	0.71
1:E:60[B]:ARG:NH2	1:E:258:ALA:HB1	2.06	0.70
1:F:107[B]:MSE:HG2	1:F:109[B]:MSE:CE	2.16	0.68
1:B:107:MSE:HE2	1:B:109:MSE:CB	2.24	0.67
1:D:107:MSE:HE2	1:D:109:MSE:CA	2.23	0.67
1:E:107[A]:MSE:HE2	1:E:109[A]:MSE:CB	2.07	0.63
1:D:60[A]:ARG:NH2	1:D:258:ALA:HB1	2.14	0.63
1:C:253[B]:HIS:HE1	5:C:426:HOH:O	1.81	0.63
1:C:38:LEU:HD11	1:D:267:GLU:HG3	1.81	0.62
1:B:107:MSE:HE2	1:B:109:MSE:HG3	1.82	0.61
1:E:193:THR:HG22	1:E:194:THR:H	1.65	0.61
1:C:107[B]:MSE:HE3	1:C:108:VAL:H	1.66	0.60
1:B:107:MSE:HE2	1:B:109:MSE:HA	1.85	0.59
1:A:60[A]:ARG:NH2	1:A:258:ALA:HB1	2.18	0.57
1:A:283:GLN:O	1:A:284:PRO:CB	2.52	0.56
1:B:85:ARG:HD3	5:B:382:HOH:O	2.05	0.55
1:B:107:MSE:HE2	1:B:109:MSE:CG	2.37	0.55
1:D:140:ASN:ND2	5:D:414:HOH:O	2.39	0.53
1:C:107[A]:MSE:HE3	1:C:112:PHE:HD2	1.73	0.53
1:A:107:MSE:HE2	1:A:109:MSE:HA	1.91	0.53
1:A:173:GLU:HG3	2:A:287:ACT:H3	1.90	0.53
1:F:218:GLU:O	1:F:222:THR:HG23	2.09	0.52
1:B:107:MSE:HE2	1:B:109:MSE:CA	2.40	0.52
1:E:77:ASN:O	1:E:80:VAL:HG12	2.10	0.51
1:F:107[A]:MSE:HE3	1:F:112:PHE:HD2	1.76	0.51
1:A:221:ARG:HD2	5:A:392:HOH:O	2.12	0.49
1:A:147:SER:HB3	1:A:150:GLN:NE2	2.28	0.48
1:E:20:GLN:O	1:E:24:ARG:HG3	2.14	0.47
4:B:290:GOL:C3	5:B:336:HOH:O	2.64	0.46
1:E:97:LEU:HD12	1:E:97:LEU:N	2.30	0.46
1:A:107:MSE:CE	1:A:109:MSE:CG	2.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ILE:HD12	1:F:274:THR:HG23	1.96	0.46
1:B:106:PHE:HB3	1:C:85[A]:ARG:HG2	1.97	0.45
1:E:107[A]:MSE:HE3	1:E:112:PHE:HD2	1.82	0.45
1:B:263:ARG:O	1:B:267:GLU:HB2	2.17	0.45
1:B:117:LYS:NZ	1:B:161:LEU:O	2.35	0.44
1:B:50:LEU:C	1:B:50:LEU:HD12	2.38	0.44
1:C:218:GLU:O	1:C:222:THR:HG23	2.17	0.44
1:B:238:ASN:HB2	1:B:239:PRO:HD2	2.00	0.43
1:B:82:ASP:O	1:B:85:ARG:HG2	2.17	0.43
1:A:107:MSE:CE	1:A:109:MSE:HA	2.48	0.43
1:C:224:ARG:HD2	5:C:401:HOH:O	2.18	0.43
1:B:97:LEU:N	1:B:97:LEU:HD12	2.33	0.43
1:A:88:LEU:N	1:A:89:PRO:CD	2.81	0.43
1:F:97:LEU:HD12	1:F:97:LEU:N	2.34	0.43
1:B:186:LEU:HG	1:B:227:ILE:HD11	2.01	0.43
1:B:107:MSE:CE	1:B:109:MSE:HG3	2.48	0.42
1:A:176:VAL:HG23	1:A:219:ALA:HB1	2.01	0.42
1:A:238:ASN:HB2	1:A:239:PRO:HD2	2.02	0.42
1:B:217:ILE:HG21	1:B:251:GLY:HA3	2.00	0.42
1:A:267:GLU:HG3	1:B:38:LEU:HD11	2.01	0.42
1:A:38:LEU:C	1:A:38:LEU:HD23	2.39	0.42
1:A:147:SER:HB3	1:A:150:GLN:HE22	1.85	0.42
1:E:167:PRO:HD2	1:E:185:ILE:O	2.20	0.42
1:D:88:LEU:N	1:D:89:PRO:CD	2.83	0.41
1:B:109:MSE:HE2	1:B:154:MSE:HB2	2.02	0.41
1:D:9:ARG:HA	1:D:10:PRO:HD3	1.98	0.41
1:E:127:PHE:HA	1:E:128:PRO:C	2.40	0.41
1:E:278:LYS:CE	1:F:49:ASP:OD2	2.69	0.41
1:E:62:ALA:O	1:E:64:ARG:NH1	2.53	0.41
1:D:60[A]:ARG:NH2	5:D:314:HOH:O	2.35	0.41
1:E:170:PHE:CE2	1:E:189:HIS:HB3	2.56	0.41
1:D:193:THR:HG22	1:D:194:THR:N	2.35	0.41
1:D:176:VAL:HG23	1:D:219:ALA:HB1	2.02	0.40
1:F:36:THR:HG23	1:F:61:MSE:HG3	2.02	0.40
1:F:104:ASP:HA	1:F:105:PRO:HD3	1.89	0.40
1:C:165:THR:OG1	1:C:183:ALA:HA	2.21	0.40
1:C:167:PRO:HD2	1:C:185:ILE:O	2.21	0.40
1:E:193:THR:HG22	1:E:194:THR:N	2.34	0.40
1:B:32:GLY:HA2	1:B:257:GLY:O	2.22	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	267/286 (93%)	262 (98%)	5 (2%)	0	100	100
1	B	267/286 (93%)	263 (98%)	4 (2%)	0	100	100
1	C	270/286 (94%)	266 (98%)	4 (2%)	0	100	100
1	D	267/286 (93%)	263 (98%)	4 (2%)	0	100	100
1	E	270/286 (94%)	264 (98%)	6 (2%)	0	100	100
1	F	265/286 (93%)	260 (98%)	5 (2%)	0	100	100
All	All	1606/1716 (94%)	1578 (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	213/213 (100%)	210 (99%)	3 (1%)	74	80
1	B	206/213 (97%)	205 (100%)	1 (0%)	92	95
1	C	216/213 (101%)	212 (98%)	4 (2%)	65	69
1	D	213/213 (100%)	210 (99%)	3 (1%)	74	80
1	E	208/213 (98%)	197 (95%)	11 (5%)	28	23
1	F	202/213 (95%)	199 (98%)	3 (2%)	72	78
All	All	1258/1278 (98%)	1233 (98%)	25 (2%)	65	67

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	85	ARG
1	A	150	GLN
1	B	107	MSE
1	C	107[A]	MSE
1	C	107[B]	MSE
1	C	202	SER
1	C	225	ASP
1	D	9	ARG
1	D	50	LEU
1	D	224	ARG
1	E	13	SER
1	E	48	ILE
1	E	53	ILE
1	E	54	TYR
1	E	92	ARG
1	E	107[A]	MSE
1	E	107[B]	MSE
1	E	215	GLU
1	E	263	ARG
1	E	268	GLU
1	E	281	ARG
1	F	66	SER
1	F	136	LEU
1	F	224	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	ACT	A	286	-	1,3,3	1.13	0	0,3,3	0.00	-
2	ACT	A	287	-	1,3,3	1.56	0	0,3,3	0.00	-
2	ACT	A	288	-	1,3,3	1.71	0	0,3,3	0.00	-
4	GOL	A	291	-	5,5,5	0.42	0	5,5,5	0.64	0
4	GOL	A	292	-	5,5,5	0.36	0	5,5,5	0.61	0
2	ACT	B	286	-	1,3,3	1.74	0	0,3,3	0.00	-
2	ACT	B	287	-	1,3,3	2.10	1 (100%)	0,3,3	0.00	-
4	GOL	B	289	-	5,5,5	0.29	0	5,5,5	0.45	0
4	GOL	B	290	-	5,5,5	0.28	0	5,5,5	0.70	0
2	ACT	C	286	-	1,3,3	1.04	0	0,3,3	0.00	-
2	ACT	C	287	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
2	ACT	C	288	-	1,3,3	1.86	0	0,3,3	0.00	-
2	ACT	C	289	-	1,3,3	1.79	0	0,3,3	0.00	-
2	ACT	D	286	-	1,3,3	0.95	0	0,3,3	0.00	-
2	ACT	D	287	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
2	ACT	E	286	-	1,3,3	1.26	0	0,3,3	0.00	-
2	ACT	F	286	-	1,3,3	0.45	0	0,3,3	0.00	-

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	ACT	A	286	-	-	0/0/0/0	0/0/0/0
2	ACT	A	287	-	-	0/0/0/0	0/0/0/0
2	ACT	A	288	-	-	0/0/0/0	0/0/0/0
4	GOL	A	291	-	-	0/4/4/4	0/0/0/0
4	GOL	A	292	-	-	0/4/4/4	0/0/0/0
2	ACT	B	286	-	-	0/0/0/0	0/0/0/0
2	ACT	B	287	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	289	-	-	0/4/4/4	0/0/0/0
4	GOL	B	290	-	-	0/4/4/4	0/0/0/0
2	ACT	C	286	-	-	0/0/0/0	0/0/0/0
2	ACT	C	287	-	-	0/0/0/0	0/0/0/0
2	ACT	C	288	-	-	0/0/0/0	0/0/0/0
2	ACT	C	289	-	-	0/0/0/0	0/0/0/0
2	ACT	D	286	-	-	0/0/0/0	0/0/0/0
2	ACT	D	287	-	-	0/0/0/0	0/0/0/0
2	ACT	E	286	-	-	0/0/0/0	0/0/0/0
2	ACT	F	286	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	287	ACT	CH3-C	2.01	1.51	1.48
2	D	287	ACT	CH3-C	2.02	1.51	1.48
2	B	287	ACT	CH3-C	2.10	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	287	ACT	1	0
4	B	290	GOL	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	258/286 (90%)	0.25	5 (1%) 70 78	46, 52, 66, 83	0
1	B	258/286 (90%)	0.49	13 (5%) 32 43	46, 52, 65, 84	0
1	C	260/286 (90%)	0.37	15 (5%) 26 36	46, 52, 68, 94	0
1	D	258/286 (90%)	0.38	12 (4%) 35 46	46, 52, 65, 87	0
1	E	259/286 (90%)	0.81	35 (13%) 4 7	45, 53, 65, 85	0
1	F	256/286 (89%)	1.13	58 (22%) 1 2	45, 53, 65, 81	0
All	All	1549/1716 (90%)	0.57	138 (8%) 12 18	45, 52, 66, 94	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	27	GLU	5.8
1	F	226	ASP	5.2
1	F	227	ILE	5.0
1	F	251	GLY	4.9
1	F	23	ILE	4.6
1	F	16	VAL	4.6
1	E	283	GLN	4.6
1	F	250	GLN	4.5
1	A	284	PRO	4.4
1	F	24	ARG	4.3
1	B	205	SER	4.3
1	D	284	PRO	4.3
1	F	253	HIS	4.2
1	F	221	ARG	4.1
1	F	252	CYS	4.0
1	F	203	GLY	4.0
1	E	24	ARG	3.9
1	E	85[A]	ARG	3.8
1	C	26	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	249	CYS	3.8
1	D	85[A]	ARG	3.7
1	C	25	ALA	3.7
1	E	276	ALA	3.7
1	F	244	PHE	3.7
1	F	225	ASP	3.6
1	F	188	CYS	3.5
1	E	26	GLY	3.4
1	F	220	ALA	3.4
1	E	281	ARG	3.3
1	C	246	LEU	3.3
1	B	114	ARG	3.3
1	C	194	THR	3.2
1	C	252	CYS	3.2
1	E	179	ALA	3.2
1	E	181	ALA	3.2
1	D	221	ARG	3.1
1	E	193	THR	3.1
1	F	217	ILE	3.0
1	F	223	ILE	3.0
1	F	47	ASP	3.0
1	F	21	LYS	3.0
1	C	23	ILE	3.0
1	C	24	ARG	3.0
1	C	251	GLY	3.0
1	E	201	ARG	3.0
1	C	9	ARG	2.9
1	B	227	ILE	2.9
1	F	280	ILE	2.9
1	E	275	LEU	2.9
1	C	253[A]	HIS	2.9
1	E	21	LYS	2.9
1	F	238	ASN	2.9
1	F	183	ALA	2.9
1	E	13	SER	2.9
1	E	202	SER	2.9
1	E	282	ARG	2.8
1	B	223	ILE	2.8
1	F	279	ALA	2.8
1	D	106	PHE	2.8
1	B	11	THR	2.8
1	E	225	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	26	GLY	2.7
1	F	233	GLY	2.7
1	A	192	LEU	2.7
1	A	283	GLN	2.7
1	E	17	ASP	2.7
1	E	226	ASP	2.7
1	F	192	LEU	2.7
1	F	245	ILE	2.7
1	F	193	THR	2.7
1	D	24	ARG	2.6
1	E	28	PRO	2.6
1	E	81	VAL	2.6
1	F	17	ASP	2.6
1	F	182	GLY	2.6
1	E	27	GLU	2.6
1	F	81	VAL	2.6
1	F	187	VAL	2.6
1	E	249	CYS	2.6
1	E	250	GLN	2.5
1	C	217	ILE	2.5
1	E	12	ARG	2.5
1	F	231	SER	2.5
1	F	243	ARG	2.5
1	E	79	ILE	2.4
1	F	239	PRO	2.4
1	F	222	THR	2.4
1	F	283	GLN	2.4
1	C	249	CYS	2.4
1	E	182	GLY	2.4
1	F	25	ALA	2.4
1	F	79	ILE	2.4
1	B	73	TYR	2.4
1	F	15	LEU	2.4
1	F	246	LEU	2.4
1	B	235	PRO	2.4
1	E	223	ILE	2.4
1	F	19	PHE	2.4
1	B	79	ILE	2.3
1	F	28	PRO	2.3
1	B	243[A]	ARG	2.3
1	F	240	GLU	2.3
1	D	253	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	221	ARG	2.3
1	D	194	THR	2.3
1	F	157	GLU	2.3
1	F	212	LEU	2.3
1	E	25	ALA	2.3
1	C	213	ILE	2.3
1	D	79	ILE	2.3
1	F	162	ASP	2.3
1	B	211	SER	2.3
1	D	160	LYS	2.3
1	A	8	LYS	2.2
1	F	275	LEU	2.2
1	D	282	ARG	2.2
1	F	62	ALA	2.2
1	E	19	PHE	2.2
1	A	218[A]	GLU	2.2
1	C	228	ILE	2.2
1	B	159	HIS	2.2
1	F	13	SER	2.2
1	F	208	ASP	2.2
1	D	218	GLU	2.1
1	E	246	LEU	2.1
1	F	181	ALA	2.1
1	D	17	ASP	2.1
1	F	232	HIS	2.1
1	E	243	ARG	2.1
1	F	11	THR	2.1
1	F	14	GLU	2.0
1	B	182	GLY	2.0
1	B	16	VAL	2.0
1	E	222	THR	2.0
1	C	245	ILE	2.0
1	F	165	THR	2.0
1	E	159	HIS	2.0
1	E	82[A]	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	B	290	6/6	0.60	0.32	3.96	89,91,93,97	0
4	GOL	B	289	6/6	0.92	0.20	2.51	95,96,97,97	0
4	GOL	A	292	6/6	0.87	0.18	1.60	63,81,84,87	0
2	ACT	C	288	4/4	0.83	0.22	1.24	83,85,86,87	0
2	ACT	C	289	4/4	0.95	0.14	0.79	62,64,65,67	0
4	GOL	A	291	6/6	0.86	0.26	0.70	55,69,73,77	0
2	ACT	A	288	4/4	0.89	0.22	0.27	79,80,81,82	0
2	ACT	B	287	4/4	0.93	0.15	0.21	62,63,64,64	0
2	ACT	A	287	4/4	0.91	0.15	0.16	61,65,65,67	0
2	ACT	D	286	4/4	0.97	0.13	-0.82	44,46,47,49	0
3	CL	A	290	1/1	0.97	0.10	-1.22	76,76,76,76	0
2	ACT	D	287	4/4	0.97	0.10	-1.27	58,61,61,61	0
2	ACT	C	286	4/4	0.97	0.10	-1.52	45,48,49,49	0
2	ACT	E	286	4/4	0.94	0.11	-1.54	43,46,47,48	0
2	ACT	B	286	4/4	0.99	0.10	-1.66	45,45,48,50	0
3	CL	D	288	1/1	0.99	0.08	-1.69	51,51,51,51	0
3	CL	B	288	1/1	0.99	0.07	-2.34	52,52,52,52	0
2	ACT	F	286	4/4	0.98	0.09	-2.57	48,50,50,50	0
2	ACT	A	286	4/4	0.98	0.08	-2.76	42,44,45,45	0
3	CL	C	290	1/1	0.98	0.08	-2.81	44,44,44,44	0
3	CL	A	289	1/1	1.00	0.05	-5.08	46,46,46,46	0
2	ACT	C	287	4/4	0.47	0.43	-	85,88,89,89	0
3	CL	C	291	1/1	0.96	0.07	-	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.