Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2017 – 06:40 PM EDT

PDB ID	:	2Q78
Title	:	Crystal structure of a thioesterase-like protein (tm0581) from thermotoga maritima msb8 at 2.20 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	unknown
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

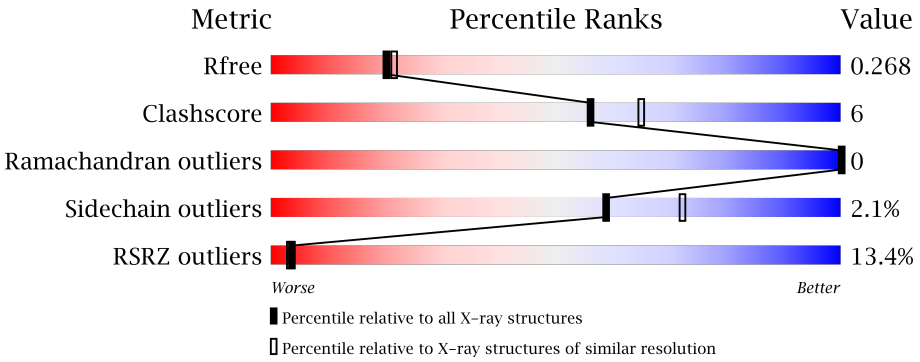
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	11% 80% 8% 12%
1	B	153	4% 79% 7% 14%
1	C	153	14% 76% 9% 14%
1	D	153	10% 77% 7% • 15%
1	E	153	20% 72% 13% • 14%

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Mol	Chain	Length	Quality of chain
1	F	153	12% 78% 9% • 11%
1	G	153	8% 69% 16% • 14%
1	H	153	9% 76% 10% 14%

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	MLC	A	200	X	-	-	-
2	MLC	B	200	X	-	-	-
2	MLC	C	200	X	-	-	-
2	MLC	D	200	X	-	-	-
2	MLC	E	200	X	-	-	-
2	MLC	F	200	X	-	-	-
2	MLC	G	200	X	-	-	-
2	MLC	H	200	X	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9110 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	Se	0	0	0
			1064	679	190	190	5			
1	B	131	Total	C	N	O	Se	0	6	0
			1061	684	185	186	6			
1	C	131	Total	C	N	O	Se	0	5	0
			1052	674	189	184	5			
1	D	130	Total	C	N	O	Se	0	7	0
			1055	676	186	188	5			
1	E	131	Total	C	N	O	Se	0	2	0
			1027	656	184	182	5			
1	F	136	Total	C	N	O	Se	0	1	0
			1052	674	188	185	5			
1	G	131	Total	C	N	O	Se	0	7	0
			1069	683	195	186	5			
1	H	131	Total	C	N	O	Se	0	0	0
			1014	649	179	181	5			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
A	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
A	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
B	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
B	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
B	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
B	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
C	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
C	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
C	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
C	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
C	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
D	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
D	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
D	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
D	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
D	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
E	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
E	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
E	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
E	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
E	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
E	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
E	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
E	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
E	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
E	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
E	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
E	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
E	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
E	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
E	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
E	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
F	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
F	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
F	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
F	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
F	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
F	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
F	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
F	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
F	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
F	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
F	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
F	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50

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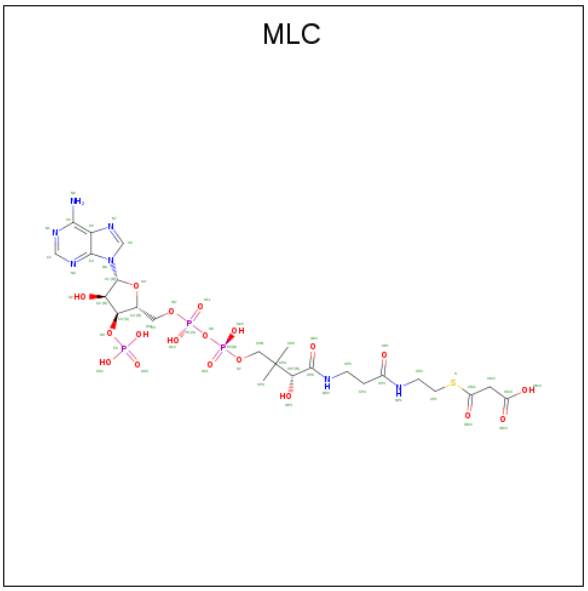
Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
F	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
F	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
F	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
F	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
G	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
G	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
G	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
G	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
G	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
G	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
G	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
G	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
G	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
G	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
G	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
G	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
G	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
G	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
G	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
G	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
H	-11	MSE	-	LEADER SEQUENCE	UNP Q9WZ50
H	-10	GLY	-	LEADER SEQUENCE	UNP Q9WZ50
H	-9	SER	-	LEADER SEQUENCE	UNP Q9WZ50
H	-8	ASP	-	LEADER SEQUENCE	UNP Q9WZ50
H	-7	LYS	-	LEADER SEQUENCE	UNP Q9WZ50
H	-6	ILE	-	LEADER SEQUENCE	UNP Q9WZ50
H	-5	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
H	-4	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
H	-3	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
H	-2	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
H	-1	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
H	0	HIS	-	LEADER SEQUENCE	UNP Q9WZ50
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
H	2	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
H	22	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
H	30	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50
H	103	MSE	MET	MODIFIED RESIDUE	UNP Q9WZ50

- Molecule 2 is MALONYL-COENZYME A (three-letter code: MLC) (formula: $C_{24}H_{38}N_7O_{19}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			54	24	7	19	3	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

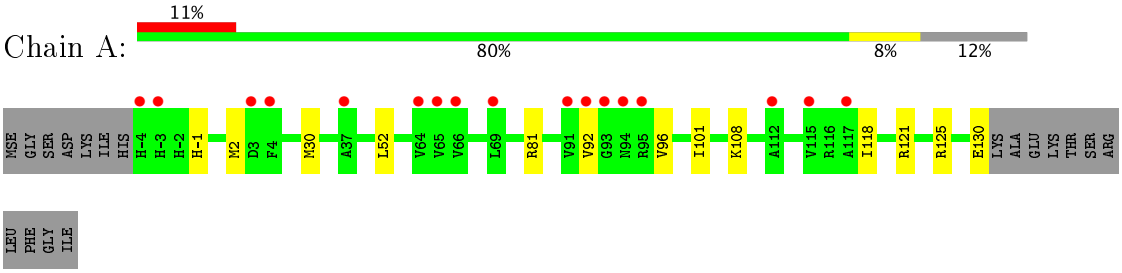
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total O 63 63	0	0
4	B	38	Total O 38 38	0	0
4	C	39	Total O 39 39	0	0
4	D	60	Total O 60 60	0	0
4	E	9	Total O 9 9	0	0
4	F	29	Total O 29 29	0	0
4	G	17	Total O 17 17	0	0
4	H	27	Total O 27 27	0	0

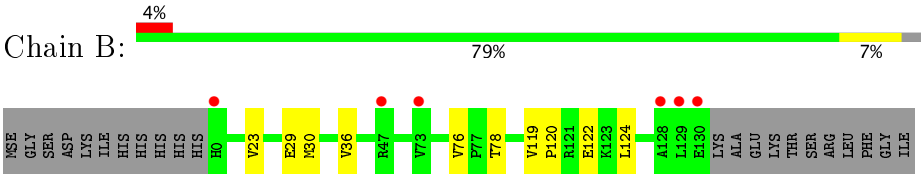
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

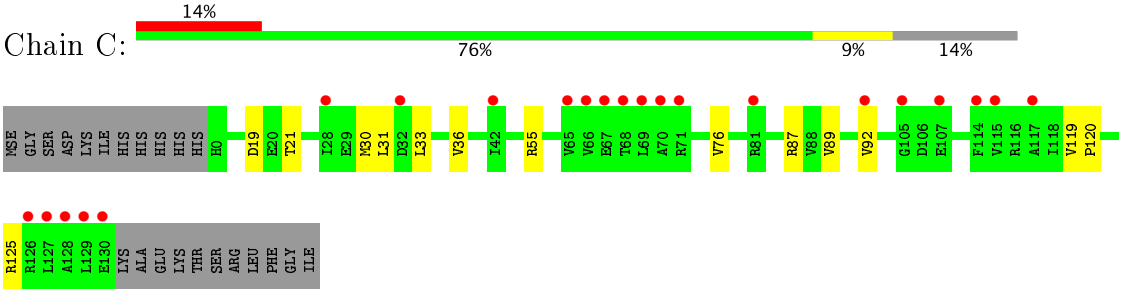
- Molecule 1: Uncharacterized protein



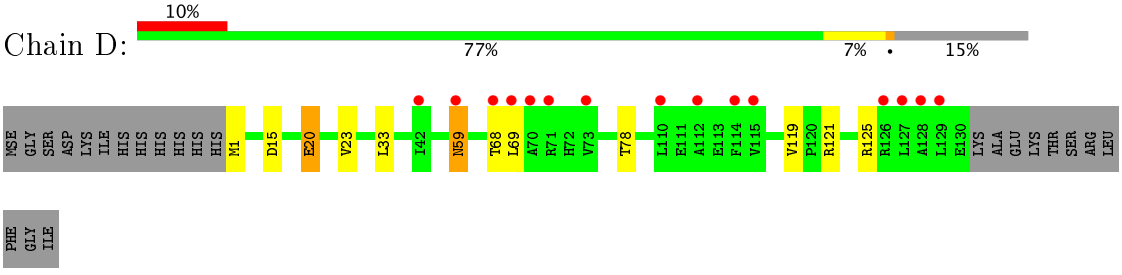
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein

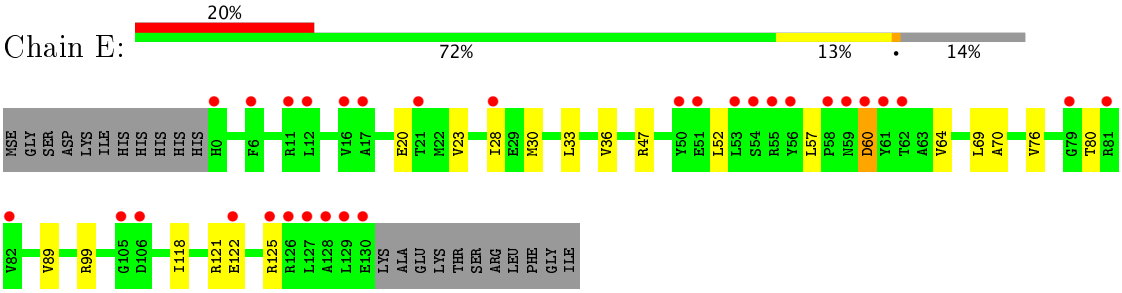


- Molecule 1: Uncharacterized protein



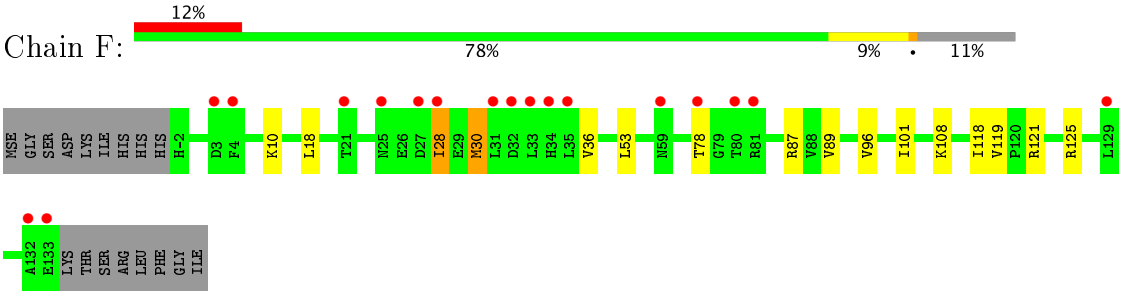
- Molecule 1: Uncharacterized protein

Chain E:



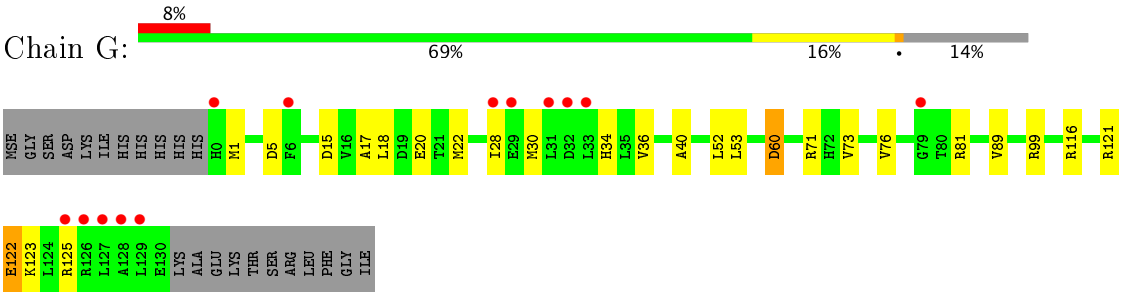
• Molecule 1: Uncharacterized protein

Chain F:



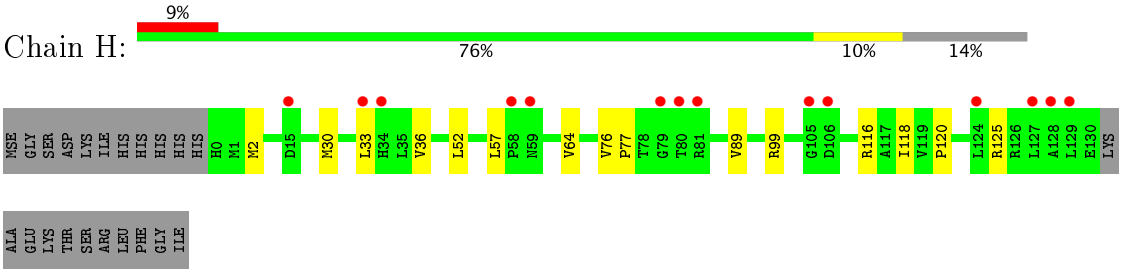
• Molecule 1: Uncharacterized protein

Chain G:



• Molecule 1: Uncharacterized protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.35Å 90.71Å 230.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.20 29.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.98-2.20) 99.7 (29.98-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.20Å)	Xtriage
Refinement program	PHENIX, REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.224 0.228 , 0.268	Depositor DCC
R_{free} test set	3296 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9110	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: MLC, 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	0.73	0/1077	0.82	0/1451
1	B	0.66	0/1086	0.72	0/1462
1	C	0.65	0/1075	0.75	0/1446
1	D	0.70	0/1086	0.75	0/1465
1	E	0.49	0/1042	0.65	0/1403
1	F	0.53	0/1066	0.69	0/1438
1	G	0.53	0/1100	0.70	0/1479
1	H	0.55	0/1023	0.68	1/1379 (0.1%)
All	All	0.61	0/8555	0.72	1/11523 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	116	ARG	NE-CZ-NH2	-5.60	117.50	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1	MSE	Peptide

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	1064	0	1082	10	0
1	B	1061	0	1118	9	0
1	C	1052	0	1108	19	0
1	D	1055	0	1107	12	0
1	E	1027	0	1059	16	0
1	F	1052	0	1076	17	0
1	G	1069	0	1120	23	0
1	H	1014	0	1040	13	0
2	A	54	0	33	0	0
2	B	54	0	33	1	0
2	C	54	0	33	0	0
2	D	54	0	33	1	0
2	E	54	0	33	1	0
2	F	54	0	33	1	0
2	G	54	0	33	1	0
2	H	54	0	33	4	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	63	0	0	0	0
4	B	38	0	0	1	0
4	C	39	0	0	0	0
4	D	60	0	0	0	0
4	E	9	0	0	0	0
4	F	29	0	0	1	0
4	G	17	0	0	0	0
4	H	27	0	0	0	0
All	All	9110	0	8974	103	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 6.

All (103) 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:2:MSE:CE	1:A:2:MSE:SE	2.15	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:MSE:HE3	1:F:121:ARG:HD3	1.55	0.89
1:C:36:VAL:CG1	1:C:76:VAL:HG13	2.10	0.81
1:C:36:VAL:CG1	1:C:76:VAL:CG1	2.60	0.80
1:C:36:VAL:HG12	1:C:76:VAL:HG13	1.69	0.73
1:G:121:ARG:HD3	1:H:30:MSE:HE3	1.70	0.72
1:C:36:VAL:HG11	1:C:76:VAL:CG1	2.19	0.71
1:C:36:VAL:HG12	1:C:76:VAL:CG1	2.22	0.69
1:G:89:VAL:HG11	1:G:99[B]:ARG:HG3	1.73	0.69
1:G:60:ASP:OD1	1:G:60:ASP:N	2.28	0.67
1:F:10:LYS:NZ	4:F:218:HOH:O	2.21	0.66
1:A:96:VAL:HG21	1:A:118:ILE:HD11	1.77	0.66
1:A:121:ARG:HD3	1:B:30[A]:MSE:HE3	1.78	0.66
1:C:36:VAL:HG11	1:C:76:VAL:HG13	1.79	0.65
1:A:30:MSE:HA	1:A:30:MSE:HE2	1.78	0.64
1:E:57:LEU:HD21	1:E:118:ILE:HD13	1.82	0.62
1:A:96:VAL:CG2	1:A:118:ILE:HD11	2.30	0.62
1:H:64:VAL:HG21	2:H:200:MLC:HP81	1.83	0.61
1:F:18:LEU:HD13	1:F:36:VAL:HG21	1.83	0.60
1:H:52:LEU:C	1:H:52:LEU:HD23	2.23	0.59
1:F:101:ILE:HD11	1:F:108:LYS:HG3	1.87	0.57
1:H:89:VAL:HG11	1:H:99:ARG:HD2	1.87	0.57
1:E:30:MSE:HE2	1:F:125:ARG:NH2	2.20	0.56
1:E:64:VAL:HG21	2:E:200:MLC:HP81	1.86	0.56
1:G:18:LEU:HD13	1:G:36[B]:VAL:HG21	1.88	0.55
1:E:30:MSE:HE2	1:F:125:ARG:HH21	1.71	0.55
1:C:30:MSE:HE3	1:D:121:ARG:HD3	1.88	0.55
1:B:36:VAL:HG12	1:B:76:VAL:HG12	1.88	0.54
1:E:20:GLU:O	1:E:23:VAL:HG12	2.07	0.54
1:E:33:LEU:HD21	1:F:125:ARG:HG2	1.90	0.53
1:H:64:VAL:CG2	2:H:200:MLC:HP81	2.37	0.53
1:E:121:ARG:O	1:E:125[B]:ARG:HG3	2.10	0.52
1:A:52:LEU:C	1:A:52:LEU:HD23	2.30	0.52
1:B:29:GLU:O	1:B:30[A]:MSE:HE2	2.11	0.51
1:F:96:VAL:CG2	1:F:118:ILE:HD11	2.41	0.51
1:C:87[A]:ARG:HH11	1:C:89:VAL:HG12	1.76	0.51
1:F:28:ILE:HD12	1:F:28:ILE:N	2.26	0.50
1:G:30:MSE:HE3	1:H:125:ARG:NH2	2.26	0.50
1:G:125[B]:ARG:CZ	1:H:30:MSE:HE1	2.42	0.50
1:F:28:ILE:CD1	1:F:28:ILE:N	2.75	0.49
2:B:200:MLC:O22	2:H:200:MLC:O22	2.31	0.49
1:G:123:LYS:HG2	2:G:200:MLC:H4'	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125[B]:ARG:HG2	1:D:33:LEU:HD11	1.93	0.49
1:E:52:LEU:HD23	1:E:52:LEU:C	2.33	0.49
1:G:122[B]:GLU:OE2	1:G:125[B]:ARG:HD2	2.13	0.48
1:G:52:LEU:C	1:G:52:LEU:HD23	2.33	0.48
1:G:89:VAL:CG1	1:G:99[B]:ARG:HG3	2.39	0.48
1:G:28:ILE:HD12	1:G:28:ILE:H	1.79	0.48
1:G:28:ILE:HD12	1:G:28:ILE:N	2.29	0.48
1:C:36:VAL:CG1	1:C:76:VAL:HG12	2.41	0.48
1:G:20:GLU:OE2	1:G:34[B]:HIS:ND1	2.47	0.48
1:C:87[A]:ARG:NH1	1:C:89:VAL:HG12	2.28	0.47
1:G:22:MSE:HB3	1:G:40:ALA:HB1	1.96	0.47
1:A:101:ILE:HD11	1:A:108:LYS:CD	2.43	0.47
1:G:36[A]:VAL:CG1	1:G:76:VAL:CG1	2.93	0.47
1:F:30:MSE:HA	1:F:30:MSE:HE2	1.96	0.46
1:B:36:VAL:CG1	1:B:76:VAL:HG12	2.45	0.46
1:B:119[B]:VAL:HG21	1:B:124:LEU:HD13	1.97	0.46
1:G:17:ALA:HB2	1:G:81:ARG:NH2	2.31	0.46
1:C:33:LEU:HD21	1:D:125:ARG:HG2	1.97	0.45
1:E:89:VAL:HG11	1:E:99:ARG:HD2	1.97	0.45
1:D:119[A]:VAL:HG13	2:D:200:MLC:H4'	1.97	0.45
1:C:125[A]:ARG:HG2	1:D:33:LEU:HD11	1.98	0.45
1:E:60:ASP:N	1:E:60:ASP:OD1	2.42	0.45
1:G:71:ARG:NH2	1:G:73:VAL:HG12	2.31	0.45
1:H:57:LEU:HD21	1:H:118:ILE:HD13	1.99	0.45
1:A:92:VAL:CG2	1:C:92:VAL:HG23	2.47	0.45
1:C:19:ASP:OD1	1:C:21:THR:HG23	2.17	0.45
1:C:36:VAL:HG12	1:C:76:VAL:O	2.17	0.44
1:B:119[A]:VAL:HG12	1:B:120:PRO:O	2.17	0.44
1:E:30:MSE:HE1	1:F:125:ARG:NE	2.33	0.43
1:B:23[B]:VAL:HG22	1:B:78:THR:HG21	2.00	0.43
1:G:36[A]:VAL:HG11	1:G:76:VAL:CG1	2.49	0.43
1:D:23[B]:VAL:HG22	1:D:78:THR:HG21	1.99	0.43
1:F:87:ARG:NH1	1:F:89:VAL:HG12	2.34	0.43
1:H:120:PRO:HD3	2:H:200:MLC:H1'	2.01	0.43
1:H:30:MSE:HA	1:H:30:MSE:HE2	2.00	0.43
1:E:30:MSE:HE1	1:F:125:ARG:HE	1.84	0.43
1:E:69:LEU:HD12	1:E:70:ALA:N	2.35	0.42
1:H:76:VAL:HG22	1:H:77:PRO:HD2	2.00	0.42
1:A:-1:HIS:O	1:A:-1:HIS:CD2	2.72	0.42
1:C:119[A]:VAL:HG13	1:C:120:PRO:HD2	2.01	0.42
1:A:125:ARG:HH21	1:B:30[A]:MSE:HE2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:ASP:OD1	1:G:81:ARG:HG2	2.19	0.41
1:B:30[A]:MSE:CE	4:B:225:HOH:O	2.67	0.41
1:E:36:VAL:HG12	1:E:76:VAL:O	2.20	0.41
1:G:125[A]:ARG:NH1	1:H:33:LEU:HD21	2.36	0.41
1:D:68:THR:C	1:D:69:LEU:HD12	2.40	0.41
1:E:28:ILE:H	1:E:28:ILE:HD12	1.85	0.41
1:D:59:ASN:O	1:D:121:ARG:NH1	2.54	0.41
1:F:119:VAL:HG22	2:F:200:MLC:H4'	2.02	0.41
1:D:20:GLU:HG3	1:D:23[B]:VAL:HG21	2.03	0.41
1:F:36:VAL:HG22	1:F:78:THR:HG22	2.02	0.41
1:G:36[A]:VAL:HG12	1:G:76:VAL:CG1	2.51	0.41
1:C:36:VAL:HG12	1:C:76:VAL:HG12	2.00	0.41
1:D:20:GLU:HA	1:D:23[B]:VAL:HG23	2.03	0.41
1:G:121:ARG:O	1:G:125[B]:ARG:HG3	2.20	0.41
1:F:53:LEU:HA	1:F:53:LEU:HD23	1.93	0.40
1:C:31:LEU:HA	1:C:31:LEU:HD23	1.96	0.40
1:D:20:GLU:O	1:D:23[B]:VAL:HG23	2.20	0.40
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.88	0.40
1:H:36:VAL:HG12	1:H:76:VAL:O	2.22	0.40
1:G:53:LEU:HD12	1:G:116:ARG:HD2	2.04	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	133/153 (87%)	129 (97%)	4 (3%)	0	100	100
1	B	135/153 (88%)	133 (98%)	2 (2%)	0	100	100
1	C	134/153 (88%)	133 (99%)	1 (1%)	0	100	100
1	D	135/153 (88%)	131 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	131/153 (86%)	127 (97%)	4 (3%)	0	100	100
1	F	135/153 (88%)	134 (99%)	1 (1%)	0	100	100
1	G	136/153 (89%)	135 (99%)	1 (1%)	0	100	100
1	H	129/153 (84%)	127 (98%)	2 (2%)	0	100	100
All	All	1068/1224 (87%)	1049 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/126 (90%)	111 (98%)	2 (2%)	64	77
1	B	115/126 (91%)	114 (99%)	1 (1%)	82	91
1	C	112/126 (89%)	111 (99%)	1 (1%)	82	91
1	D	115/126 (91%)	111 (96%)	4 (4%)	41	51
1	E	108/126 (86%)	104 (96%)	4 (4%)	39	49
1	F	109/126 (86%)	107 (98%)	2 (2%)	64	77
1	G	115/126 (91%)	111 (96%)	4 (4%)	41	51
1	H	106/126 (84%)	105 (99%)	1 (1%)	82	91
All	All	893/1008 (89%)	874 (98%)	19 (2%)	59	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	130	GLU
1	B	122	GLU
1	C	55	ARG
1	D	1	MSE
1	D	15	ASP

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Mol	Chain	Res	Type
1	D	20	GLU
1	D	59	ASN
1	E	47	ARG
1	E	60	ASP
1	E	80	THR
1	E	122	GLU
1	F	28	ILE
1	F	30	MSE
1	G	5	ASP
1	G	60	ASP
1	G	122[A]	GLU
1	G	122[B]	GLU
1	H	2	MSE

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	-1	HIS
1	A	0	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	MLC	A	200	-	46,56,56	1.03	3 (6%)	53,83,83	3.41	16 (30%)
2	MLC	B	200	-	46,56,56	0.91	1 (2%)	53,83,83	3.03	11 (20%)
2	MLC	C	200	-	46,56,56	0.93	3 (6%)	53,83,83	3.27	7 (13%)
2	MLC	D	200	-	46,56,56	1.01	2 (4%)	53,83,83	2.82	9 (16%)
2	MLC	E	200	-	46,56,56	1.02	3 (6%)	53,83,83	1.96	8 (15%)
2	MLC	F	200	-	46,56,56	0.92	3 (6%)	53,83,83	2.57	7 (13%)
2	MLC	G	200	-	46,56,56	0.98	3 (6%)	53,83,83	3.10	6 (11%)
2	MLC	H	200	-	46,56,56	1.05	3 (6%)	53,83,83	2.24	9 (16%)

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	MLC	A	200	-	1/1/13/15	0/48/71/71	0/3/3/3
2	MLC	B	200	-	1/1/13/15	0/48/71/71	0/3/3/3
2	MLC	C	200	-	1/1/13/15	0/48/71/71	0/3/3/3
2	MLC	D	200	-	1/1/13/15	0/48/71/71	0/3/3/3
2	MLC	E	200	-	1/1/13/15	1/48/71/71	0/3/3/3
2	MLC	F	200	-	1/1/13/15	0/48/71/71	0/3/3/3
2	MLC	G	200	-	1/1/13/15	0/48/71/71	0/3/3/3
2	MLC	H	200	-	1/1/13/15	0/48/71/71	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	200	MLC	CM1-S	-3.70	1.68	1.76
2	H	200	MLC	CM1-S	-3.65	1.68	1.76
2	D	200	MLC	CM1-S	-2.82	1.70	1.76
2	G	200	MLC	CM1-S	-2.52	1.71	1.76
2	F	200	MLC	CM1-S	-2.05	1.72	1.76
2	H	200	MLC	P3-O3'	2.02	1.63	1.59
2	F	200	MLC	C2-N3	2.03	1.35	1.32
2	E	200	MLC	C2-N3	2.04	1.35	1.32
2	A	200	MLC	P3-O3'	2.07	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200	MLC	CM2-CM1	2.24	1.58	1.50
2	G	200	MLC	C2-N3	2.36	1.36	1.32
2	A	200	MLC	OM2-CM1	2.50	1.24	1.21
2	C	200	MLC	C2-N3	2.58	1.36	1.32
2	F	200	MLC	C5-C4	2.68	1.46	1.40
2	C	200	MLC	C5-C4	2.77	1.46	1.40
2	E	200	MLC	C5-C4	3.05	1.47	1.40
2	G	200	MLC	C5-C4	3.15	1.47	1.40
2	A	200	MLC	C5-C4	3.22	1.47	1.40
2	B	200	MLC	C5-C4	3.28	1.47	1.40
2	H	200	MLC	C5-C4	3.41	1.48	1.40
2	D	200	MLC	C5-C4	3.47	1.48	1.40

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	200	MLC	OM2-CM1-S	-9.46	112.94	122.84
2	C	200	MLC	OM2-CM1-S	-8.92	113.50	122.84
2	A	200	MLC	OM2-CM1-CM2	-7.91	111.17	123.08
2	D	200	MLC	OM2-CM1-S	-7.63	114.85	122.84
2	B	200	MLC	N3-C2-N1	-7.56	122.27	128.86
2	C	200	MLC	N3-C2-N1	-7.40	122.41	128.86
2	E	200	MLC	N3-C2-N1	-7.15	122.63	128.86
2	D	200	MLC	N3-C2-N1	-6.95	122.81	128.86
2	B	200	MLC	OM2-CM1-S	-6.86	115.66	122.84
2	H	200	MLC	N3-C2-N1	-6.77	122.96	128.86
2	H	200	MLC	OM2-CM1-S	-6.72	115.81	122.84
2	A	200	MLC	OM2-CM1-S	-6.56	115.97	122.84
2	F	200	MLC	N3-C2-N1	-6.47	123.22	128.86
2	B	200	MLC	OM2-CM1-CM2	-6.47	113.34	123.08
2	A	200	MLC	N3-C2-N1	-6.21	123.45	128.86
2	C	200	MLC	OM2-CM1-CM2	-6.15	113.81	123.08
2	G	200	MLC	N3-C2-N1	-6.11	123.53	128.86
2	F	200	MLC	OM2-CM1-CM2	-6.03	114.00	123.08
2	G	200	MLC	OM2-CM1-CM2	-5.16	115.30	123.08
2	A	200	MLC	O2'-C2'-C3'	-4.80	97.53	111.18
2	D	200	MLC	OM2-CM1-CM2	-4.78	115.89	123.08
2	F	200	MLC	OM2-CM1-S	-4.63	117.99	122.84
2	E	200	MLC	OM2-CM1-S	-4.23	118.41	122.84
2	A	200	MLC	O31-P3-O3'	-2.95	92.58	106.00
2	B	200	MLC	CP8-CPA-CPB	-2.72	104.37	108.37
2	H	200	MLC	C4-C5-N7	-2.65	106.85	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	200	MLC	C4-C5-N7	-2.64	106.86	109.41
2	E	200	MLC	OM2-CM1-CM2	-2.54	119.25	123.08
2	D	200	MLC	C4-C5-N7	-2.34	107.15	109.41
2	C	200	MLC	O2'-C2'-C3'	-2.25	104.79	111.18
2	A	200	MLC	CP8-CPA-CPB	-2.21	105.12	108.37
2	C	200	MLC	C4-C5-N7	-2.20	107.29	109.41
2	E	200	MLC	C4-C5-N7	-2.20	107.29	109.41
2	B	200	MLC	C4-C5-N7	-2.18	107.31	109.41
2	D	200	MLC	CP8-CPA-CPB	-2.13	105.23	108.37
2	A	200	MLC	CP5-CP4-CP3	-2.12	108.80	112.22
2	A	200	MLC	OP1-CP3-CP4	-2.10	118.06	122.01
2	F	200	MLC	O2'-C2'-C1'	-2.08	105.09	111.61
2	B	200	MLC	CP4-CP5-NP2	-2.08	107.57	111.87
2	A	200	MLC	CP4-CP5-NP2	-2.02	107.69	111.87
2	E	200	MLC	C3'-C2'-C1'	2.06	104.58	99.95
2	H	200	MLC	O22-P2-O21	2.08	123.04	112.28
2	A	200	MLC	C4'-O4'-C1'	2.09	111.99	109.77
2	A	200	MLC	O22-P2-O21	2.09	123.10	112.28
2	D	200	MLC	CP7-CP6-NP2	2.10	120.95	116.58
2	E	200	MLC	O32-P3-O31	2.16	116.33	107.61
2	B	200	MLC	C2-N1-C6	2.16	122.55	118.77
2	B	200	MLC	CP8-CPA-CP7	2.18	112.59	108.82
2	H	200	MLC	C2-N1-C6	2.23	122.66	118.77
2	E	200	MLC	N6-C6-N1	2.23	123.19	118.77
2	H	200	MLC	CP2-CP1-S	2.28	117.85	111.23
2	B	200	MLC	O32-P3-O31	2.28	116.82	107.61
2	D	200	MLC	C2-N1-C6	2.30	122.80	118.77
2	D	200	MLC	C3'-C2'-C1'	2.30	105.12	99.95
2	A	200	MLC	C2-N1-C6	2.33	122.85	118.77
2	F	200	MLC	N6-C6-N1	2.40	123.51	118.77
2	A	200	MLC	N6-C6-N1	2.41	123.54	118.77
2	H	200	MLC	CP4-CP5-NP2	2.56	117.17	111.87
2	B	200	MLC	C3'-C2'-C1'	2.58	105.75	99.95
2	G	200	MLC	C3'-C2'-C1'	2.59	105.76	99.95
2	F	200	MLC	C3'-C2'-C1'	3.05	106.80	99.95
2	A	200	MLC	O3'-C3'-C2'	3.26	123.72	111.63
2	H	200	MLC	C3'-C2'-C1'	3.34	107.46	99.95
2	C	200	MLC	C3'-C2'-C1'	3.39	107.56	99.95
2	A	200	MLC	C3'-C2'-C1'	3.68	108.23	99.95
2	E	200	MLC	CM2-CM1-S	8.41	122.34	113.42
2	H	200	MLC	CM2-CM1-S	9.63	123.63	113.42
2	F	200	MLC	CM2-CM1-S	13.74	128.00	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	200	MLC	CM2-CM1-S	14.90	129.22	113.42
2	B	200	MLC	CM2-CM1-S	16.55	130.98	113.42
2	G	200	MLC	CM2-CM1-S	17.24	131.71	113.42
2	C	200	MLC	CM2-CM1-S	18.12	132.64	113.42
2	A	200	MLC	CM2-CM1-S	18.30	132.84	113.42

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	200	MLC	C3'
2	A	200	MLC	C3'
2	G	200	MLC	C3'
2	E	200	MLC	C3'
2	H	200	MLC	C3'
2	B	200	MLC	C3'
2	F	200	MLC	C3'
2	D	200	MLC	C3'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	200	MLC	P3-O3'-C3'-C2'

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200	MLC	1	0
2	D	200	MLC	1	0
2	E	200	MLC	1	0
2	F	200	MLC	1	0
2	G	200	MLC	1	0
2	H	200	MLC	4	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	130/153 (84%)	0.57	17 (13%) 4 3	42, 51, 69, 97	0
1	B	126/153 (82%)	0.36	6 (4%) 31 30	43, 51, 66, 92	0
1	C	126/153 (82%)	0.83	22 (17%) 2 2	44, 50, 69, 83	0
1	D	125/153 (81%)	0.68	15 (12%) 5 4	43, 50, 67, 82	0
1	E	126/153 (82%)	1.16	31 (24%) 1 1	44, 53, 67, 82	0
1	F	131/153 (85%)	0.76	18 (13%) 3 3	43, 52, 72, 84	0
1	G	126/153 (82%)	0.62	13 (10%) 7 6	43, 52, 64, 89	0
1	H	126/153 (82%)	0.62	14 (11%) 6 5	45, 52, 66, 82	0
All	All	1016/1224 (83%)	0.70	136 (13%) 4 3	42, 51, 70, 97	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	128	ALA	8.1
1	H	129	LEU	6.9
1	G	128	ALA	5.6
1	E	129	LEU	5.5
1	F	34	HIS	5.5
1	D	69	LEU	5.2
1	C	69	LEU	4.9
1	G	129	LEU	4.9
1	C	115	VAL	4.8
1	E	59	ASN	4.8
1	B	129	LEU	4.8
1	C	129	LEU	4.7
1	F	28	ILE	4.4
1	F	21	THR	4.4
1	D	126	ARG	4.3
1	E	126	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	128	ALA	4.2
1	H	58	PRO	4.2
1	G	33	LEU	4.0
1	C	68	THR	4.0
1	F	33	LEU	3.9
1	E	28	ILE	3.9
1	C	128	ALA	3.9
1	D	70	ALA	3.9
1	G	28	ILE	3.9
1	E	106	ASP	3.8
1	E	61	TYR	3.8
1	D	129	LEU	3.8
1	F	31	LEU	3.8
1	G	127	LEU	3.8
1	C	66	VAL	3.7
1	E	12	LEU	3.6
1	E	127	LEU	3.5
1	E	11	ARG	3.5
1	E	79	GLY	3.5
1	H	79	GLY	3.5
1	E	53	LEU	3.5
1	F	132	ALA	3.4
1	H	106	ASP	3.3
1	H	34	HIS	3.3
1	D	128	ALA	3.3
1	A	117	ALA	3.3
1	C	107	GLU	3.3
1	F	80	THR	3.3
1	B	0	HIS	3.2
1	D	112	ALA	3.1
1	E	55	ARG	3.1
1	D	114	PHE	3.1
1	C	126	ARG	3.1
1	E	82	VAL	3.1
1	E	54	SER	3.0
1	A	92	VAL	3.0
1	E	21	THR	3.0
1	C	105	GLY	3.0
1	E	62	THR	3.0
1	D	71	ARG	2.9
1	A	-3	HIS	2.9
1	G	6	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	79	GLY	2.9
1	E	81	ARG	2.9
1	C	65	VAL	2.9
1	C	117	ALA	2.9
1	H	81	ARG	2.9
1	F	35	LEU	2.9
1	D	127	LEU	2.8
1	B	47[A]	ARG	2.8
1	E	105	GLY	2.8
1	E	0	HIS	2.8
1	D	68	THR	2.8
1	F	78	THR	2.8
1	C	42	ILE	2.7
1	A	65	VAL	2.7
1	E	51	GLU	2.6
1	C	67	GLU	2.6
1	H	105	GLY	2.6
1	E	130	GLU	2.6
1	C	32	ASP	2.6
1	D	115	VAL	2.5
1	C	81	ARG	2.5
1	A	64	VAL	2.5
1	C	114	PHE	2.5
1	F	27	ASP	2.5
1	G	32	ASP	2.5
1	A	93	GLY	2.5
1	A	69	LEU	2.5
1	A	37	ALA	2.5
1	F	32	ASP	2.5
1	F	133	GLU	2.5
1	A	4	PHE	2.5
1	E	56	TYR	2.5
1	C	71[A]	ARG	2.4
1	G	0	HIS	2.4
1	E	125[A]	ARG	2.4
1	H	59	ASN	2.4
1	E	50	TYR	2.4
1	F	129[A]	LEU	2.4
1	H	124	LEU	2.4
1	F	59	ASN	2.4
1	A	91	VAL	2.4
1	C	92	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	6	PHE	2.4
1	B	128	ALA	2.4
1	E	122	GLU	2.4
1	E	60	ASP	2.3
1	G	29	GLU	2.3
1	H	127	LEU	2.3
1	F	81	ARG	2.3
1	F	3	ASP	2.3
1	C	28	ILE	2.3
1	A	66	VAL	2.3
1	H	15	ASP	2.3
1	C	70	ALA	2.3
1	F	4	PHE	2.2
1	E	17	ALA	2.2
1	A	-4	HIS	2.2
1	A	3	ASP	2.2
1	D	110	LEU	2.2
1	A	115	VAL	2.2
1	E	16	VAL	2.2
1	E	58	PRO	2.2
1	G	125[A]	ARG	2.2
1	G	126	ARG	2.2
1	G	31	LEU	2.2
1	B	73	VAL	2.1
1	H	33	LEU	2.1
1	A	112	ALA	2.1
1	C	130	GLU	2.1
1	D	73	VAL	2.1
1	D	42	ILE	2.0
1	A	94	ASN	2.0
1	D	59	ASN	2.0
1	B	130	GLU	2.0
1	H	80	THR	2.0
1	F	25	ASN	2.0
1	C	127	LEU	2.0
1	A	95	ARG	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MLC	H	200	54/54	0.68	0.29	2.73	43,100,113,118	0
2	MLC	D	200	54/54	0.78	0.21	0.67	39,78,122,124	0
2	MLC	E	200	54/54	0.84	0.20	0.22	68,96,105,106	0
2	MLC	B	200	54/54	0.85	0.17	-0.31	36,67,83,86	0
2	MLC	G	200	54/54	0.88	0.15	-0.37	44,72,87,96	0
2	MLC	F	200	54/54	0.95	0.12	-0.83	41,52,71,79	0
2	MLC	A	200	54/54	0.96	0.16	-1.08	28,38,48,48	0
2	MLC	C	200	54/54	0.94	0.14	-1.16	33,47,70,76	0
3	CL	F	142	1/1	0.81	0.06	-1.77	89,89,89,89	0
3	CL	D	142	1/1	0.96	0.10	-	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.