Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:09 am BST

PDB ID	:	5NNP
Title	:	Structure of Naa15/Naa10 bound to HypK-THB
Authors	:	Weyer, F.A.; Gumiero, A.; Kopp, J.; Sinning, I.
Deposited on	:	2017-04-10
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

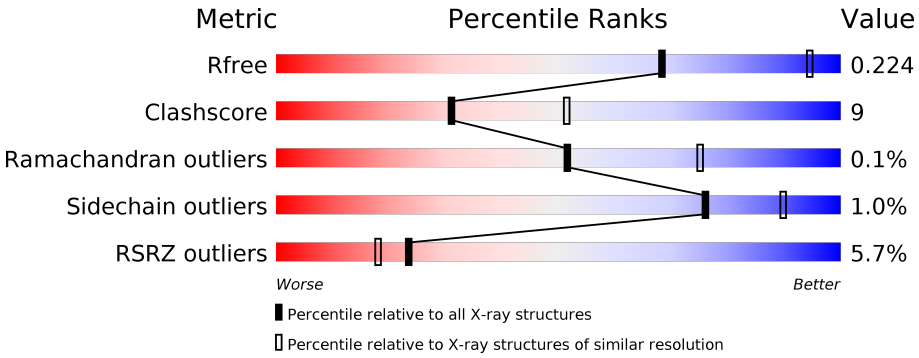
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	745	6% 74% 16% 11%
1	E	745	6% 73% 15% 12%
2	B	195	4% 78% 14% 8%
2	F	195	2% 75% 16% • 9%
3	C	62	2% 60% 13% 27%
3	G	62	2% 48% 24% 27%

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Mol	Chain	Length	Quality of chain
4	I	4	
4	L	4	

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
5	GOL	A	801	-	-	X	X
5	GOL	A	805	-	-	-	X
5	GOL	A	807	-	-	-	X
5	GOL	C	202	-	-	-	X
5	GOL	F	201	-	-	-	X
6	PO4	E	807	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15101 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 N-terminal acetyltransferase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	665	Total	C	N	O	S	0	0	0
			5390	3428	943	997	22			
1	E	658	Total	C	N	O	S	0	1	0
			5346	3400	934	990	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP G0S4M4
A	1	GLY	-	expression tag	UNP G0S4M4
A	707	LYS	ASN	conflict	UNP G0S4M4
A	724	ASP	GLY	conflict	UNP G0S4M4
E	0	MET	-	initiating methionine	UNP G0S4M4
E	1	GLY	-	expression tag	UNP G0S4M4
E	707	LYS	ASN	conflict	UNP G0S4M4
E	724	ASP	GLY	conflict	UNP G0S4M4

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	0	0
			1458	930	251	270	7			
2	F	178	Total	C	N	O	S	0	0	0
			1450	926	250	267	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	FME	-	expression tag	UNP G0SEE8
B	190	HIS	-	expression tag	UNP G0SEE8
B	191	HIS	-	expression tag	UNP G0SEE8
B	192	HIS	-	expression tag	UNP G0SEE8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	193	HIS	-	expression tag	UNP G0SEE8
B	194	HIS	-	expression tag	UNP G0SEE8
B	195	HIS	-	expression tag	UNP G0SEE8
F	1	FME	-	expression tag	UNP G0SEE8
F	190	HIS	-	expression tag	UNP G0SEE8
F	191	HIS	-	expression tag	UNP G0SEE8
F	192	HIS	-	expression tag	UNP G0SEE8
F	193	HIS	-	expression tag	UNP G0SEE8
F	194	HIS	-	expression tag	UNP G0SEE8
F	195	HIS	-	expression tag	UNP G0SEE8

- Molecule 3 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	45	Total	C	N	O	S	0	0	0
			337	214	55	66	2			
3	G	45	Total	C	N	O	S	0	0	0
			337	214	55	66	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	79	GLY	-	expression tag	UNP G0SCY6
C	80	ALA	-	expression tag	UNP G0SCY6
C	81	MET	-	expression tag	UNP G0SCY6
C	82	GLY	-	expression tag	UNP G0SCY6
C	127	GLY	-	expression tag	UNP G0SCY6
C	128	SER	-	expression tag	UNP G0SCY6
C	129	GLY	-	expression tag	UNP G0SCY6
C	130	SER	-	expression tag	UNP G0SCY6
C	131	GLY	-	expression tag	UNP G0SCY6
C	132	SER	-	expression tag	UNP G0SCY6
C	133	TRP	-	expression tag	UNP G0SCY6
C	134	SER	-	expression tag	UNP G0SCY6
C	135	HIS	-	expression tag	UNP G0SCY6
C	136	PRO	-	expression tag	UNP G0SCY6
C	137	GLN	-	expression tag	UNP G0SCY6
C	138	PHE	-	expression tag	UNP G0SCY6
C	139	GLU	-	expression tag	UNP G0SCY6
C	140	LYS	-	expression tag	UNP G0SCY6
G	79	GLY	-	expression tag	UNP G0SCY6
G	80	ALA	-	expression tag	UNP G0SCY6

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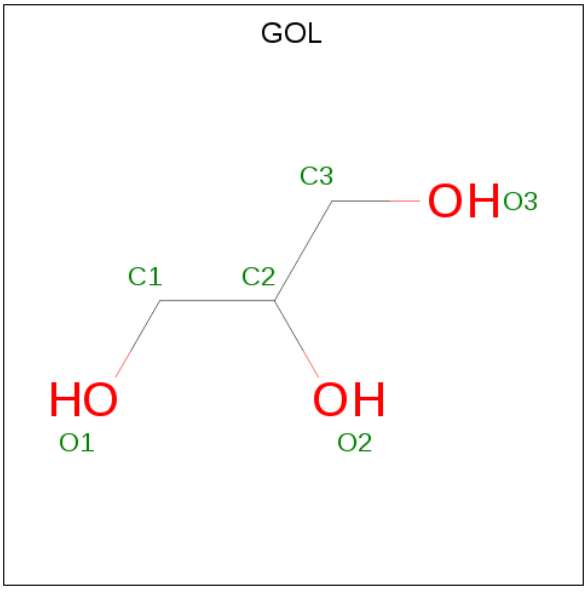
Chain	Residue	Modelled	Actual	Comment	Reference
G	81	MET	-	expression tag	UNP G0SCY6
G	82	GLY	-	expression tag	UNP G0SCY6
G	127	GLY	-	expression tag	UNP G0SCY6
G	128	SER	-	expression tag	UNP G0SCY6
G	129	GLY	-	expression tag	UNP G0SCY6
G	130	SER	-	expression tag	UNP G0SCY6
G	131	GLY	-	expression tag	UNP G0SCY6
G	132	SER	-	expression tag	UNP G0SCY6
G	133	TRP	-	expression tag	UNP G0SCY6
G	134	SER	-	expression tag	UNP G0SCY6
G	135	HIS	-	expression tag	UNP G0SCY6
G	136	PRO	-	expression tag	UNP G0SCY6
G	137	GLN	-	expression tag	UNP G0SCY6
G	138	PHE	-	expression tag	UNP G0SCY6
G	139	GLU	-	expression tag	UNP G0SCY6
G	140	LYS	-	expression tag	UNP G0SCY6

- Molecule 4 is a protein called Ser-Glu-Ser-Ser.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	4	Total	C	N	O	0	0	0
			28	14	4	10			
4	L	4	Total	C	N	O	0	0	0
			28	14	4	10			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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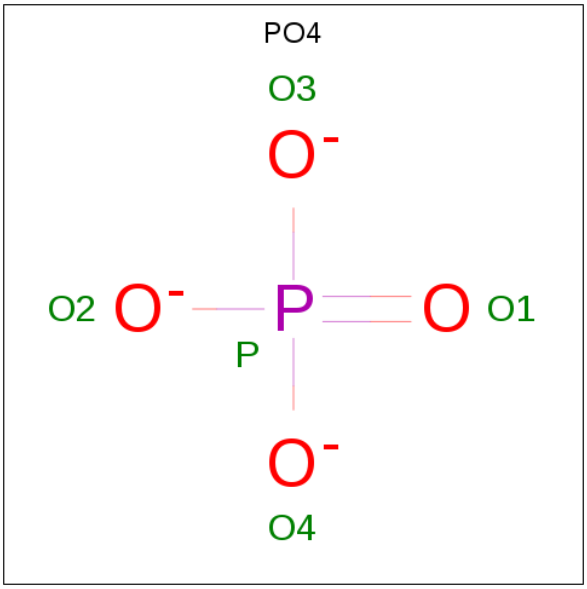
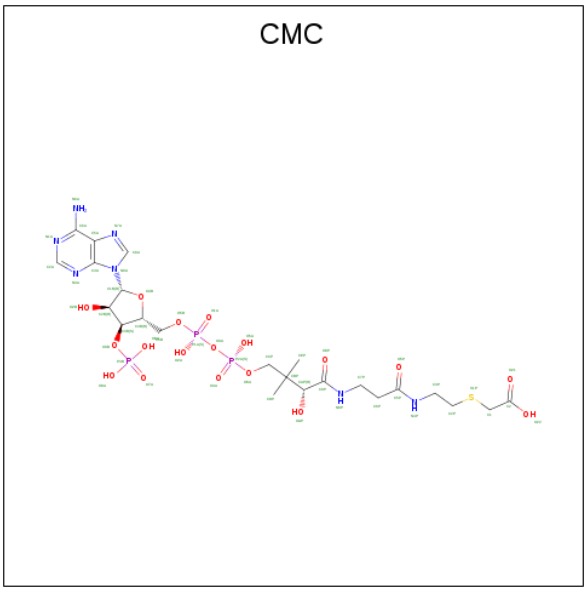
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	F	1	Total O P 5 4 1	0	0

- Molecule 7 is CARBOXYMETHYL COENZYME *A (three-letter code: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
7	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 8 is water.

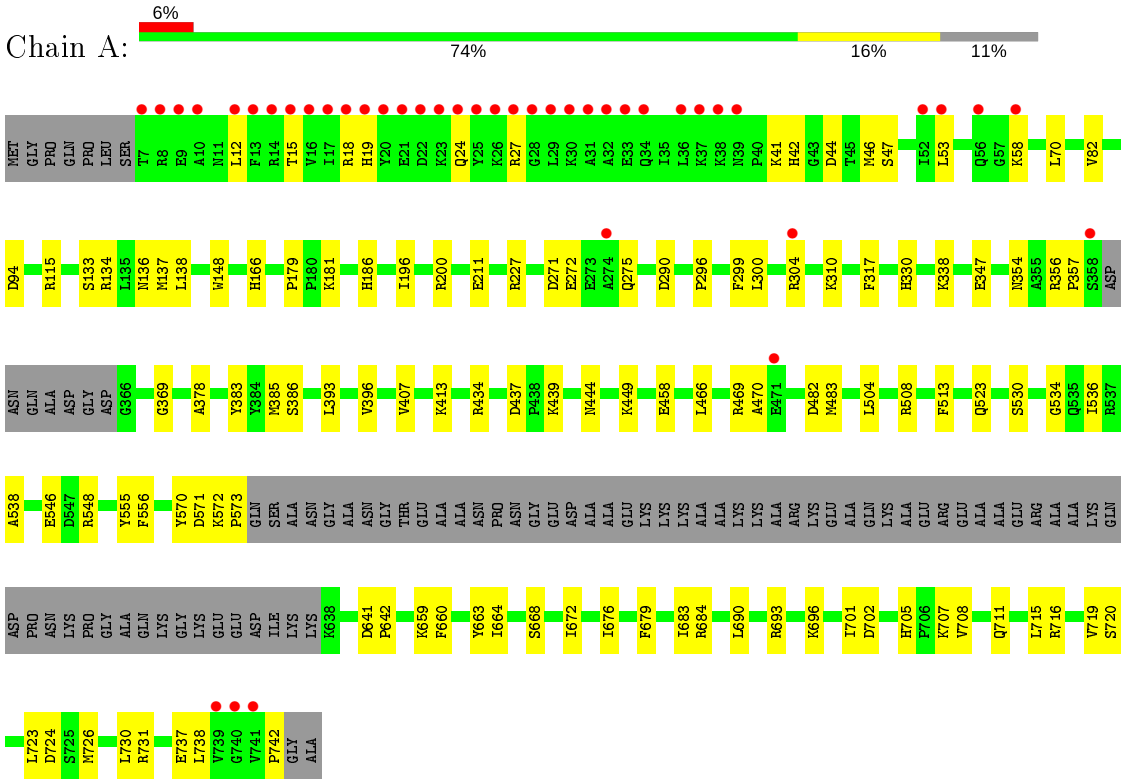
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	155	Total	O	0	0
			155	155		
8	B	52	Total	O	0	0
			52	52		
8	C	4	Total	O	0	0
			4	4		
8	E	159	Total	O	0	0
			159	159		
8	F	54	Total	O	0	0
			54	54		
8	G	6	Total	O	0	0
			6	6		
8	I	8	Total	O	0	0
			8	8		
8	L	5	Total	O	0	0
			5	5		

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 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.

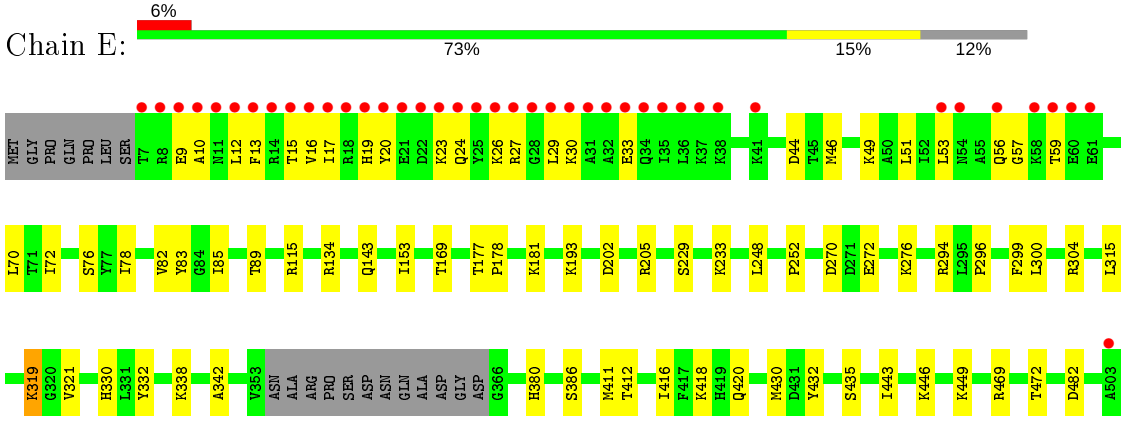
- Molecule 1: N-terminal acetyltransferase-like protein

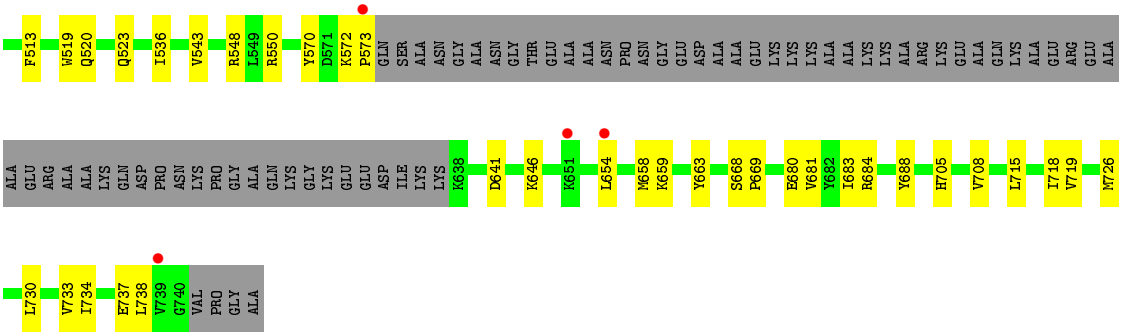
Chain A:



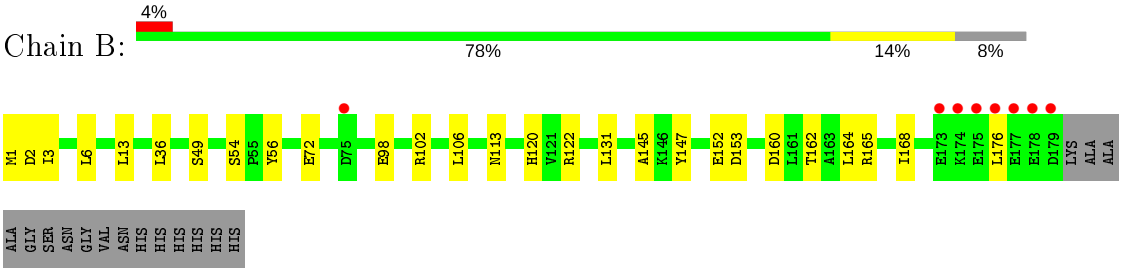
- Molecule 1: N-terminal acetyltransferase-like protein

Chain E:

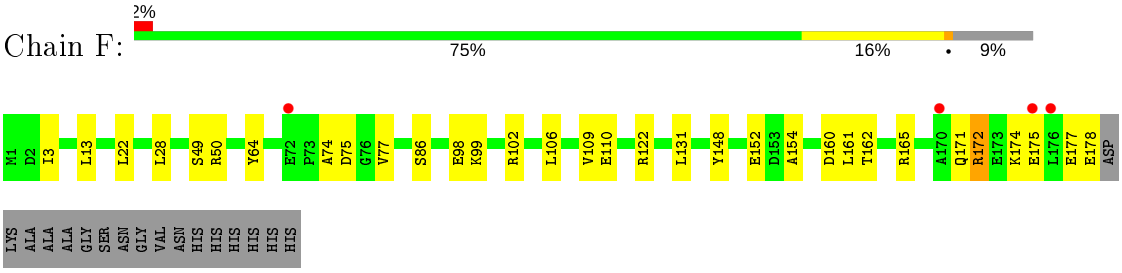




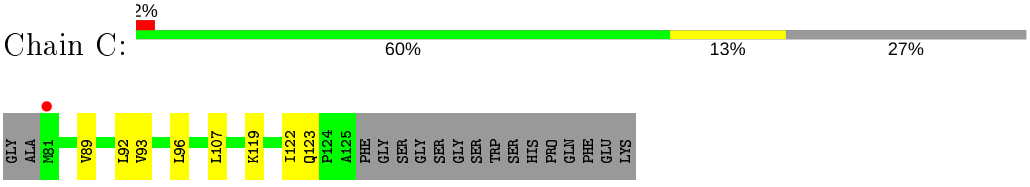
• Molecule 2: Putative uncharacterized protein



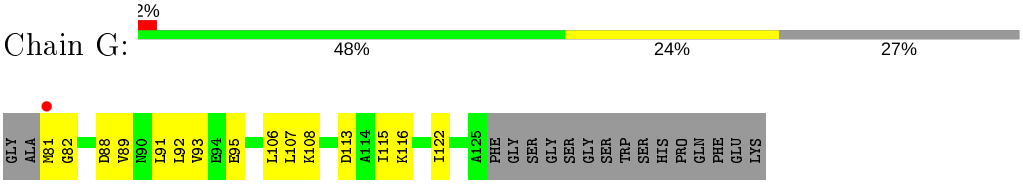
• Molecule 2: Putative uncharacterized protein



• Molecule 3: Putative uncharacterized protein



• Molecule 3: Putative uncharacterized protein



• Molecule 4: Ser-Glu-Ser-Ser

- Molecule 4: Ser-Glu-Ser-Ser

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.32Å 106.04Å 130.94Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	49.32 – 2.60 49.32 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.32-2.60) 99.7 (49.32-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.161 , 0.220 0.166 , 0.224	Depositor DCC
R_{free} test set	3925 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.3	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	0.95	EDS
Total number of atoms	15101	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: GOL, PO4, FME, CMC

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	0.38	0/5501	0.49	0/7413
1	E	0.38	0/5455	0.49	0/7348
2	B	0.40	0/1482	0.53	0/2008
2	F	0.40	0/1474	0.54	0/1997
3	C	0.35	0/340	0.47	0/457
3	G	0.31	0/340	0.47	0/457
4	I	2.03	1/27 (3.7%)	1.44	0/33
4	L	2.07	1/27 (3.7%)	1.44	0/33
All	All	0.40	2/14646 (0.0%)	0.50	0/19746

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	4	SER	C-N	5.88	1.47	1.34
4	I	4	SER	C-N	5.63	1.47	1.34

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	5390	0	5391	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5346	0	5339	107	0
2	B	1458	0	1449	23	0
2	F	1450	0	1445	23	0
3	C	337	0	352	5	0
3	G	337	0	352	13	0
4	I	28	0	20	2	0
4	L	28	0	20	3	0
5	A	72	0	96	14	0
5	B	6	0	8	2	0
5	C	12	0	16	0	0
5	E	36	0	48	5	0
5	F	36	0	48	4	0
6	A	5	0	0	0	0
6	E	10	0	0	3	0
6	F	5	0	0	1	0
7	I	51	0	33	4	0
7	L	51	0	33	1	0
8	A	155	0	0	9	0
8	B	52	0	0	1	0
8	C	4	0	0	0	0
8	E	159	0	0	4	0
8	F	54	0	0	5	0
8	G	6	0	0	0	0
8	I	8	0	0	2	0
8	L	5	0	0	0	0
All	All	15101	0	14650	267	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 9.

All (267) 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:E:19:HIS:CB	1:E:24:GLN:HG3	1.73	1.16
1:E:19:HIS:O	1:E:24:GLN:HG2	1.52	1.10
1:E:654:LEU:HD12	1:E:681:VAL:HG13	1.33	1.08
1:E:19:HIS:HB3	1:E:24:GLN:HG3	1.01	1.00
1:E:19:HIS:HB3	1:E:24:GLN:CG	1.91	0.99
1:E:730:LEU:HD11	3:G:95:GLU:HG3	1.48	0.95
1:E:19:HIS:O	1:E:24:GLN:CG	2.15	0.94
1:A:723:LEU:HD13	1:A:731:ARG:HE	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ALA:HB1	1:A:396:VAL:CG2	2.01	0.91
1:E:572:LYS:HB3	1:E:573:PRO:HD3	1.52	0.89
1:A:134:ARG:NH2	8:A:901:HOH:O	2.00	0.83
1:A:469:ARG:NH1	8:A:903:HOH:O	2.13	0.82
1:A:538:ALA:N	5:A:801:GOL:H32	1.94	0.82
1:A:378:ALA:HB1	1:A:396:VAL:HG23	1.62	0.81
1:E:19:HIS:CA	1:E:24:GLN:HG3	2.11	0.81
1:E:26:LYS:HA	1:E:29:LEU:HB3	1.64	0.80
1:A:272:GLU:CD	1:A:304:ARG:HH21	1.88	0.78
1:E:12:LEU:O	1:E:16:VAL:HG23	1.86	0.76
1:E:469:ARG:HH21	4:L:5:SER:HA	1.50	0.76
1:E:570:TYR:CD1	1:E:654:LEU:HD23	2.20	0.76
1:E:688:TYR:HE1	1:E:718:ILE:HD13	1.51	0.76
1:E:19:HIS:C	1:E:24:GLN:CG	2.55	0.75
1:E:548:ARG:HH21	5:E:803:GOL:C1	1.99	0.74
1:E:658:MET:CE	1:E:681:VAL:HG11	2.17	0.73
1:E:24:GLN:OE1	1:E:27:ARG:HB2	1.88	0.73
1:E:338:LYS:HD2	1:E:386:SER:HB3	1.71	0.73
1:A:548:ARG:NH2	8:A:904:HOH:O	2.23	0.71
1:E:134:ARG:NH1	8:E:901:HOH:O	2.09	0.71
1:E:294:ARG:NH1	8:E:902:HOH:O	2.25	0.70
1:A:413:LYS:NZ	5:A:808:GOL:H31	2.07	0.69
1:A:211:GLU:OE2	1:A:227:ARG:HD3	1.92	0.69
1:E:19:HIS:C	1:E:24:GLN:HG3	2.11	0.69
1:A:271:ASP:O	1:A:275:GLN:HG3	1.92	0.69
1:A:705:HIS:CE1	1:A:707:LYS:HB2	2.25	0.69
1:E:411:MET:HE2	1:E:443:ILE:HD13	1.74	0.69
1:A:383:TYR:CE2	1:A:385:MET:HG3	2.28	0.69
1:A:378:ALA:HB1	1:A:396:VAL:HG22	1.75	0.69
2:F:172:ARG:NH1	6:F:207:PO4:O2	2.26	0.68
2:F:174:LYS:O	2:F:177:GLU:HG2	1.93	0.68
5:A:805:GOL:O2	8:A:902:HOH:O	2.11	0.67
2:B:98:GLU:OE2	2:B:102:ARG:NH1	2.26	0.67
1:A:716:ARG:HH12	1:A:742:PRO:HB3	1.59	0.67
4:L:4:SER:O	4:L:5:SER:HB2	1.94	0.67
1:A:523:GLN:CD	1:A:546:GLU:HG2	2.15	0.67
1:E:688:TYR:CE1	1:E:718:ILE:HD13	2.29	0.67
3:G:82:GLY:H	3:G:108:LYS:HE3	1.59	0.67
1:E:548:ARG:HH21	5:E:803:GOL:H11	1.61	0.66
3:G:81:MET:N	3:G:108:LYS:HZ1	1.94	0.66
1:A:338:LYS:HD2	1:A:386:SER:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LYS:HB2	8:A:912:HOH:O	1.96	0.65
2:F:98:GLU:OE2	2:F:102:ARG:NH1	2.28	0.65
1:A:272:GLU:OE2	1:A:304:ARG:NH2	2.26	0.65
1:E:272:GLU:CD	1:E:304:ARG:HH21	2.01	0.64
1:E:469:ARG:NH2	4:L:5:SER:HA	2.12	0.63
1:E:229:SER:O	1:E:233:LYS:HG3	1.98	0.63
2:F:171:GLN:O	2:F:175:GLU:HG2	1.98	0.62
1:E:730:LEU:HD13	3:G:91:LEU:HD11	1.81	0.62
1:A:672:ILE:HD11	1:A:701:ILE:HB	1.81	0.61
2:B:1:FME:O	5:B:201:GOL:O2	2.18	0.61
1:A:523:GLN:NE2	1:A:546:GLU:HG2	2.15	0.61
1:E:15:THR:HG23	1:E:19:HIS:CE1	2.36	0.61
1:E:513:PHE:CZ	1:E:659:LYS:HG2	2.36	0.61
5:A:801:GOL:H11	8:A:1032:HOH:O	2.01	0.60
1:A:19:HIS:CE1	1:A:27:ARG:HE	2.19	0.60
1:A:723:LEU:HD13	1:A:731:ARG:NE	2.11	0.60
1:A:458:GLU:HG2	8:A:984:HOH:O	2.00	0.60
1:E:70:LEU:HD21	1:E:83:TYR:CD2	2.36	0.60
1:E:432:TYR:O	1:E:435:SER:OG	2.19	0.60
1:A:434:ARG:HB3	1:A:434:ARG:NH1	2.17	0.60
5:F:204:GOL:H32	8:F:316:HOH:O	2.00	0.60
1:E:49:LYS:O	1:E:53:LEU:HG	2.02	0.60
1:A:449:LYS:HD2	5:A:809:GOL:H2	1.84	0.60
1:E:19:HIS:CB	1:E:24:GLN:CG	2.65	0.60
1:A:693:ARG:HB2	3:C:122:ILE:HG22	1.84	0.59
1:E:13:PHE:CZ	1:E:44:ASP:HB3	2.36	0.59
1:A:179:PRO:HG2	1:A:186:HIS:CD2	2.37	0.59
1:E:19:HIS:CA	1:E:24:GLN:CG	2.80	0.59
2:F:161:LEU:O	2:F:165:ARG:HG3	2.02	0.59
1:A:660:PHE:O	1:A:664:ILE:HG13	2.03	0.59
1:A:716:ARG:HG2	1:A:738:LEU:HD21	1.84	0.58
1:A:407:VAL:HG21	1:A:437:ASP:HB2	1.85	0.58
7:I:101:CMC:H2B	8:I:202:HOH:O	2.02	0.58
1:E:411:MET:CE	1:E:443:ILE:HD13	2.33	0.58
1:A:672:ILE:CD1	1:A:701:ILE:HB	2.33	0.57
1:E:51:LEU:HD13	1:E:82:VAL:HG13	1.86	0.57
1:A:15:THR:HG22	1:A:18:ARG:HH21	1.69	0.57
1:A:679:PHE:CE1	1:A:683:ILE:HD13	2.39	0.57
1:E:658:MET:HE1	1:E:681:VAL:HG11	1.87	0.56
1:A:378:ALA:CB	1:A:396:VAL:HG22	2.35	0.56
2:B:106:LEU:CD1	2:B:168:ILE:HD11	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:ILE:CD1	2:F:99:LYS:HB2	2.35	0.56
1:E:252:PRO:HG2	5:F:201:GOL:H31	1.88	0.56
1:A:548:ARG:HH22	5:A:810:GOL:H32	1.70	0.56
1:A:356:ARG:N	1:A:357:PRO:HD3	2.21	0.56
1:A:378:ALA:CB	1:A:396:VAL:CG2	2.80	0.55
1:E:734:ILE:O	1:E:738:LEU:HB2	2.06	0.55
1:A:716:ARG:NH1	1:A:742:PRO:HB3	2.21	0.55
1:E:446:LYS:NZ	6:E:807:PO4:O1	2.39	0.55
2:F:110:GLU:OE1	8:F:301:HOH:O	2.18	0.55
1:A:705:HIS:O	1:A:708:VAL:HG22	2.08	0.54
1:E:570:TYR:CG	1:E:654:LEU:HD23	2.43	0.54
3:C:92:LEU:HD22	3:C:107:LEU:HG	1.90	0.54
2:F:172:ARG:NH2	8:F:301:HOH:O	2.21	0.54
1:A:413:LYS:HZ1	5:A:808:GOL:H31	1.71	0.54
1:A:310:LYS:NZ	1:A:347:GLU:OE1	2.26	0.54
1:E:26:LYS:O	1:E:30:LYS:HD3	2.08	0.53
1:E:737:GLU:HG3	3:G:122:ILE:HD11	1.89	0.53
1:A:296:PRO:HA	1:A:299:PHE:CE2	2.44	0.53
1:A:672:ILE:HD11	1:A:701:ILE:CG2	2.39	0.53
1:E:733:VAL:HG22	3:G:115:ILE:HG23	1.91	0.53
1:E:26:LYS:HG2	1:E:29:LEU:HD23	1.89	0.52
1:A:470:ALA:HB1	1:E:270:ASP:OD2	2.09	0.52
1:A:290:ASP:HB3	5:B:201:GOL:H2	1.92	0.52
2:F:74:ALA:O	2:F:77:VAL:HG12	2.09	0.52
1:A:47:SER:HB3	1:A:82:VAL:HG21	1.90	0.52
1:E:169:THR:OG1	1:E:193:LYS:HE3	2.10	0.52
1:A:705:HIS:HE1	1:A:707:LYS:HB2	1.71	0.52
1:E:733:VAL:CG2	3:G:115:ILE:HG23	2.40	0.51
1:A:115:ARG:NE	8:A:906:HOH:O	2.35	0.51
3:G:92:LEU:HD23	3:G:106:LEU:HD23	1.91	0.51
1:A:570:TYR:CD2	1:A:684:ARG:HD3	2.46	0.51
1:E:572:LYS:HB3	1:E:573:PRO:CD	2.34	0.51
3:G:89:VAL:O	3:G:93:VAL:HG23	2.10	0.51
1:A:641:ASP:N	1:A:642:PRO:HD3	2.26	0.50
3:C:119:LYS:O	3:C:123:GLN:HG2	2.11	0.50
1:E:411:MET:HG3	1:E:430:MET:SD	2.51	0.50
1:A:538:ALA:HB2	5:A:801:GOL:H31	1.93	0.50
1:E:319:LYS:HB3	1:E:321:VAL:HG23	1.92	0.50
2:B:147:TYR:CE2	4:I:4:SER:HB3	2.46	0.50
1:E:153:ILE:HD11	1:E:536:ILE:HG23	1.94	0.50
1:A:504:LEU:O	1:A:508:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:SER:HA	2:B:56:TYR:CZ	2.47	0.49
1:A:672:ILE:HD11	1:A:701:ILE:CB	2.42	0.49
2:F:177:GLU:HG3	2:F:178:GLU:N	2.27	0.49
1:A:723:LEU:HA	1:A:726:MET:HG2	1.93	0.49
2:B:113:ASN:OD1	2:B:165:ARG:NH1	2.35	0.49
1:E:49:LYS:HE2	1:E:53:LEU:HD11	1.94	0.49
1:A:133:SER:O	1:A:137:MET:HG3	2.12	0.49
1:A:534:GLY:O	1:A:536:ILE:HG12	2.12	0.48
1:E:85:ILE:O	1:E:89:THR:HG23	2.13	0.48
1:E:449:LYS:NZ	6:E:807:PO4:O1	2.44	0.48
1:E:654:LEU:CD1	1:E:681:VAL:HG13	2.24	0.48
2:F:122:ARG:HD3	2:F:152:GLU:OE2	2.13	0.48
2:F:74:ALA:O	2:F:75:ASP:HB2	2.12	0.48
1:A:720:SER:HA	1:A:723:LEU:HD23	1.93	0.48
8:B:321:HOH:O	4:I:2:SER:HB2	2.12	0.48
1:A:548:ARG:HH22	5:A:810:GOL:C3	2.27	0.48
1:A:434:ARG:HG3	1:A:444:ASN:HA	1.95	0.48
2:B:3:ILE:N	2:B:3:ILE:HD12	2.29	0.48
1:E:730:LEU:HD21	3:G:95:GLU:CD	2.35	0.48
5:E:806:GOL:H31	2:F:106:LEU:HB2	1.95	0.47
2:F:64:TYR:CE1	2:F:86:SER:HB3	2.49	0.47
1:E:570:TYR:HB2	1:E:654:LEU:CD2	2.45	0.47
1:E:418:LYS:NZ	6:E:807:PO4:O2	2.47	0.47
5:E:806:GOL:H11	2:F:106:LEU:HD22	1.97	0.47
1:A:672:ILE:HG12	1:A:701:ILE:HD12	1.97	0.47
1:E:641:ASP:HB2	1:E:646:LYS:HD2	1.97	0.47
1:E:680:GLU:O	1:E:683:ILE:HG22	2.15	0.47
1:A:138:LEU:HD11	1:A:148:TRP:CE2	2.50	0.47
2:F:50:ARG:NH2	8:F:304:HOH:O	2.48	0.47
2:B:131:LEU:HD13	7:I:101:CMC:H52A	1.96	0.47
1:E:296:PRO:HA	1:E:299:PHE:CE2	2.50	0.47
1:A:300:LEU:HD22	1:A:304:ARG:HB3	1.97	0.47
1:E:115:ARG:HD3	8:E:1012:HOH:O	2.14	0.47
1:E:29:LEU:O	1:E:33:GLU:HG3	2.15	0.47
1:E:469:ARG:HB2	1:E:472:THR:OG1	2.15	0.47
1:E:520:GLN:O	1:E:523:GLN:HG2	2.15	0.47
1:A:317:PHE:O	1:A:369:GLY:HA2	2.16	0.46
2:F:49:SER:HB2	8:F:328:HOH:O	2.15	0.46
1:A:166:HIS:CG	5:A:806:GOL:H11	2.50	0.46
1:E:9:GLU:HG2	1:E:10:ALA:N	2.30	0.46
1:A:555:TYR:OH	1:A:663:TYR:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:570:TYR:CB	1:E:654:LEU:CD2	2.94	0.46
1:A:548:ARG:HG2	5:A:811:GOL:O3	2.15	0.46
1:E:570:TYR:CG	1:E:654:LEU:CD2	2.99	0.46
2:B:145:ALA:HA	2:B:153:ASP:OD1	2.16	0.46
1:E:19:HIS:C	1:E:24:GLN:HG2	2.23	0.46
2:F:160:ASP:OD1	2:F:162:THR:OG1	2.18	0.46
1:A:12:LEU:O	1:A:12:LEU:HD13	2.15	0.45
1:A:556:PHE:CE1	1:A:664:ILE:HG23	2.51	0.45
1:E:332:TYR:CD2	1:E:338:LYS:HG3	2.51	0.45
2:B:176:LEU:HD23	2:B:176:LEU:O	2.16	0.45
1:A:181:LYS:HD3	1:A:181:LYS:HA	1.76	0.45
1:A:19:HIS:CE1	1:A:27:ARG:HH11	2.34	0.45
1:E:19:HIS:O	1:E:24:GLN:CB	2.64	0.45
1:A:715:LEU:O	1:A:719:VAL:HG23	2.16	0.45
1:A:272:GLU:OE2	1:A:304:ARG:NE	2.48	0.45
1:E:684:ARG:HH11	1:E:684:ARG:HG3	1.81	0.45
1:A:469:ARG:HH22	1:A:483:MET:CE	2.30	0.44
1:E:668:SER:N	1:E:669:PRO:CD	2.80	0.44
1:E:276:LYS:HD2	1:E:300:LEU:HD11	1.99	0.44
2:B:122:ARG:HB3	2:B:152:GLU:OE1	2.17	0.44
1:E:44:ASP:OD2	1:E:78:ILE:HD12	2.17	0.44
1:E:53:LEU:O	1:E:56:GLN:HB2	2.18	0.44
2:F:13:LEU:HD23	2:F:13:LEU:HA	1.78	0.44
1:A:196:ILE:O	1:A:200:ARG:HG3	2.18	0.44
2:B:106:LEU:HD11	2:B:168:ILE:HD11	1.99	0.44
2:B:164:LEU:O	2:B:168:ILE:HG12	2.18	0.44
1:E:315:LEU:C	1:E:315:LEU:HD23	2.38	0.44
1:E:548:ARG:NH2	5:E:803:GOL:O1	2.51	0.44
1:A:354:ASN:O	1:A:357:PRO:HG3	2.19	0.43
1:E:143[B]:GLN:CD	1:E:143[B]:GLN:H	2.19	0.43
1:A:723:LEU:HD12	1:A:724:ASP:N	2.33	0.43
1:A:726:MET:HB2	1:A:730:LEU:HD23	2.00	0.43
1:A:434:ARG:HB3	1:A:434:ARG:HH11	1.83	0.43
3:G:113:ASP:HB3	3:G:116:LYS:HB3	1.99	0.43
3:C:89:VAL:O	3:C:93:VAL:HG23	2.18	0.43
1:A:42:HIS:O	1:A:46:MET:HG3	2.18	0.43
1:A:672:ILE:HD11	1:A:701:ILE:HG22	1.99	0.43
1:A:723:LEU:HD12	1:A:723:LEU:C	2.39	0.43
1:E:550:ARG:HD3	1:E:663:TYR:CD2	2.54	0.43
1:E:330:HIS:HB2	8:E:902:HOH:O	2.17	0.43
1:A:572:LYS:N	1:A:573:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ASP:HB3	1:A:705:HIS:HB2	2.01	0.43
1:E:181:LYS:HA	1:E:181:LYS:HD3	1.68	0.43
1:A:41:LYS:NZ	8:A:922:HOH:O	2.52	0.43
1:E:248:LEU:HD23	1:E:248:LEU:HA	1.92	0.43
1:E:449:LYS:NZ	5:F:206:GOL:O3	2.43	0.43
1:A:378:ALA:CB	1:A:396:VAL:HG23	2.41	0.43
1:A:672:ILE:CG1	1:A:701:ILE:HG21	2.49	0.43
1:A:676:ILE:HG23	1:A:711:GLN:NE2	2.34	0.42
1:E:705:HIS:HB3	1:E:708:VAL:HG23	2.01	0.42
2:F:109:VAL:HG13	2:F:165:ARG:HG2	2.01	0.42
1:E:519:TRP:CD2	2:F:28:LEU:HD13	2.54	0.42
7:I:101:CMC:O7A	8:I:201:HOH:O	2.22	0.42
1:A:530:SER:OG	2:B:36:LEU:HD23	2.19	0.42
2:B:13:LEU:HA	2:B:13:LEU:HD23	1.70	0.42
2:B:122:ARG:HD3	2:B:152:GLU:OE2	2.19	0.42
1:A:413:LYS:HZ3	5:A:808:GOL:H31	1.80	0.42
1:E:12:LEU:O	1:E:15:THR:HB	2.20	0.42
1:E:177:THR:HG23	1:E:178:PRO:HD2	2.01	0.42
1:A:668:SER:HA	2:B:56:TYR:CE2	2.55	0.42
1:E:46:MET:SD	1:E:72:ILE:HD12	2.60	0.42
1:E:730:LEU:CD1	3:G:95:GLU:HG3	2.35	0.42
1:E:15:THR:O	1:E:19:HIS:HB2	2.20	0.41
1:A:513:PHE:CZ	1:A:659:LYS:HD2	2.55	0.41
2:B:160:ASP:OD1	2:B:162:THR:OG1	2.19	0.41
1:E:202:ASP:HB3	1:E:205:ARG:HB3	2.01	0.41
1:A:571:ASP:C	1:A:573:PRO:HD3	2.41	0.41
1:E:412:THR:O	1:E:416:ILE:HG13	2.20	0.41
2:B:120:HIS:O	7:I:101:CMC:H12	2.20	0.41
1:A:42:HIS:CE1	1:A:44:ASP:HB2	2.56	0.41
1:E:342:ALA:HB2	1:E:380:HIS:CE1	2.55	0.41
2:B:72:GLU:HG3	2:B:72:GLU:O	2.20	0.41
1:E:416:ILE:O	1:E:420:GLN:HG3	2.21	0.41
1:E:715:LEU:O	1:E:718:ILE:HG22	2.21	0.41
1:A:24:GLN:HG3	1:A:27:ARG:CZ	2.51	0.41
1:A:538:ALA:H	5:A:801:GOL:H32	1.78	0.41
1:E:57:GLY:O	1:E:59:THR:N	2.51	0.41
2:F:22:LEU:HD21	7:L:101:CMC:C5P	2.51	0.41
1:A:15:THR:O	1:A:19:HIS:CD2	2.74	0.41
1:A:690:LEU:HD21	3:C:96:LEU:HA	2.02	0.41
2:F:148:TYR:CE2	2:F:154:ALA:HB2	2.56	0.41
1:E:15:THR:O	1:E:19:HIS:ND1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:NZ	1:A:737:GLU:OE2	2.54	0.41
2:B:6:LEU:HD23	2:B:6:LEU:C	2.41	0.41
1:E:719:VAL:HG13	1:E:726:MET:CE	2.51	0.41
3:G:88:ASP:HB3	3:G:107:LEU:HD21	2.03	0.41
1:A:166:HIS:HA	5:A:805:GOL:H31	2.02	0.41
1:A:70:LEU:C	1:A:70:LEU:HD12	2.42	0.41
1:A:53:LEU:HB3	1:A:58:LYS:HB2	2.03	0.40
1:A:330:HIS:HB2	2:B:49:SER:HB3	2.04	0.40
2:B:2:ASP:C	2:B:3:ILE:HD12	2.42	0.40
1:E:202:ASP:HB3	1:E:205:ARG:CB	2.51	0.40
1:E:134:ARG:HA	1:E:134:ARG:HD3	1.78	0.40
1:E:20:TYR:CZ	1:E:51:LEU:HG	2.56	0.40
1:E:449:LYS:HD2	5:F:206:GOL:O3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	659/745 (88%)	648 (98%)	11 (2%)	0	100	100
1	E	653/745 (88%)	638 (98%)	13 (2%)	2 (0%)	41	64
2	B	177/195 (91%)	176 (99%)	1 (1%)	0	100	100
2	F	176/195 (90%)	175 (99%)	1 (1%)	0	100	100
3	C	43/62 (69%)	43 (100%)	0	0	100	100
3	G	43/62 (69%)	43 (100%)	0	0	100	100
4	I	2/4 (50%)	2 (100%)	0	0	100	100
4	L	2/4 (50%)	2 (100%)	0	0	100	100
All	All	1755/2012 (87%)	1727 (98%)	26 (2%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	23	LYS
1	E	17	ILE

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	560/614 (91%)	555 (99%)	5 (1%)	78 91
1	E	554/614 (90%)	550 (99%)	4 (1%)	84 94
2	B	155/166 (93%)	154 (99%)	1 (1%)	86 95
2	F	154/166 (93%)	152 (99%)	2 (1%)	69 86
3	C	35/47 (74%)	35 (100%)	0	100 100
3	G	35/47 (74%)	35 (100%)	0	100 100
4	I	4/4 (100%)	2 (50%)	2 (50%)	0 0
4	L	4/4 (100%)	3 (75%)	1 (25%)	0 1
All	All	1501/1662 (90%)	1486 (99%)	15 (1%)	76 90

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	136	ASN
1	A	393	LEU
1	A	466	LEU
1	A	482	ASP
2	B	54	SER
1	E	76	SER
1	E	319	LYS
1	E	482	ASP
1	E	543	VAL
2	F	131	LEU
2	F	172	ARG

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Mol	Chain	Res	Type
4	I	2	SER
4	I	5	SER
4	L	5	SER

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	19	HIS
1	E	132	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	FME	B	1	2	8,9,10	0.83	0	7,9,11	1.00	0
2	FME	F	1	2	8,9,10	0.83	0	7,9,11	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	3/7/9/11	-
2	FME	F	1	2	-	2/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FME	O-C-CA-CB
2	F	1	FME	O-C-CA-CB
2	F	1	FME	CB-CG-SD-CE
2	B	1	FME	CB-CG-SD-CE
2	B	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

33 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	$\#\|Z\| > 2$
7	CMC	I	101	4	45,53,54	1.72	8 (17%)	55,78,80	1.57	10 (18%)
5	GOL	F	203	-	5,5,5	0.43	0	5,5,5	0.28	0
5	GOL	A	805	-	5,5,5	0.31	0	5,5,5	0.34	0
5	GOL	A	802	-	5,5,5	0.39	0	5,5,5	0.24	0
5	GOL	B	201	-	5,5,5	0.44	0	5,5,5	0.14	0
6	PO4	E	807	-	4,4,4	0.91	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	C	201	-	5,5,5	0.37	0	5,5,5	0.28	0
5	GOL	E	804	-	5,5,5	0.34	0	5,5,5	0.37	0
5	GOL	A	807	-	5,5,5	0.36	0	5,5,5	0.19	0
5	GOL	A	810	-	5,5,5	0.47	0	5,5,5	0.23	0
5	GOL	E	802	-	5,5,5	0.35	0	5,5,5	0.50	0
5	GOL	F	204	-	5,5,5	0.42	0	5,5,5	0.22	0
5	GOL	E	801	-	5,5,5	0.37	0	5,5,5	0.61	0
5	GOL	E	806	-	5,5,5	0.45	0	5,5,5	0.45	0
5	GOL	A	801	-	5,5,5	0.37	0	5,5,5	0.43	0
5	GOL	E	803	-	5,5,5	0.49	0	5,5,5	0.25	0
5	GOL	F	202	-	5,5,5	0.38	0	5,5,5	0.31	0
5	GOL	A	806	-	5,5,5	0.35	0	5,5,5	0.33	0
5	GOL	A	811	-	5,5,5	0.34	0	5,5,5	0.26	0
6	PO4	F	207	-	4,4,4	0.95	0	6,6,6	0.44	0
5	GOL	E	805	-	5,5,5	0.42	0	5,5,5	0.21	0
5	GOL	A	804	-	5,5,5	0.36	0	5,5,5	0.33	0
5	GOL	F	206	-	5,5,5	0.38	0	5,5,5	0.28	0
6	PO4	E	808	-	4,4,4	0.88	0	6,6,6	0.58	0
7	CMC	L	101	4	45,53,54	1.70	9 (20%)	55,78,80	1.37	6 (10%)
5	GOL	A	803	-	5,5,5	0.33	0	5,5,5	0.50	0
5	GOL	A	808	-	5,5,5	0.36	0	5,5,5	0.41	0
6	PO4	A	813	-	4,4,4	0.84	0	6,6,6	0.56	0
5	GOL	A	812	-	5,5,5	0.34	0	5,5,5	0.67	0
5	GOL	C	202	-	5,5,5	0.35	0	5,5,5	0.16	0
5	GOL	F	201	-	5,5,5	0.36	0	5,5,5	0.27	0
5	GOL	A	809	-	5,5,5	0.34	0	5,5,5	0.28	0
5	GOL	F	205	-	5,5,5	0.40	0	5,5,5	0.37	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
7	CMC	I	101	4	-	6/46/67/68	0/3/3/3
5	GOL	F	203	-	-	2/4/4/4	-
5	GOL	A	805	-	-	2/4/4/4	-
5	GOL	A	802	-	-	2/4/4/4	-
5	GOL	B	201	-	-	4/4/4/4	-
5	GOL	C	201	-	-	3/4/4/4	-
5	GOL	E	804	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	807	-	-	0/4/4/4	-
5	GOL	A	810	-	-	4/4/4/4	-
5	GOL	E	802	-	-	4/4/4/4	-
5	GOL	F	204	-	-	2/4/4/4	-
5	GOL	E	801	-	-	4/4/4/4	-
5	GOL	E	806	-	-	0/4/4/4	-
5	GOL	A	801	-	-	3/4/4/4	-
5	GOL	E	803	-	-	2/4/4/4	-
5	GOL	F	202	-	-	2/4/4/4	-
5	GOL	A	806	-	-	2/4/4/4	-
5	GOL	A	811	-	-	2/4/4/4	-
5	GOL	E	805	-	-	4/4/4/4	-
5	GOL	A	804	-	-	0/4/4/4	-
5	GOL	F	206	-	-	2/4/4/4	-
7	CMC	L	101	4	-	4/46/67/68	0/3/3/3
5	GOL	A	803	-	-	2/4/4/4	-
5	GOL	A	808	-	-	2/4/4/4	-
5	GOL	A	812	-	-	0/4/4/4	-
5	GOL	C	202	-	-	4/4/4/4	-
5	GOL	F	201	-	-	2/4/4/4	-
5	GOL	A	809	-	-	2/4/4/4	-
5	GOL	F	205	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	101	CMC	C9P-N8P	5.51	1.45	1.33
7	I	101	CMC	C9P-N8P	5.51	1.45	1.33
7	L	101	CMC	C5P-N4P	4.83	1.44	1.33
7	I	101	CMC	C5P-N4P	4.48	1.43	1.33
7	I	101	CMC	C2B-C1B	-3.88	1.47	1.53
7	L	101	CMC	C2B-C3B	-3.30	1.45	1.52
7	I	101	CMC	C2B-C3B	-3.18	1.45	1.52
7	I	101	CMC	O4B-C1B	3.03	1.45	1.41
7	L	101	CMC	C2B-C1B	-2.97	1.49	1.53
7	I	101	CMC	C2A-N3A	2.90	1.36	1.32
7	L	101	CMC	C2A-N3A	2.83	1.36	1.32
7	L	101	CMC	O4B-C1B	2.69	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	101	CMC	C5A-N7A	2.52	1.48	1.39
7	I	101	CMC	C5A-N7A	2.35	1.48	1.39
7	L	101	CMC	OAP-CAP	-2.29	1.38	1.42
7	I	101	CMC	P3B-O9A	-2.18	1.46	1.54
7	L	101	CMC	P3B-O9A	-2.04	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	101	CMC	N3A-C2A-N1A	-4.92	120.99	128.68
7	L	101	CMC	N3A-C2A-N1A	-4.59	121.50	128.68
7	I	101	CMC	C2P-S1P-C1	4.11	108.58	101.71
7	L	101	CMC	C2P-S1P-C1	3.26	107.15	101.71
7	I	101	CMC	C7P-C6P-C5P	-3.10	107.20	112.36
7	L	101	CMC	C1B-N9A-C4A	-3.01	121.35	126.64
7	I	101	CMC	C4A-C5A-N7A	-3.00	106.27	109.40
7	L	101	CMC	C4A-C5A-N7A	-2.77	106.51	109.40
7	I	101	CMC	C3B-C2B-C1B	2.73	105.94	99.89
7	L	101	CMC	O9A-P3B-O7A	-2.72	100.02	110.68
7	I	101	CMC	O9A-P3B-O7A	-2.34	101.51	110.68
7	I	101	CMC	CDP-CBP-CAP	2.24	112.70	108.82
7	L	101	CMC	P2A-O3A-P1A	-2.08	125.67	132.83
7	I	101	CMC	C1B-N9A-C4A	-2.08	122.99	126.64
7	I	101	CMC	C5B-C4B-C3B	-2.05	107.60	114.40
7	I	101	CMC	P2A-O3A-P1A	-2.00	125.96	132.83

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	101	CMC	CCP-O6A-P2A-O4A
5	A	805	GOL	O1-C1-C2-O2
5	A	805	GOL	O1-C1-C2-C3
5	A	802	GOL	O1-C1-C2-C3
5	B	201	GOL	O1-C1-C2-C3
5	C	201	GOL	O1-C1-C2-C3
5	A	810	GOL	O1-C1-C2-O2
5	A	810	GOL	O1-C1-C2-C3
5	E	802	GOL	O1-C1-C2-C3
5	F	204	GOL	O1-C1-C2-C3
5	E	801	GOL	O1-C1-C2-O2
5	E	801	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	801	GOL	O1-C1-C2-C3
5	E	803	GOL	O1-C1-C2-C3
5	F	203	GOL	O1-C1-C2-O2
5	F	203	GOL	O1-C1-C2-C3
5	E	805	GOL	C1-C2-C3-O3
5	F	206	GOL	C1-C2-C3-O3
7	L	101	CMC	CCP-O6A-P2A-O3A
7	L	101	CMC	CCP-O6A-P2A-O4A
5	A	803	GOL	O1-C1-C2-C3
5	A	808	GOL	O1-C1-C2-C3
5	C	202	GOL	O1-C1-C2-C3
5	C	202	GOL	C1-C2-C3-O3
5	F	201	GOL	O1-C1-C2-C3
5	A	801	GOL	O1-C1-C2-O2
5	F	206	GOL	O2-C2-C3-O3
7	I	101	CMC	C2-C1-S1P-C2P
5	B	201	GOL	C1-C2-C3-O3
5	E	804	GOL	O1-C1-C2-C3
5	E	804	GOL	C1-C2-C3-O3
5	A	810	GOL	C1-C2-C3-O3
5	E	802	GOL	C1-C2-C3-O3
5	F	202	GOL	O1-C1-C2-C3
5	A	811	GOL	O1-C1-C2-C3
5	E	805	GOL	O1-C1-C2-C3
5	A	809	GOL	O1-C1-C2-C3
5	A	802	GOL	O1-C1-C2-O2
5	C	201	GOL	O1-C1-C2-O2
5	E	802	GOL	O1-C1-C2-O2
5	F	204	GOL	O1-C1-C2-O2
5	E	803	GOL	O1-C1-C2-O2
5	A	811	GOL	O1-C1-C2-O2
5	E	805	GOL	O1-C1-C2-O2
5	E	805	GOL	O2-C2-C3-O3
5	A	803	GOL	O1-C1-C2-O2
5	A	808	GOL	O1-C1-C2-O2
5	C	202	GOL	O2-C2-C3-O3
5	F	201	GOL	O1-C1-C2-O2
5	B	201	GOL	O2-C2-C3-O3
5	E	804	GOL	O1-C1-C2-O2
5	C	202	GOL	O1-C1-C2-O2
7	L	101	CMC	C2-C1-S1P-C2P
5	B	201	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	E	804	GOL	O2-C2-C3-O3
5	E	802	GOL	O2-C2-C3-O3
7	L	101	CMC	C6P-C7P-N8P-C9P
7	I	101	CMC	CCP-O6A-P2A-O3A
5	A	806	GOL	O1-C1-C2-O2
5	A	810	GOL	O2-C2-C3-O3
5	A	809	GOL	O1-C1-C2-O2
5	F	202	GOL	O1-C1-C2-O2
7	I	101	CMC	C6P-C7P-N8P-C9P
5	C	201	GOL	O2-C2-C3-O3
7	I	101	CMC	C3P-C2P-S1P-C1
5	E	801	GOL	O2-C2-C3-O3
5	A	806	GOL	O1-C1-C2-C3
5	E	801	GOL	C1-C2-C3-O3
5	A	801	GOL	C1-C2-C3-O3
7	I	101	CMC	C5B-O5B-P1A-O1A

There are no ring outliers.

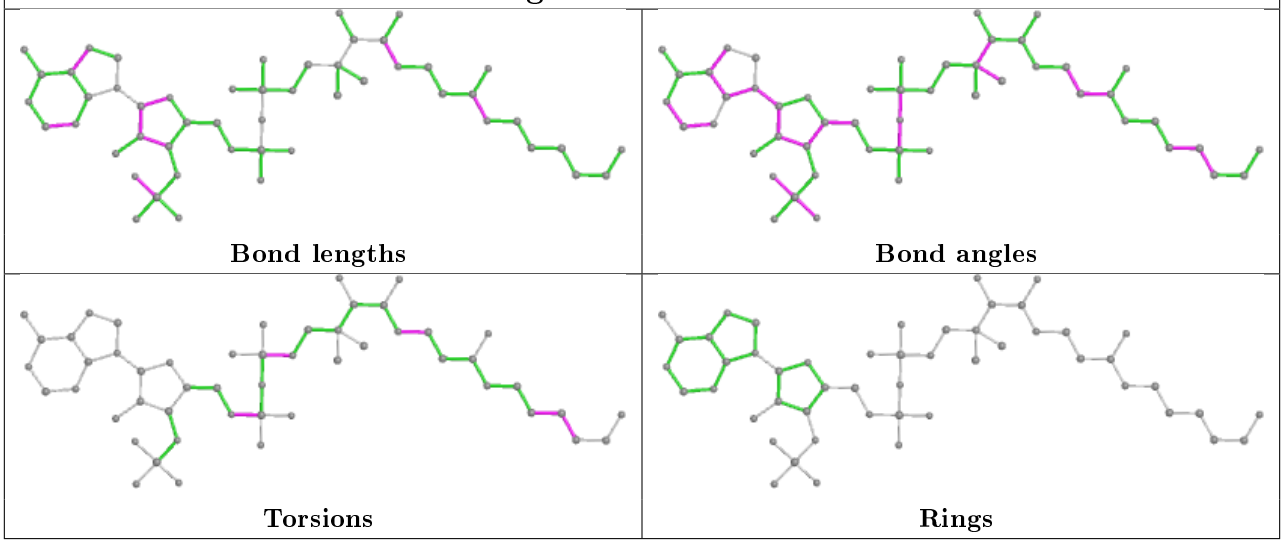
17 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	101	CMC	4	0
5	A	805	GOL	2	0
5	B	201	GOL	2	0
6	E	807	PO4	3	0
5	A	810	GOL	2	0
5	F	204	GOL	1	0
5	E	806	GOL	2	0
5	A	801	GOL	4	0
5	E	803	GOL	3	0
5	A	806	GOL	1	0
5	A	811	GOL	1	0
6	F	207	PO4	1	0
5	F	206	GOL	2	0
7	L	101	CMC	1	0
5	A	808	GOL	3	0
5	F	201	GOL	1	0
5	A	809	GOL	1	0

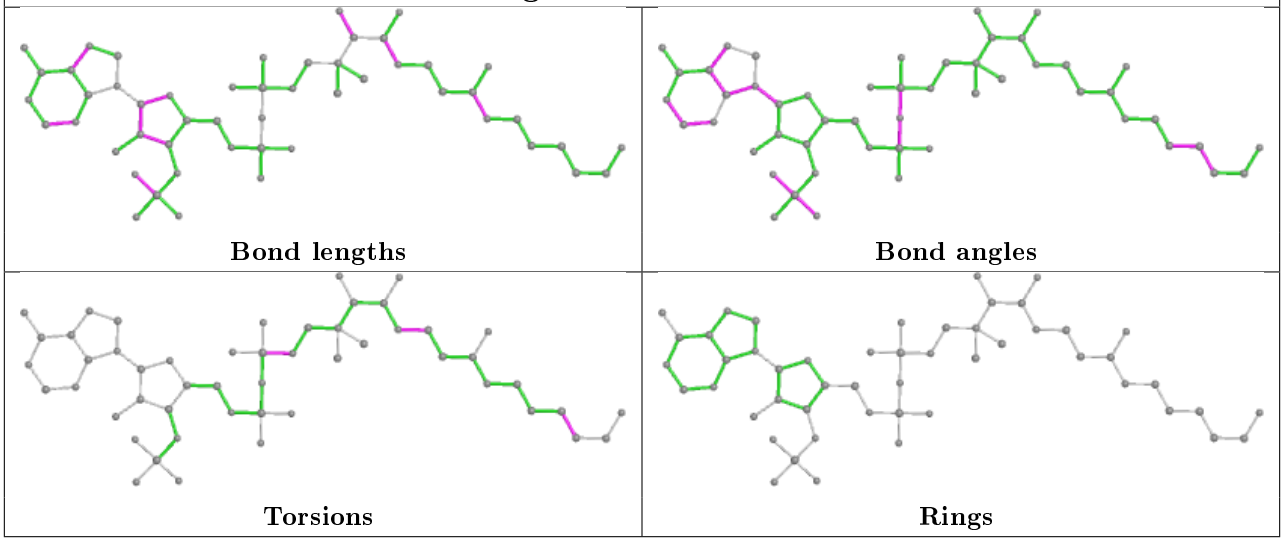
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CMC I 101



Ligand CMC L 101



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	665/745 (89%)	0.00	42 (6%) 20 15	28, 49, 104, 151	0
1	E	658/745 (88%)	0.07	45 (6%) 17 12	28, 51, 122, 184	0
2	B	178/195 (91%)	0.11	8 (4%) 33 26	27, 37, 123, 153	0
2	F	177/195 (90%)	-0.03	4 (2%) 60 54	25, 38, 121, 179	0
3	C	45/62 (72%)	-0.16	1 (2%) 62 56	47, 57, 89, 107	0
3	G	45/62 (72%)	-0.07	1 (2%) 62 56	50, 65, 83, 113	0
4	I	4/4 (100%)	0.72	1 (25%) 0 0	41, 46, 70, 99	0
4	L	4/4 (100%)	0.22	0 100 100	35, 42, 56, 90	0
All	All	1776/2012 (88%)	0.03	102 (5%) 23 18	25, 49, 113, 184	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	TYR	7.8
1	E	573	PRO	6.9
1	E	32	ALA	6.0
2	B	176	LEU	5.6
1	E	36	LEU	5.6
1	A	25	TYR	5.5
1	E	7	THR	5.4
1	E	27	ARG	5.3
1	E	14	ARG	5.1
1	E	28	GLY	5.1
1	E	19	HIS	5.0
1	E	34	GLN	4.8
1	E	13	PHE	4.8
1	E	22	ASP	4.8
1	E	56	GLN	4.7
1	E	20	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	58	LYS	4.5
1	A	30	LYS	4.5
2	B	179	ASP	4.4
1	E	18	ARG	4.4
1	E	10	ALA	4.2
1	A	24	GLN	4.1
3	G	81	MET	4.1
1	A	18	ARG	4.0
2	B	177	GLU	4.0
1	E	24	GLN	3.9
1	E	29	LEU	3.7
1	A	38	LYS	3.7
1	E	53	LEU	3.6
1	E	30	LYS	3.6
1	E	26	LYS	3.6
1	E	503	ALA	3.5
1	A	8	ARG	3.5
1	A	19	HIS	3.5
1	A	31	ALA	3.5
1	A	741	VAL	3.5
1	A	13	PHE	3.5
2	B	173	GLU	3.4
1	E	17	ILE	3.4
1	E	37	LYS	3.4
1	A	17	ILE	3.4
1	E	38	LYS	3.4
1	A	739	VAL	3.3
1	A	28	GLY	3.2
1	E	31	ALA	3.2
1	A	20	TYR	3.2
1	A	34	GLN	3.2
2	F	176	LEU	3.2
1	E	11	ASN	3.2
1	A	23	LYS	3.2
1	A	740	GLY	3.1
1	A	27	ARG	3.1
1	A	56	GLN	3.1
1	A	12	LEU	3.0
1	E	12	LEU	3.0
1	A	358	SER	3.0
2	B	175	GLU	2.9
1	A	58	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	39	ASN	2.9
1	E	23	LYS	2.8
1	E	8	ARG	2.8
1	A	9	GLU	2.8
1	E	35	ILE	2.8
1	E	16	VAL	2.7
2	B	178	GLU	2.7
2	F	175	GLU	2.6
3	C	81	MET	2.6
1	A	37	LYS	2.5
1	E	15	THR	2.5
1	A	16	VAL	2.5
2	B	174	LYS	2.5
1	E	739	VAL	2.5
1	A	26	LYS	2.4
2	F	170	ALA	2.4
1	A	21	GLU	2.4
1	A	32	ALA	2.4
1	E	54	ASN	2.4
1	A	304	ARG	2.3
1	A	36	LEU	2.3
1	A	22	ASP	2.3
4	I	5	SER	2.3
1	A	52	ILE	2.3
1	E	654	LEU	2.3
1	A	15	THR	2.3
1	A	7	THR	2.3
2	B	75	ASP	2.2
1	E	41	LYS	2.2
1	E	21	GLU	2.2
1	A	53	LEU	2.2
2	F	72	GLU	2.2
1	A	471	GLU	2.2
1	A	14	ARG	2.2
1	E	651	LYS	2.1
1	A	29	LEU	2.1
1	E	59	THR	2.1
1	E	33	GLU	2.1
1	E	60	GLU	2.1
1	A	10	ALA	2.1
1	E	9	GLU	2.1
1	A	33	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	61	GLU	2.1
1	A	274	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
2	FME	F	1	10/11	0.96	0.20	39,59,78,79	0
2	FME	B	1	10/11	0.98	0.16	26,49,60,69	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
5	GOL	F	201	6/6	0.59	0.51	104,107,109,110	0
5	GOL	E	805	6/6	0.70	0.31	67,73,83,84	0
5	GOL	A	807	6/6	0.72	0.42	89,90,96,101	0
5	GOL	E	806	6/6	0.72	0.31	62,70,72,76	0
5	GOL	A	805	6/6	0.74	0.40	79,84,92,99	0
6	PO4	F	207	5/5	0.76	0.27	165,167,168,168	0
5	GOL	A	801	6/6	0.77	0.55	109,111,112,113	0
5	GOL	F	205	6/6	0.77	0.33	58,69,79,81	0
5	GOL	C	202	6/6	0.78	0.42	82,90,98,108	0
5	GOL	E	801	6/6	0.79	0.30	60,64,70,70	0
5	GOL	F	204	6/6	0.79	0.29	72,81,83,84	0
5	GOL	F	202	6/6	0.80	0.23	57,77,80,81	0
5	GOL	B	201	6/6	0.82	0.36	96,100,101,101	0
5	GOL	A	804	6/6	0.83	0.36	51,72,79,80	0

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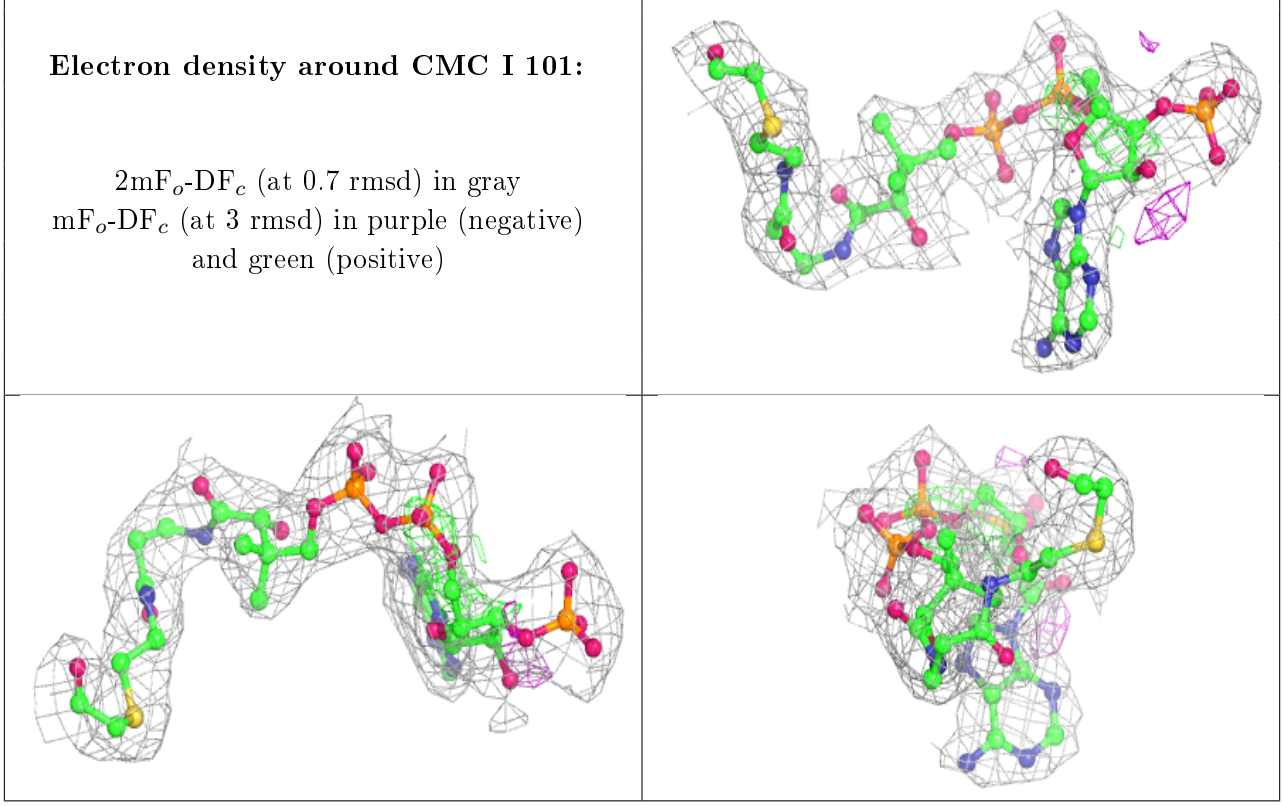
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	811	6/6	0.83	0.17	85,89,90,90	0
5	GOL	A	802	6/6	0.84	0.23	70,80,86,86	0
5	GOL	A	809	6/6	0.85	0.28	80,92,95,104	0
5	GOL	E	803	6/6	0.85	0.40	92,96,99,100	0
5	GOL	F	206	6/6	0.86	0.25	72,73,78,84	0
5	GOL	A	803	6/6	0.86	0.23	62,69,78,88	0
5	GOL	A	808	6/6	0.87	0.32	85,95,95,102	0
6	PO4	E	808	5/5	0.88	0.28	109,113,118,120	0
5	GOL	A	806	6/6	0.88	0.21	79,80,84,88	0
5	GOL	C	201	6/6	0.88	0.27	63,70,72,73	0
5	GOL	A	812	6/6	0.88	0.25	49,67,71,74	0
5	GOL	F	203	6/6	0.91	0.27	63,67,69,71	0
5	GOL	E	802	6/6	0.92	0.37	93,94,95,98	0
5	GOL	A	810	6/6	0.93	0.27	61,67,70,73	0
5	GOL	E	804	6/6	0.93	0.09	88,90,91,92	0
6	PO4	E	807	5/5	0.94	0.15	94,101,103,105	0
6	PO4	A	813	5/5	0.97	0.12	90,91,92,96	0
7	CMC	I	101	51/52	0.97	0.19	18,44,106,112	0
7	CMC	L	101	51/52	0.97	0.17	24,43,84,88	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

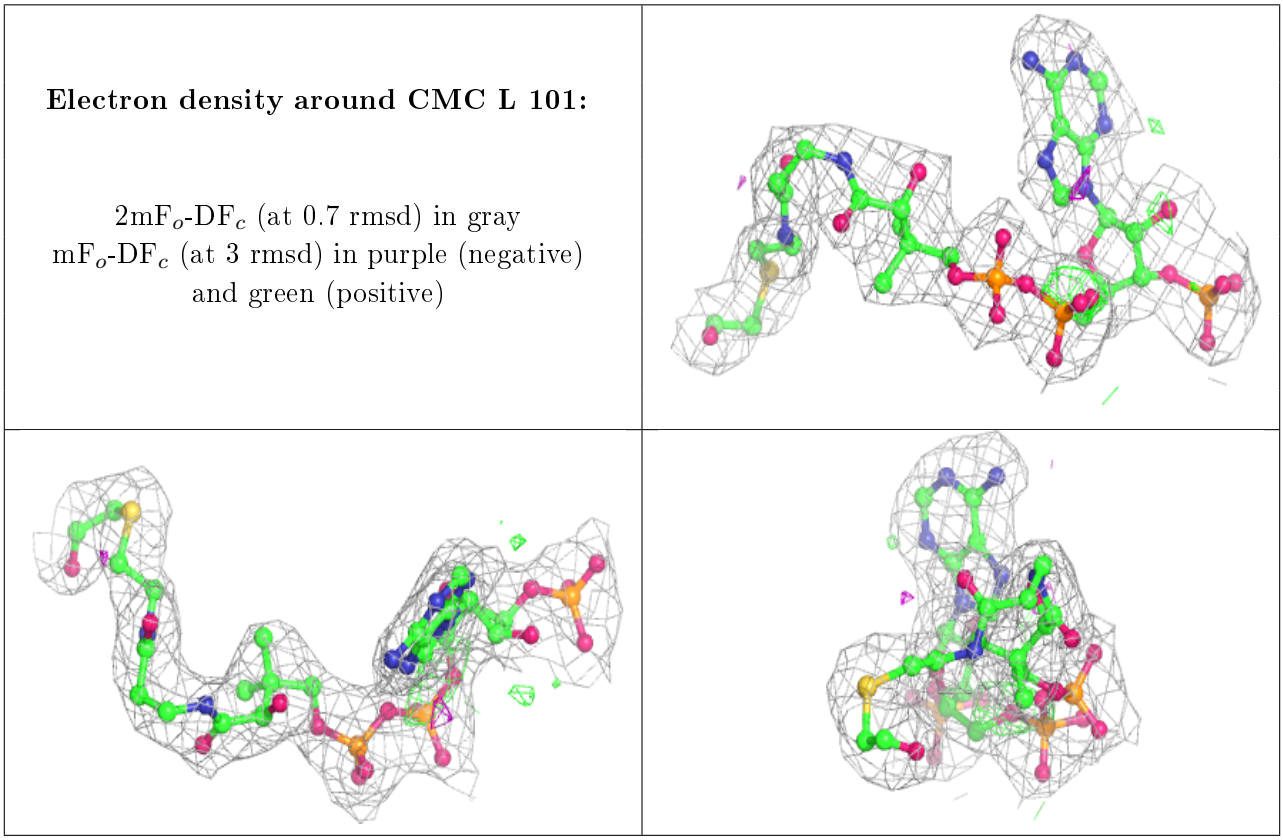
Electron density around CMC I 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CMC L 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.