



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 12:37 AM BST

PDB ID : 6S6Y
Title : X-ray crystal structure of the formyltransferase/hydrolase complex (Fh-cABCD) from *Methylobacterium extorquens* in complex with methylofuran
Authors : Wagner, T.; Hemmann, J.L.; Shima, S.; Vorholt, J.
Deposited on : 2019-07-04
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.13.1
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)	:	2.13.1

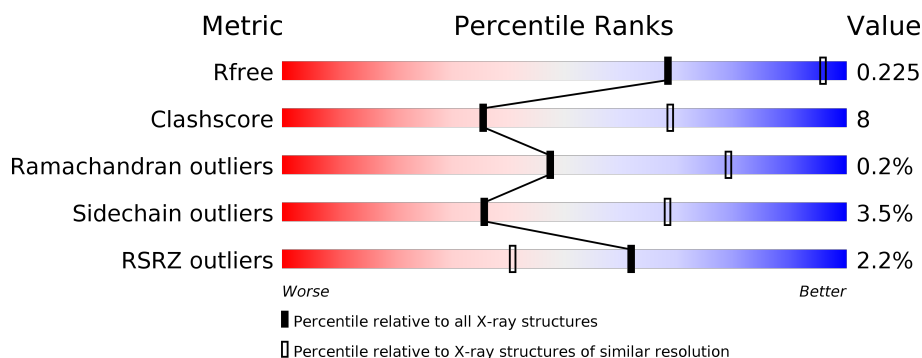
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.








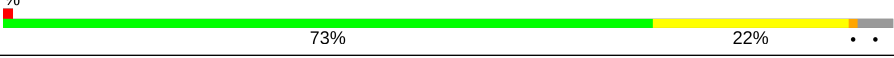
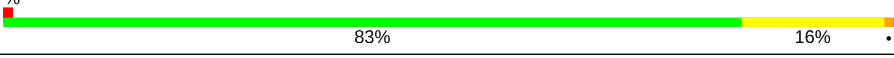

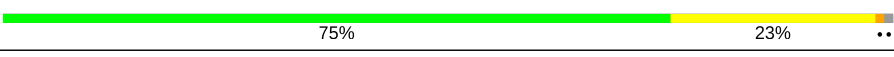

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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	548	<div> <div>79%</div> <div>20%</div> <div>•</div> </div>
1	E	548	<div> <div>6%</div> <div>80%</div> <div>18%</div> <div>••</div> </div>
1	I	548	<div> <div>77%</div> <div>21%</div> <div>••</div> </div>
1	M	548	<div> <div>6%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
2	B	361	<div> <div>82%</div> <div>16%</div> <div>••</div> </div>
2	F	361	<div> <div>7%</div> <div>80%</div> <div>18%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	361	
2	N	361	
3	C	276	
3	G	276	
3	K	276	
3	O	276	
4	D	310	
4	H	310	
4	L	310	
4	P	310	

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
11	CL	C	301	-	-	X	-
12	DGL	P	403	-	-	X	X
13	NH2	B	403	-	-	-	X
16	L6K	I	602	-	-	-	X
6	MFN	A	602	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 43288 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 Formylmethanofuran dehydrogenase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4104	2572	731	786	15			
1	E	542	Total	C	N	O	S	0	0	0
			4063	2548	724	776	15			
1	I	545	Total	C	N	O	S	0	0	0
			4087	2561	727	784	15			
1	M	546	Total	C	N	O	S	0	0	0
			4085	2561	728	781	15			

- Molecule 2 is a protein called Tungsten-containing formylmethanofuran dehydrogenase, subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	356	Total	C	N	O	S	0	0	0
			2552	1603	461	486	2			
2	F	355	Total	C	N	O	S	0	0	0
			2551	1602	460	487	2			
2	J	355	Total	C	N	O	S	0	0	0
			2558	1605	462	489	2			
2	N	355	Total	C	N	O	S	0	0	0
			2554	1603	461	488	2			

- Molecule 3 is a protein called Formylmethanofuran dehydrogenase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total	C	N	O	S	0	0	0
			1864	1152	344	363	5			
3	G	265	Total	C	N	O	S	0	0	0
			1864	1152	344	363	5			
3	K	265	Total	C	N	O	S	0	0	0
			1864	1152	344	363	5			
3	O	265	Total	C	N	O	S	0	0	0
			1864	1152	344	363	5			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	266	HIS	-	expression tag	UNP A9W3R7
C	267	GLY	-	expression tag	UNP A9W3R7
C	268	SER	-	expression tag	UNP A9W3R7
C	269	ALA	-	expression tag	UNP A9W3R7
C	270	TRP	-	expression tag	UNP A9W3R7
C	271	SER	-	expression tag	UNP A9W3R7
C	272	HIS	-	expression tag	UNP A9W3R7
C	273	PRO	-	expression tag	UNP A9W3R7
C	274	GLN	-	expression tag	UNP A9W3R7
C	275	PHE	-	expression tag	UNP A9W3R7
C	276	GLU	-	expression tag	UNP A9W3R7
C	277	LYS	-	expression tag	UNP A9W3R7
G	266	HIS	-	expression tag	UNP A9W3R7
G	267	GLY	-	expression tag	UNP A9W3R7
G	268	SER	-	expression tag	UNP A9W3R7
G	269	ALA	-	expression tag	UNP A9W3R7
G	270	TRP	-	expression tag	UNP A9W3R7
G	271	SER	-	expression tag	UNP A9W3R7
G	272	HIS	-	expression tag	UNP A9W3R7
G	273	PRO	-	expression tag	UNP A9W3R7
G	274	GLN	-	expression tag	UNP A9W3R7
G	275	PHE	-	expression tag	UNP A9W3R7
G	276	GLU	-	expression tag	UNP A9W3R7
G	277	LYS	-	expression tag	UNP A9W3R7
K	266	HIS	-	expression tag	UNP A9W3R7
K	267	GLY	-	expression tag	UNP A9W3R7
K	268	SER	-	expression tag	UNP A9W3R7
K	269	ALA	-	expression tag	UNP A9W3R7
K	270	TRP	-	expression tag	UNP A9W3R7
K	271	SER	-	expression tag	UNP A9W3R7
K	272	HIS	-	expression tag	UNP A9W3R7
K	273	PRO	-	expression tag	UNP A9W3R7
K	274	GLN	-	expression tag	UNP A9W3R7
K	275	PHE	-	expression tag	UNP A9W3R7
K	276	GLU	-	expression tag	UNP A9W3R7
K	277	LYS	-	expression tag	UNP A9W3R7
O	266	HIS	-	expression tag	UNP A9W3R7
O	267	GLY	-	expression tag	UNP A9W3R7
O	268	SER	-	expression tag	UNP A9W3R7
O	269	ALA	-	expression tag	UNP A9W3R7
O	270	TRP	-	expression tag	UNP A9W3R7
O	271	SER	-	expression tag	UNP A9W3R7

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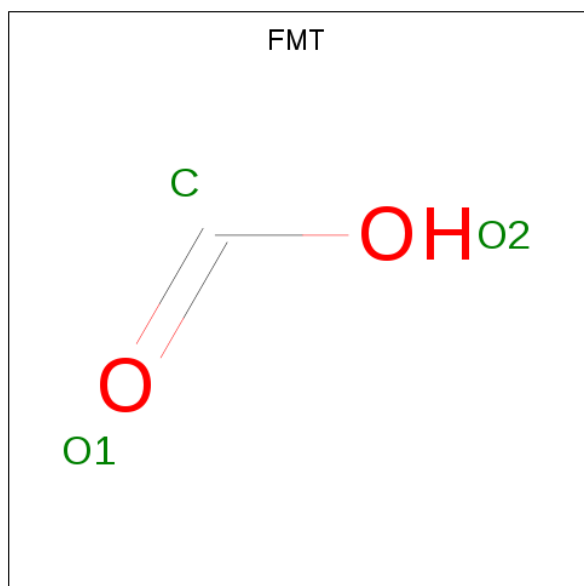
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Chain	Residue	Modelled	Actual	Comment	Reference
O	272	HIS	-	expression tag	UNP A9W3R7
O	273	PRO	-	expression tag	UNP A9W3R7
O	274	GLN	-	expression tag	UNP A9W3R7
O	275	PHE	-	expression tag	UNP A9W3R7
O	276	GLU	-	expression tag	UNP A9W3R7
O	277	LYS	-	expression tag	UNP A9W3R7

- Molecule 4 is a protein called Formylmethanofuran--tetrahydromethanopterin formyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	308	Total	C	N	O	S	0	0	0
			2252	1422	396	420	14			
4	H	308	Total	C	N	O	S	0	0	0
			2252	1422	396	420	14			
4	L	308	Total	C	N	O	S	0	0	0
			2252	1422	396	420	14			
4	P	308	Total	C	N	O	S	0	0	0
			2252	1422	396	420	14			

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



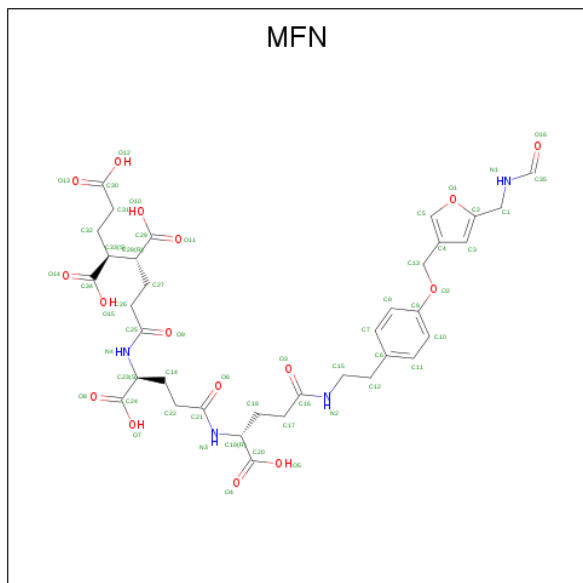
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	I	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	J	1	3	1	2	0	0

- Molecule 6 is N-[4,5,7-TRICARBOXYHEPTANOYL]-L-GAMMA-GLUTAMYL-N-{2-[4-({5-[(FORMYLAMINO)METHYL]-3-FURYL}METHOXY)PHENYL]ETHYL}-D-GLUTAMINE (three-letter code: MFN) (formula: $C_{35}H_{44}N_4O_{16}$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	21	16	2	3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	2	Total	Zn	0	0
			2	2		
8	A	2	Total	Zn	0	0
			2	2		
8	M	2	Total	Zn	0	0
			2	2		
8	E	2	Total	Zn	0	0
			2	2		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		
9	A	3	Total	Ca	0	0
			3	3		
9	L	2	Total	Ca	0	0
			2	2		

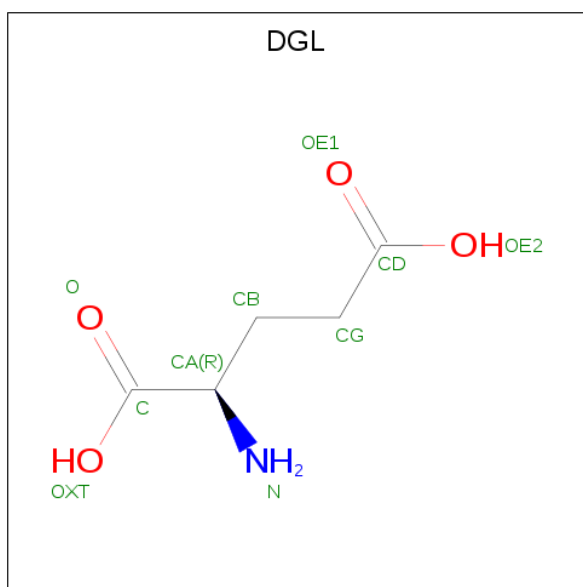
- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	P	2	Total K 2 2	0	0
10	J	1	Total K 1 1	0	0
10	D	1	Total K 1 1	0	0
10	H	1	Total K 1 1	0	0
10	I	1	Total K 1 1	0	0
10	A	2	Total K 2 2	0	0
10	L	1	Total K 1 1	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	I	1	Total Cl 1 1	0	0
11	A	2	Total Cl 2 2	0	0
11	C	1	Total Cl 1 1	0	0
11	J	1	Total Cl 1 1	0	0

- Molecule 12 is D-GLUTAMIC ACID (three-letter code: DGL) (formula: C₅H₉NO₄).



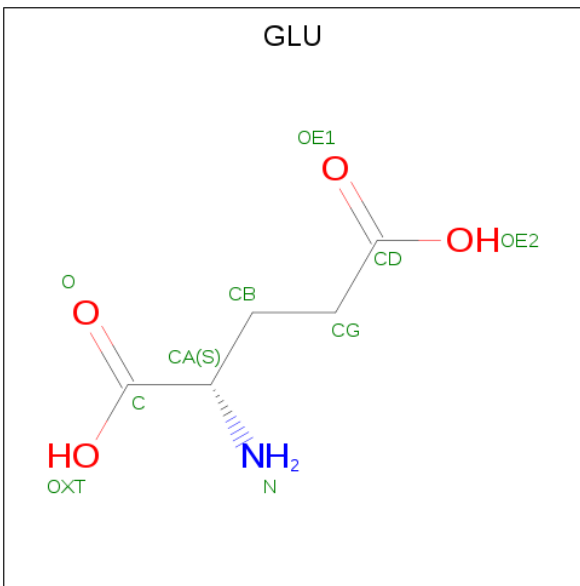
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	N	O	0	0
			9	5	1	3		
12	C	1	Total	C	N	O	0	0
			8	5	1	2		
12	D	1	Total	C	N	O	0	0
			9	5	1	3		
12	I	1	Total	C	N	O	0	0
			9	5	1	3		
12	I	1	Total	C	N	O	0	0
			10	5	1	4		
12	K	1	Total	C	N	O	0	0
			8	5	1	2		
12	L	1	Total	C	N	O	0	0
			10	5	1	4		
12	L	1	Total	C	N	O	0	0
			10	5	1	4		
12	O	1	Total	C	N	O	0	0
			8	5	1	2		
12	P	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 13 is AMINO GROUP (three-letter code: NH2) (formula: H₂N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total N 1 1	0	0

- Molecule 14 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



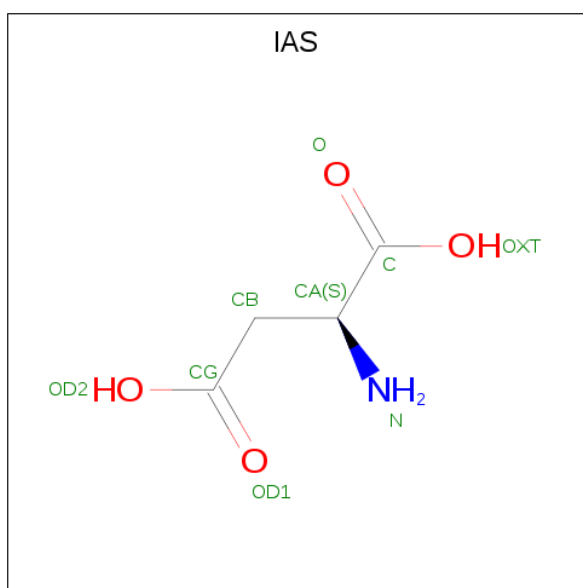
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total 9	C 5	N 1	O 3	0	0
14	C	1	Total 9	C 5	N 1	O 3	0	0
14	I	1	Total 9	C 5	N 1	O 3	0	0

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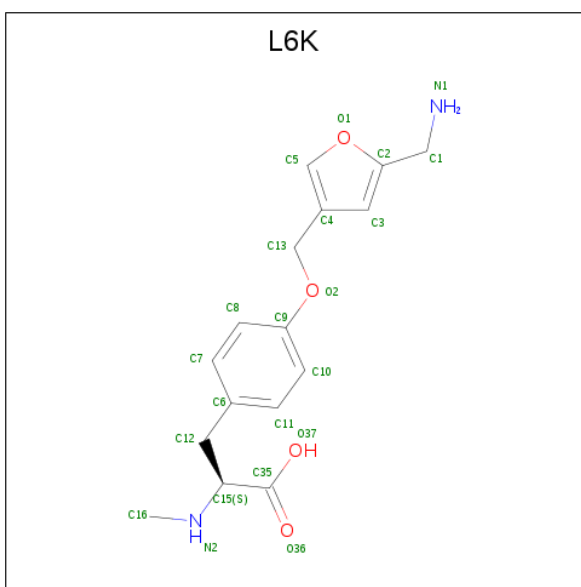
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	J	1	Total	C	N	O	0	0
			9	5	1	3		
14	K	1	Total	C	N	O	0	0
			8	5	1	2		
14	L	1	Total	C	N	O	0	0
			9	5	1	3		
14	O	1	Total	C	N	O	0	0
			9	5	1	3		
14	O	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 15 is BETA-L-ASPARTIC ACID (three-letter code: IAS) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	D	1	Total	C	N	O	0	0
			7	4	1	2		
15	P	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 16 is (2 {S})-3-[4-[[5-(aminomethyl)furan-3-yl]methoxy]phenyl]-2-(methylamino)propanoic acid (three-letter code: L6K) (formula: $C_{16}H_{20}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	I	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 17 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

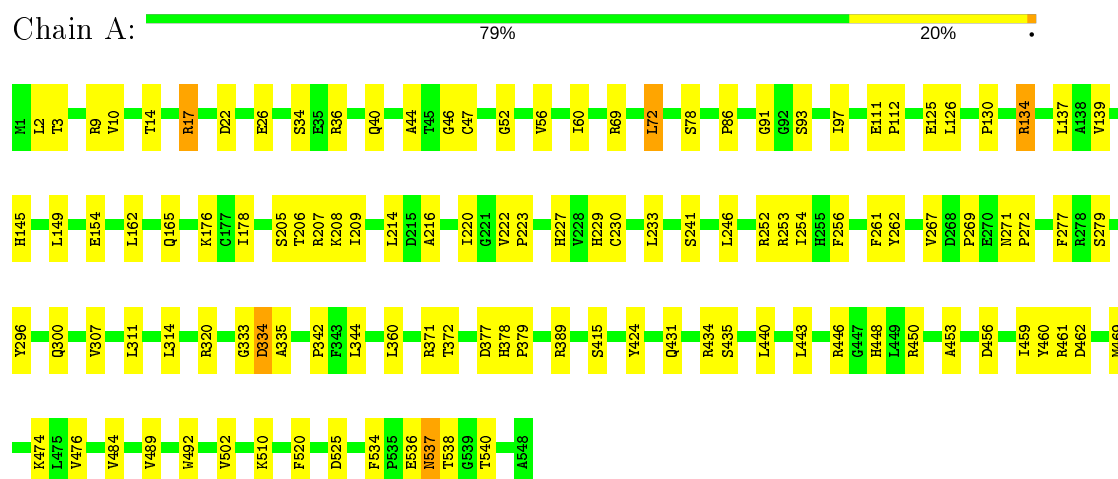
- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	J	1	Total	Na	0	0
			1	1		

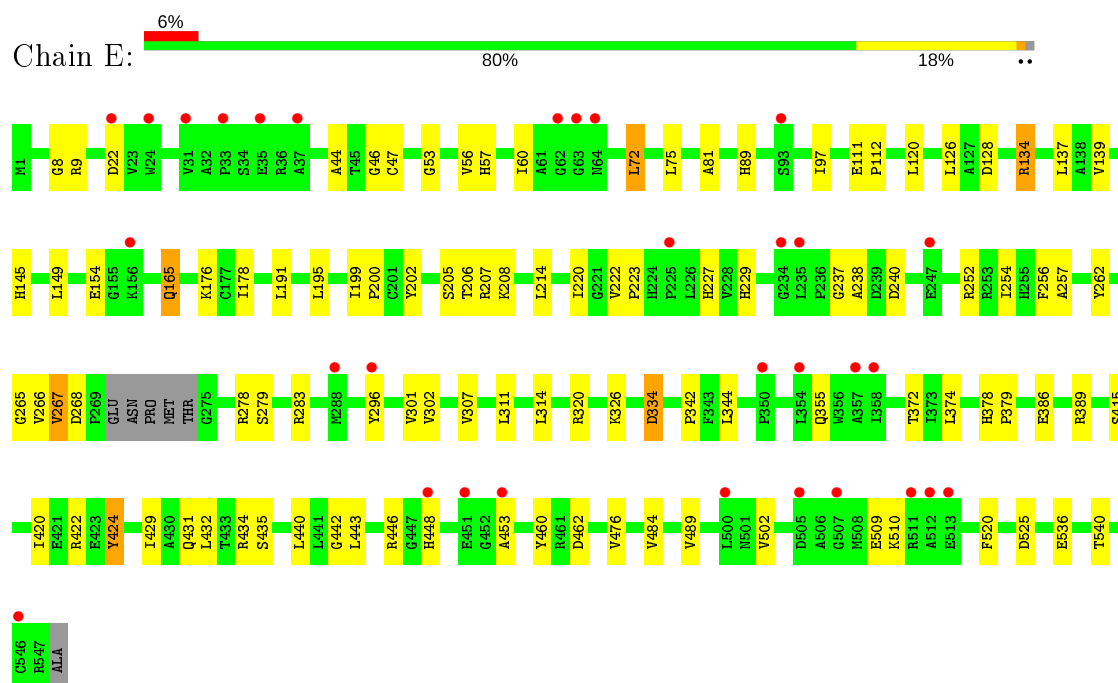
3 Residue-property plots [i](#)

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

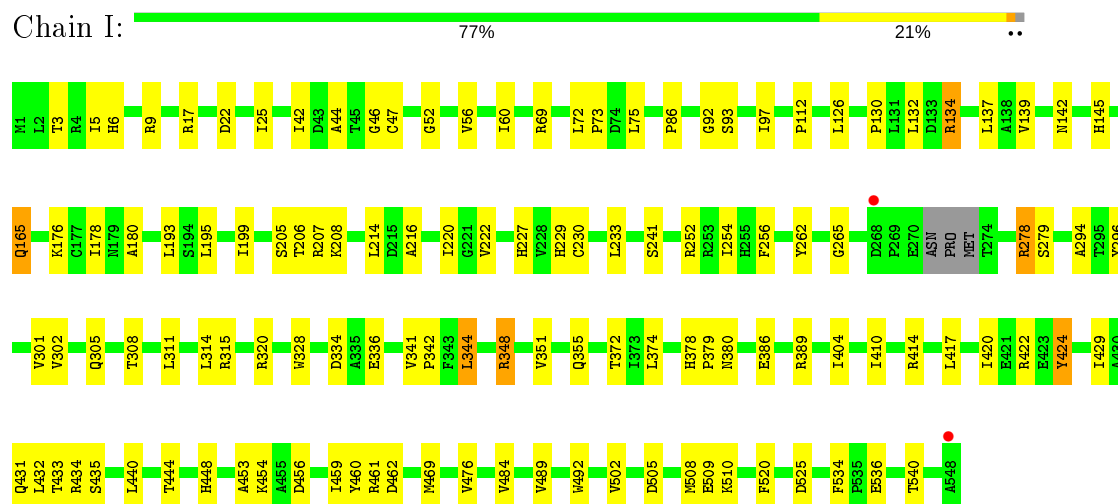
- Molecule 1: Formylmethanofuran dehydrogenase subunit A



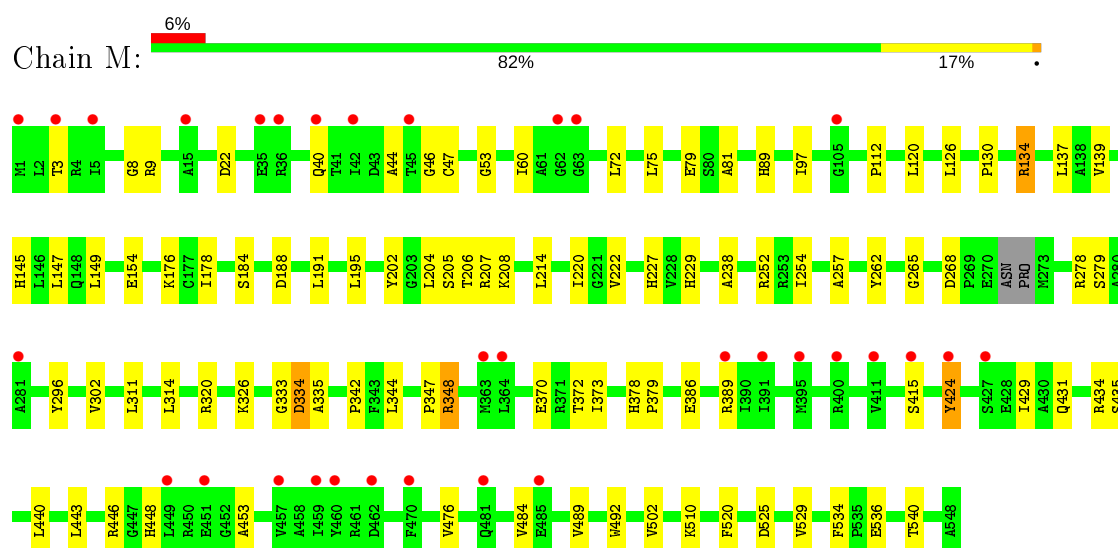
- Molecule 1: Formylmethanofuran dehydrogenase subunit A



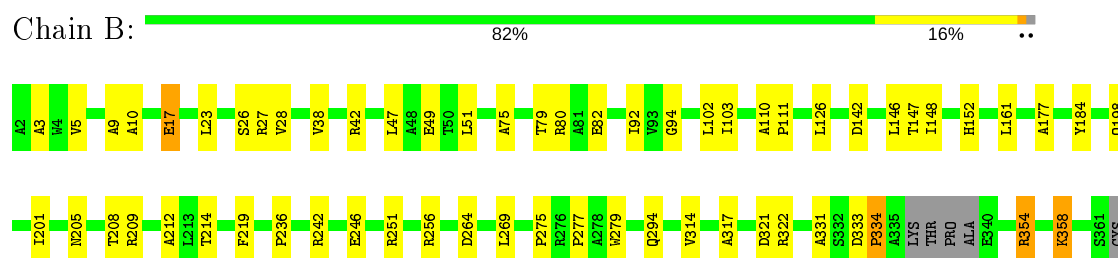
- Molecule 1: Formylmethanofuran dehydrogenase subunit A



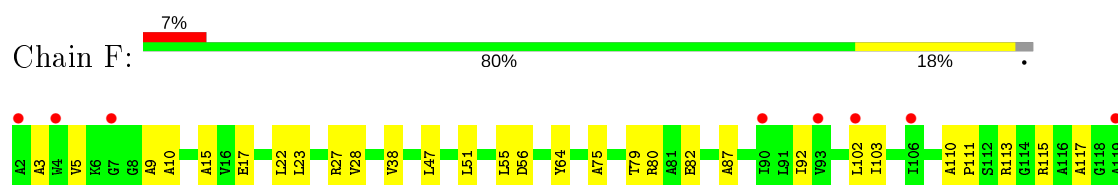
• Molecule 1: Formylmethanofuran dehydrogenase subunit A

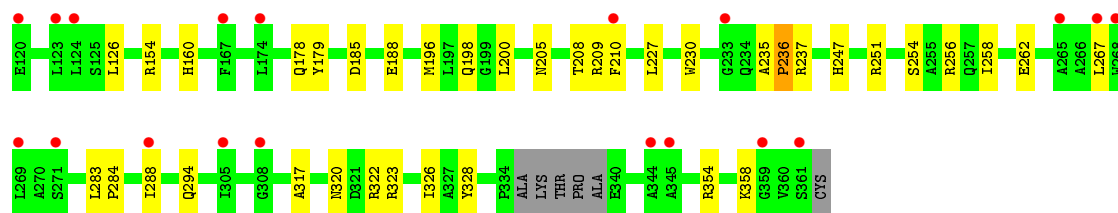


• Molecule 2: Tungsten-containing formylmethanofuran dehydrogenase, subunit B



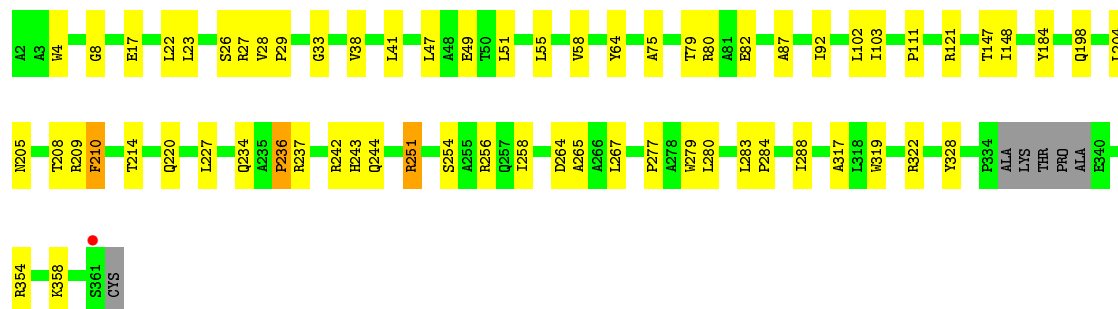
• Molecule 2: Tungsten-containing formylmethanofuran dehydrogenase, subunit B





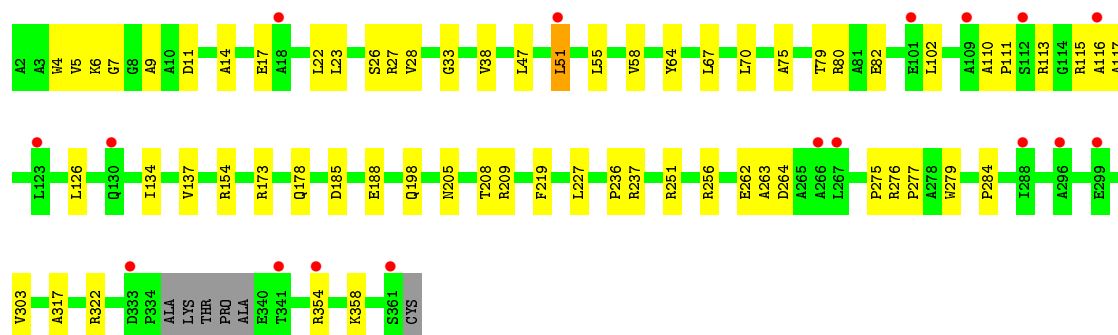
- Molecule 2: Tungsten-containing formylmethanofuran dehydrogenase, subunit B

Chain J: 80% 17% ..



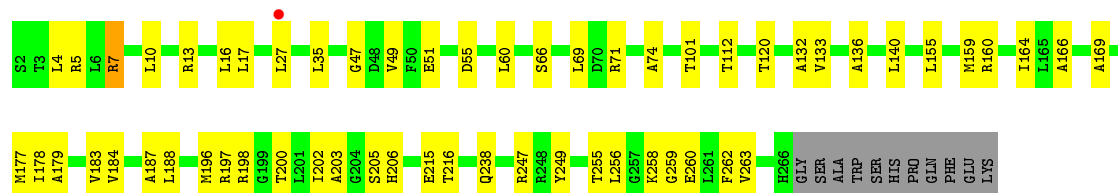
- Molecule 2: Tungsten-containing formylmethanofuran dehydrogenase, subunit B

Chain N: 5% 81% 17% .



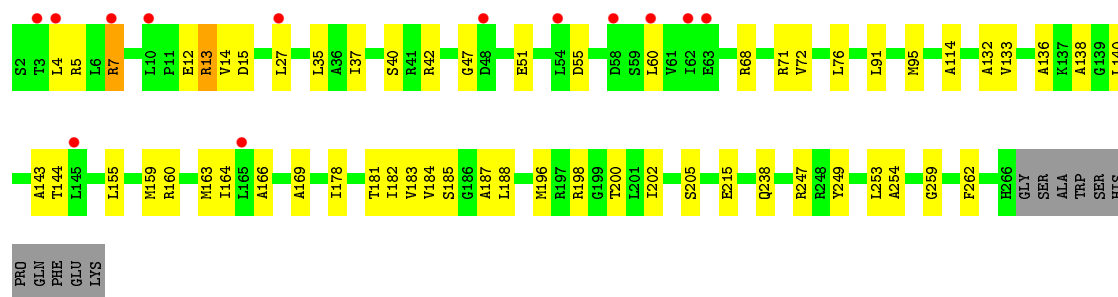
- Molecule 3: Formylmethanofuran dehydrogenase subunit C

Chain C: 75% 21% .



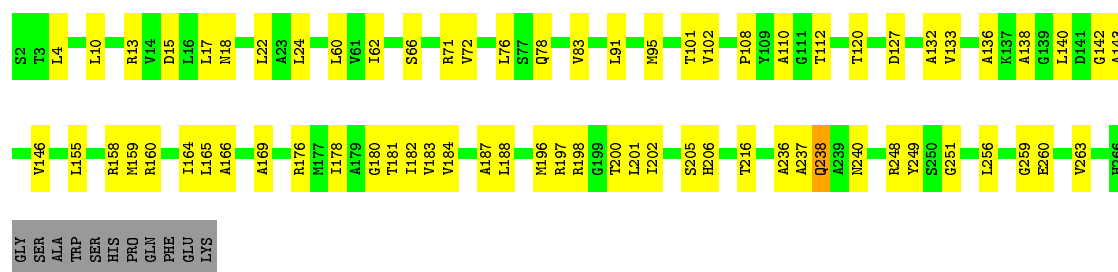
- Molecule 3: Formylmethanofuran dehydrogenase subunit C

Chain G: 5% 75% 20% ..



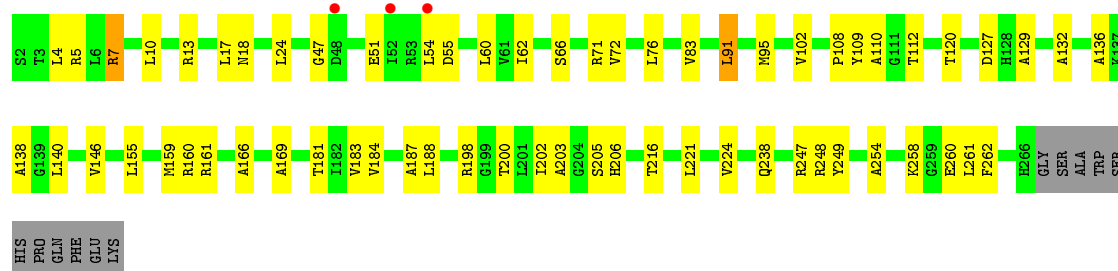
- Molecule 3: Formylmethanofuran dehydrogenase subunit C

Chain K: 71% 25%



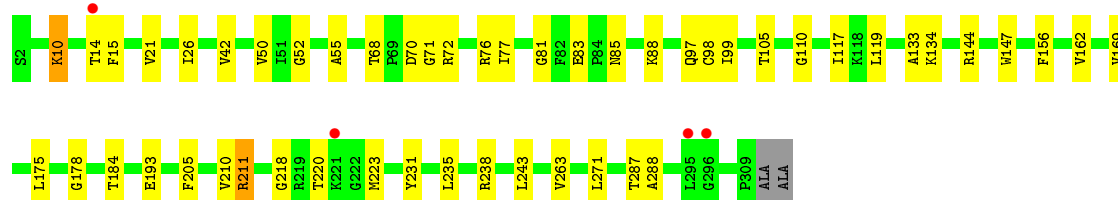
- Molecule 3: Formylmethanofuran dehydrogenase subunit C

Chain O: 73% 22%



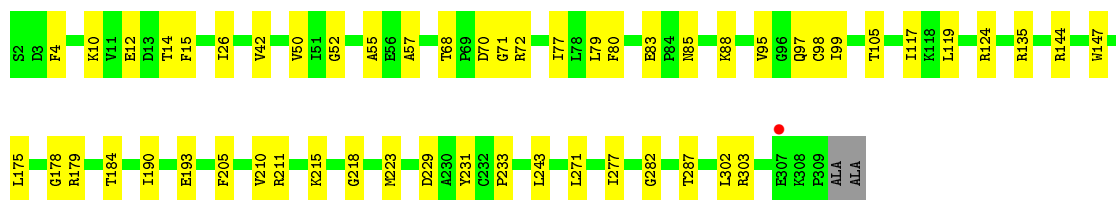
- Molecule 4: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain D: 83% 16%



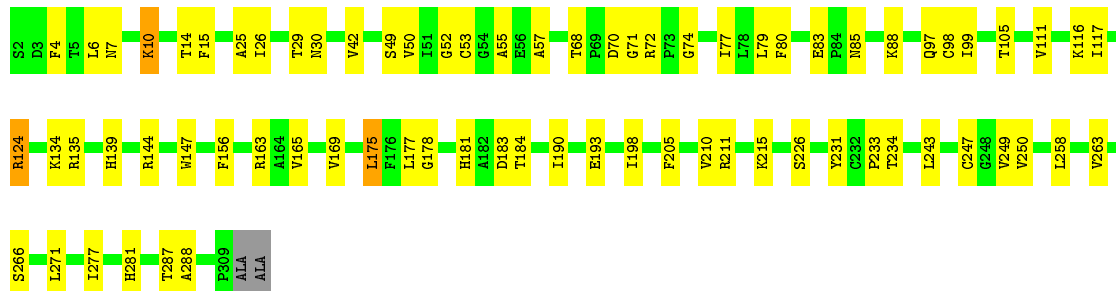
- Molecule 4: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain H: 82% 17%



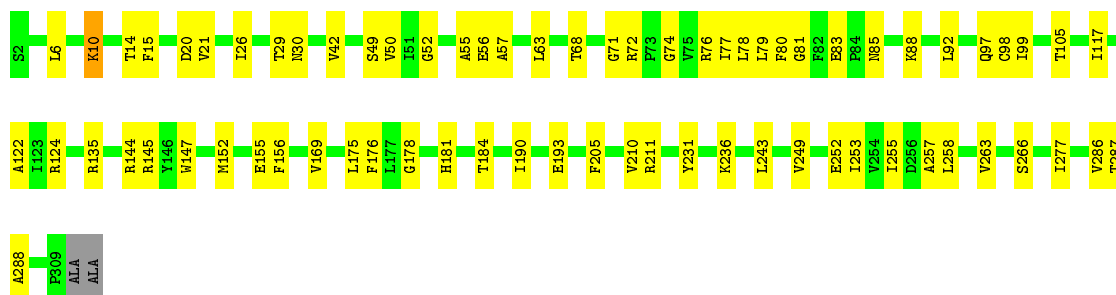
• Molecule 4: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain L: 75% 23%



• Molecule 4: Formylmethanofuran--tetrahydromethanopterin formyltransferase

Chain P: 76% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.97Å 130.32Å 172.69Å 84.97° 75.91° 82.09°	Depositor
Resolution (Å)	24.95 – 3.10 48.50 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (24.95-3.10) 96.6 (48.50-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.221 , 0.251 0.223 , 0.225	Depositor DCC
R_{free} test set	6518 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	43288	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CL, NA, FMT, EDO, DGL, MFN, NH2, K, L6K, CA, KCX, IAS

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	0.33	0/4175	0.53	0/5673
1	E	0.27	0/4132	0.46	0/5611
1	I	0.33	0/4156	0.54	0/5644
1	M	0.28	0/4154	0.47	0/5642
2	B	0.33	0/2599	0.54	0/3543
2	F	0.27	0/2598	0.48	0/3541
2	J	0.33	0/2605	0.54	0/3550
2	N	0.27	0/2601	0.48	0/3545
3	C	0.34	0/1885	0.60	0/2547
3	G	0.27	0/1885	0.54	0/2547
3	K	0.32	0/1885	0.60	0/2547
3	O	0.29	0/1885	0.54	0/2547
4	D	0.29	0/2295	0.52	0/3110
4	H	0.31	0/2295	0.53	0/3110
4	L	0.34	0/2295	0.55	0/3110
4	P	0.35	0/2295	0.58	0/3110
All	All	0.31	0/43740	0.52	0/59377

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4104	0	4039	66	0
1	E	4063	0	4005	56	0
1	I	4087	0	4025	74	0
1	M	4085	0	4021	51	0
2	B	2552	0	2519	36	0
2	F	2551	0	2518	40	0
2	J	2558	0	2527	40	0
2	N	2554	0	2522	39	0
3	C	1864	0	1890	38	0
3	G	1864	0	1890	35	0
3	K	1864	0	1890	48	0
3	O	1864	0	1890	38	0
4	D	2252	0	2265	40	0
4	H	2252	0	2265	40	0
4	L	2252	0	2265	51	0
4	P	2252	0	2265	51	0
5	A	3	0	1	0	0
5	I	3	0	1	0	0
5	J	3	0	1	0	0
6	A	21	0	15	3	0
7	A	6	0	8	1	0
7	H	6	0	8	0	0
8	A	2	0	0	0	0
8	E	2	0	0	0	0
8	I	2	0	0	0	0
8	M	2	0	0	0	0
9	A	3	0	0	0	0
9	B	1	0	0	0	0
9	L	2	0	0	0	0
10	A	2	0	0	0	0
10	D	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
10	J	1	0	0	0	0
10	L	1	0	0	0	0
10	P	2	0	0	0	0
11	A	2	0	0	1	0
11	C	1	0	0	2	0
11	I	1	0	0	1	0
11	J	1	0	0	1	0
12	B	9	0	5	0	0
12	C	8	0	5	0	0
12	D	9	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	I	19	0	12	1	0
12	K	8	0	6	1	0
12	L	20	0	11	3	0
12	O	8	0	5	3	0
12	P	9	0	7	6	0
13	B	1	0	0	0	0
14	C	18	0	11	2	0
14	I	9	0	5	0	0
14	J	9	0	5	0	0
14	K	8	0	6	1	0
14	L	9	0	5	1	0
14	O	15	0	7	0	0
15	D	7	0	5	0	0
15	P	7	0	5	1	0
16	I	22	0	0	2	0
17	I	4	0	6	1	0
18	J	1	0	0	0	0
All	All	43288	0	42943	698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 698 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)
4:D:211:ARG:HH11	4:H:105:THR:HG22	1.14	1.09
3:K:72:VAL:HG13	3:K:91:LEU:CD2	1.99	0.91
3:K:72:VAL:HG13	3:K:91:LEU:HD23	1.56	0.85
1:A:371:ARG:NH2	11:A:611:CL:CL	2.49	0.82
1:E:178:ILE:HA	1:E:229:HIS:HB3	1.60	0.82

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	545/548 (100%)	518 (95%)	26 (5%)	1 (0%)	47	79
1	E	537/548 (98%)	512 (95%)	23 (4%)	2 (0%)	34	69
1	I	540/548 (98%)	515 (95%)	24 (4%)	1 (0%)	47	79
1	M	541/548 (99%)	513 (95%)	26 (5%)	2 (0%)	34	69
2	B	352/361 (98%)	334 (95%)	16 (4%)	2 (1%)	25	59
2	F	351/361 (97%)	334 (95%)	16 (5%)	1 (0%)	41	73
2	J	351/361 (97%)	333 (95%)	16 (5%)	2 (1%)	25	59
2	N	351/361 (97%)	335 (95%)	15 (4%)	1 (0%)	41	73
3	C	263/276 (95%)	258 (98%)	5 (2%)	0	100	100
3	G	263/276 (95%)	257 (98%)	6 (2%)	0	100	100
3	K	263/276 (95%)	256 (97%)	7 (3%)	0	100	100
3	O	263/276 (95%)	258 (98%)	5 (2%)	0	100	100
4	D	306/310 (99%)	294 (96%)	12 (4%)	0	100	100
4	H	306/310 (99%)	294 (96%)	12 (4%)	0	100	100
4	L	306/310 (99%)	295 (96%)	11 (4%)	0	100	100
4	P	306/310 (99%)	295 (96%)	11 (4%)	0	100	100
All	All	5844/5980 (98%)	5601 (96%)	231 (4%)	12 (0%)	47	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	268	ASP
1	I	334	ASP
1	A	334	ASP
2	B	236	PRO
1	E	267	VAL

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	421/424 (99%)	404 (96%)	17 (4%)	31	65
1	E	417/424 (98%)	400 (96%)	17 (4%)	30	64
1	I	420/424 (99%)	401 (96%)	19 (4%)	27	60
1	M	418/424 (99%)	401 (96%)	17 (4%)	30	64
2	B	235/245 (96%)	227 (97%)	8 (3%)	37	69
2	F	236/245 (96%)	227 (96%)	9 (4%)	33	66
2	J	238/245 (97%)	231 (97%)	7 (3%)	42	72
2	N	237/245 (97%)	229 (97%)	8 (3%)	37	69
3	C	182/192 (95%)	177 (97%)	5 (3%)	44	74
3	G	182/192 (95%)	178 (98%)	4 (2%)	52	78
3	K	182/192 (95%)	180 (99%)	2 (1%)	73	89
3	O	182/192 (95%)	176 (97%)	6 (3%)	38	69
4	D	227/227 (100%)	221 (97%)	6 (3%)	46	74
4	H	227/227 (100%)	221 (97%)	6 (3%)	46	74
4	L	227/227 (100%)	218 (96%)	9 (4%)	31	65
4	P	227/227 (100%)	221 (97%)	6 (3%)	46	74
All	All	4258/4352 (98%)	4112 (97%)	146 (3%)	36	69

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	10	LYS
1	I	241	SER
3	O	7	ARG
4	H	135	ARG
1	I	17	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	285	ASN
2	J	226	GLN
3	K	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	KCX	E	176	1,8	7,11,12	0.60	0	4,12,14	0.34	0
1	KCX	A	176	1,8	7,11,12	0.58	0	4,12,14	1.06	0
1	KCX	I	176	1,8	7,11,12	0.54	0	4,12,14	0.59	0
1	KCX	M	176	1,8	7,11,12	0.64	0	4,12,14	0.82	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
1	KCX	E	176	1,8	-	4/7/10/12	-
1	KCX	A	176	1,8	-	4/7/10/12	-
1	KCX	I	176	1,8	-	4/7/10/12	-
1	KCX	M	176	1,8	-	4/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	176	KCX	N-CA-CB-CG
1	E	176	KCX	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	176	KCX	N-CA-CB-CG
1	A	176	KCX	C-CA-CB-CG
1	I	176	KCX	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	176	KCX	1	0
1	A	176	KCX	1	0
1	I	176	KCX	1	0
1	M	176	KCX	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 1 is modelled with single atom and 29 are monoatomic - leaving 28 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	$\# Z > 2$
5	FMT	A	601	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MFN	A	602	8	18,22,56	0.44	0	22,28,73	1.11	2 (9%)
15	IAS	P	404	12	3,6,8	0.78	0	1,7,10	0.29	0
5	FMT	J	401	-	0,2,2	0.00	-	0,1,1	0.00	-
16	L6K	I	602	8	16,23,23	1.34	1 (6%)	18,30,30	1.61	4 (22%)
15	IAS	D	403	12	3,6,8	0.97	0	1,7,10	0.95	0
7	GOL	H	401	-	5,5,5	0.77	0	5,5,5	1.11	1 (20%)
7	GOL	A	603	-	5,5,5	1.00	0	5,5,5	0.89	0
17	EDO	I	603	-	3,3,3	0.74	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMT	I	601	-	0,2,2	0.00	-	0,1,1	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
6	MFN	A	602	8	-	6/9/13/63	0/2/2/2
15	IAS	P	404	12	-	0/2/6/8	-
16	L6K	I	602	8	-	4/9/17/17	0/2/2/2
15	IAS	D	403	12	-	2/2/6/8	-
7	GOL	H	401	-	-	0/4/4/4	-
7	GOL	A	603	-	-	2/4/4/4	-
17	EDO	I	603	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	602	L6K	C16-N2	-4.84	1.33	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	602	L6K	C16-N2-C15	3.57	124.76	113.64
16	I	602	L6K	C13-O2-C9	2.93	124.88	117.65
16	I	602	L6K	C13-C4-C5	-2.60	124.05	127.92
16	I	602	L6K	C6-C12-C15	-2.52	108.68	112.97
6	A	602	MFN	C15-C12-C6	-2.45	107.19	112.87

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

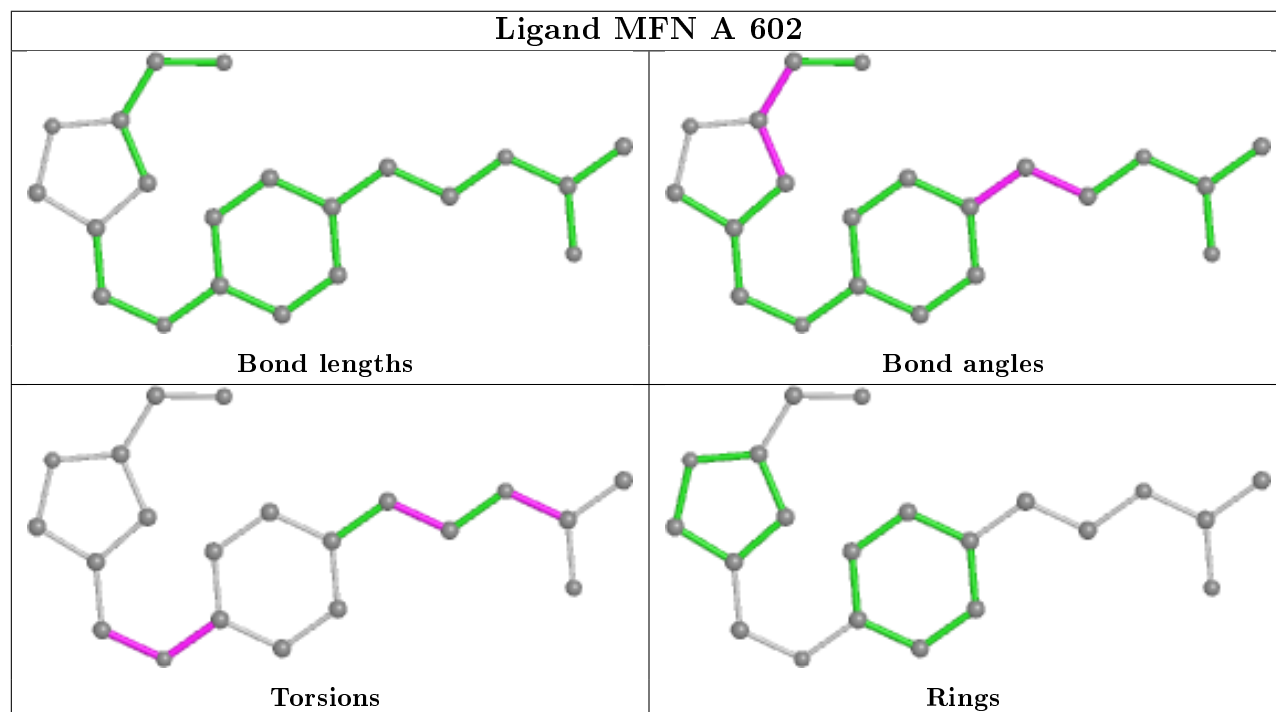
Mol	Chain	Res	Type	Atoms
15	D	403	IAS	C-CA-CB-CG
16	I	602	L6K	C35-C15-N2-C16
6	A	602	MFN	C17-C16-N2-C15
6	A	602	MFN	C10-C9-O2-C13
6	A	602	MFN	C8-C9-O2-C13

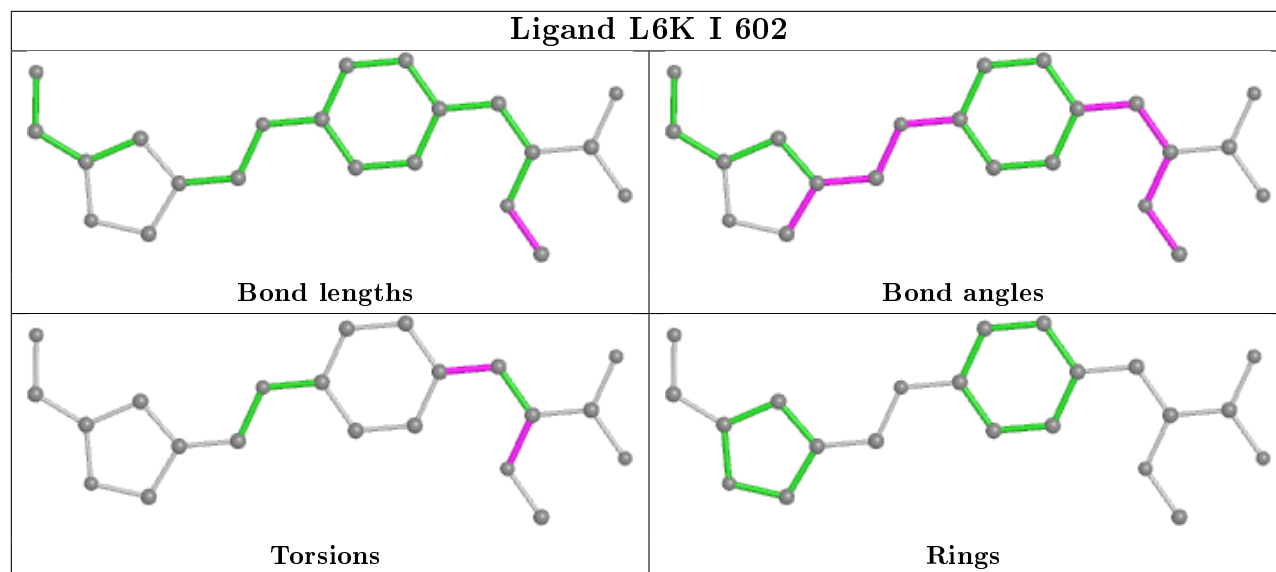
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	MFN	3	0
15	P	404	IAS	1	0
16	I	602	L6K	2	0
7	A	603	GOL	1	0
17	I	603	EDO	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	547/548 (99%)	-0.18	0 100 100	43, 80, 126, 198	0
1	E	541/548 (98%)	0.44	31 (5%) 23 11	84, 147, 203, 316	0
1	I	544/548 (99%)	-0.19	2 (0%) 92 84	42, 79, 134, 206	0
1	M	545/548 (99%)	0.34	32 (5%) 22 10	99, 146, 197, 258	0
2	B	356/361 (98%)	-0.37	0 100 100	44, 75, 132, 193	0
2	F	355/361 (98%)	0.47	27 (7%) 13 5	89, 139, 199, 247	0
2	J	355/361 (98%)	-0.25	1 (0%) 94 88	48, 85, 146, 218	0
2	N	355/361 (98%)	0.30	17 (4%) 30 14	97, 139, 192, 258	0
3	C	265/276 (96%)	-0.43	1 (0%) 92 84	48, 72, 112, 152	0
3	G	265/276 (96%)	0.17	13 (4%) 29 14	86, 126, 173, 210	0
3	K	265/276 (96%)	-0.37	0 100 100	44, 72, 116, 145	0
3	O	265/276 (96%)	-0.25	3 (1%) 80 64	69, 112, 151, 197	0
4	D	308/310 (99%)	-0.17	4 (1%) 77 59	54, 100, 150, 238	0
4	H	308/310 (99%)	-0.29	1 (0%) 94 88	62, 96, 135, 175	0
4	L	308/310 (99%)	-0.30	0 100 100	37, 85, 141, 196	0
4	P	308/310 (99%)	-0.43	0 100 100	32, 73, 114, 177	0
All	All	5890/5980 (98%)	-0.06	132 (2%) 62 41	32, 103, 176, 316	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	361	SER	7.7
2	F	361	SER	6.7
1	E	453	ALA	6.2
2	N	267	LEU	6.2
2	J	361	SER	6.1

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

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, 95th 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
1	KCX	E	176	12/13	0.83	0.33	135,140,174,180	0
1	KCX	M	176	12/13	0.90	0.35	108,116,146,150	0
1	KCX	I	176	12/13	0.93	0.28	54,64,113,138	0
1	KCX	A	176	12/13	0.97	0.32	56,68,86,92	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
13	NH2	B	403	1/1	0.53	0.63	98,98,98,98	0
16	L6K	I	602	22/22	0.72	0.47	70,70,70,70	22
6	MFN	A	602	21/55	0.74	0.41	38,47,57,59	21
12	DGL	P	403	9/10	0.75	0.43	82,86,92,93	0
12	DGL	B	402	9/10	0.76	0.39	107,112,125,129	0
12	DGL	D	402	9/10	0.76	0.37	82,86,92,93	0
12	DGL	I	610	10/10	0.77	0.36	70,70,70,70	10
14	GLU	J	405	9/10	0.78	0.30	70,70,70,70	9
14	GLU	C	304	9/10	0.81	0.41	89,111,131,143	0
12	DGL	I	608	9/10	0.81	0.31	70,70,70,70	9
10	K	H	402	1/1	0.82	0.11	80,80,80,80	0
9	CA	A	606	1/1	0.83	0.12	90,90,90,90	0
14	GLU	I	609	9/10	0.83	0.26	70,70,70,70	9
5	FMT	A	601	3/3	0.84	0.39	50,50,50,50	0
12	DGL	K	301	8/10	0.84	0.19	70,70,70,70	8
8	ZN	M	601	1/1	0.85	0.09	85,85,85,85	0
14	GLU	K	302	8/10	0.86	0.21	70,70,70,70	8
14	GLU	L	404	9/10	0.87	0.15	70,70,70,70	9

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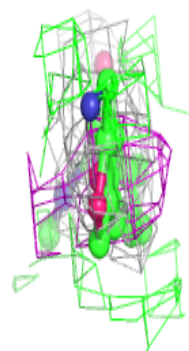
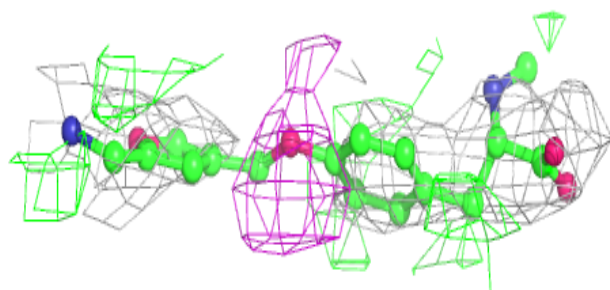
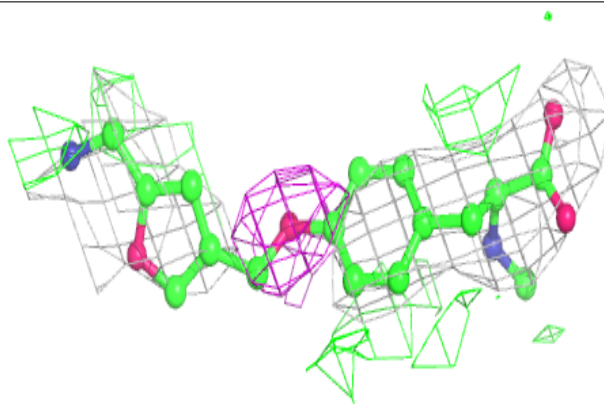
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	DGL	O	301	8/10	0.88	0.16	73,83,84,85	0
12	DGL	L	406	10/10	0.88	0.29	70,70,70,70	10
12	DGL	C	302	8/10	0.88	0.14	73,83,84,85	0
12	DGL	L	405	10/10	0.89	0.27	70,70,70,70	10
14	GLU	C	303	9/10	0.89	0.14	67,82,94,99	0
14	GLU	O	303	6/10	0.89	0.53	89,98,113,120	0
14	GLU	O	302	9/10	0.89	0.24	67,82,94,99	0
10	K	P	402	1/1	0.90	0.12	70,70,70,70	0
10	K	J	403	1/1	0.90	0.28	70,70,70,70	0
11	CL	I	607	1/1	0.91	0.20	65,65,65,65	0
17	EDO	I	603	4/4	0.91	0.22	20,20,20,20	0
5	FMT	I	601	3/3	0.91	0.34	50,50,50,50	0
10	K	I	606	1/1	0.92	0.06	70,70,70,70	0
15	IAS	D	403	7/9	0.92	0.26	55,65,73,74	0
7	GOL	A	603	6/6	0.92	0.20	60,60,60,60	0
11	CL	J	404	1/1	0.92	0.19	60,60,60,60	0
10	K	P	401	1/1	0.92	0.16	70,70,70,70	0
9	CA	L	401	1/1	0.93	0.08	65,65,65,65	0
10	K	D	401	1/1	0.94	0.22	70,70,70,70	0
8	ZN	E	601	1/1	0.94	0.23	122,122,122,122	0
11	CL	C	301	1/1	0.94	0.19	65,65,65,65	0
7	GOL	H	401	6/6	0.94	0.25	60,60,60,60	0
10	K	L	403	1/1	0.94	0.13	70,70,70,70	0
9	CA	L	402	1/1	0.95	0.09	70,70,70,70	0
8	ZN	I	605	1/1	0.95	0.27	75,75,75,75	0
15	IAS	P	404	7/9	0.95	0.20	55,65,73,74	0
9	CA	A	608	1/1	0.95	0.15	70,70,70,70	0
5	FMT	J	401	3/3	0.95	0.21	50,50,50,50	0
11	CL	A	612	1/1	0.95	0.18	65,65,65,65	0
9	CA	A	607	1/1	0.96	0.12	70,70,70,70	0
8	ZN	E	602	1/1	0.96	0.31	155,155,155,155	0
8	ZN	A	604	1/1	0.97	0.15	67,67,67,67	0
8	ZN	M	602	1/1	0.97	0.10	80,80,80,80	0
9	CA	B	401	1/1	0.97	0.14	70,70,70,70	0
10	K	A	610	1/1	0.97	0.18	70,70,70,70	0
8	ZN	I	604	1/1	0.98	0.21	65,65,65,65	0
10	K	A	609	1/1	0.98	0.22	70,70,70,70	0
11	CL	A	611	1/1	0.98	0.16	65,65,65,65	0
8	ZN	A	605	1/1	0.99	0.26	70,70,70,70	0
18	NA	J	402	1/1	0.99	0.09	60,60,60,60	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.

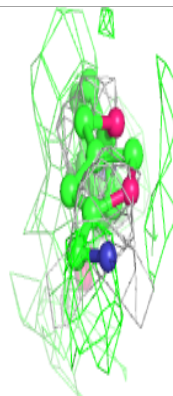
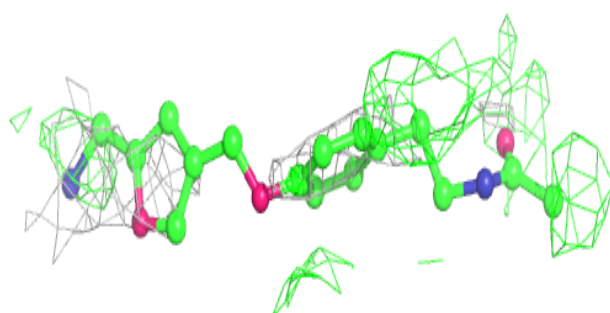
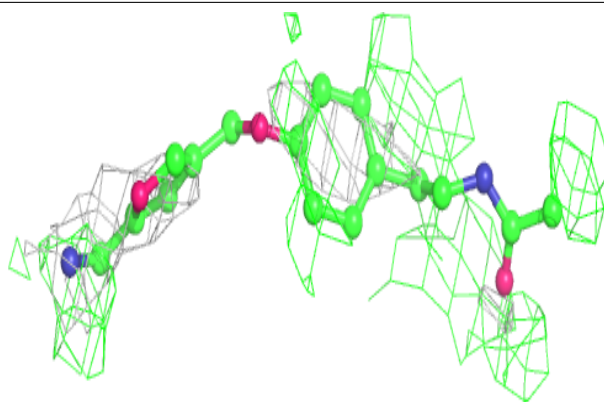
Electron density around L6K I 602:

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



Electron density around MFN A 602:

$2mF_o-DF_c$ (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.