Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 05:41 AM EDT

PDB ID	:	7KYP
Title	:	PsaBC from Streptococcus pneumoniae in complex with Fab
Authors	:	Maher, M.J.; Sjohamn, J.
Deposited on	:	2020-12-08
Resolution	:	2.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

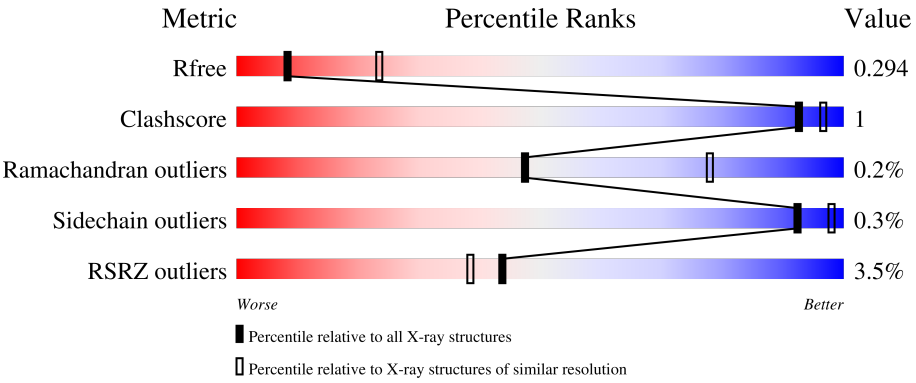
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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	240	3% 95%
1	C	240	3% 93%
1	E	240	% 95%
1	G	240	% 92%
1	I	240	3% 94%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	240	2% 92% 6%
1	M	240	4% 93%
1	O	240	3% 92% 5%
2	B	290	2% 93%
2	D	290	% 89% 6%
2	F	290	2% 94% 6%
2	H	290	4% 89% 5% 6%
2	J	290	11% 91% 6%
2	L	290	3% 93%
2	N	290	3% 92%
2	P	290	6% 90% 7%

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
3	PO4	K	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31187 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 Manganese ABC transporter, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	1	0
			1839	1188	309	337	5			
1	C	232	Total	C	N	O	S	0	1	0
			1793	1155	302	331	5			
1	E	236	Total	C	N	O	S	0	1	0
			1835	1185	308	337	5			
1	G	230	Total	C	N	O	S	0	0	0
			1775	1147	296	327	5			
1	I	234	Total	C	N	O	S	0	0	0
			1831	1182	309	335	5			
1	K	236	Total	C	N	O	S	0	0	0
			1850	1195	312	338	5			
1	M	233	Total	C	N	O	S	0	1	0
			1815	1169	308	333	5			
1	O	234	Total	C	N	O	S	0	1	0
			1810	1170	302	333	5			

- Molecule 2 is a protein called Manganese ABC transporter, permease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	S	0	0	0
			2080	1396	315	357	12			
2	D	272	Total	C	N	O	S	0	0	0
			2027	1362	303	350	12			
2	F	290	Total	C	N	O	S	0	0	0
			2173	1457	329	375	12			
2	H	272	Total	C	N	O	S	0	0	0
			2012	1355	301	345	11			
2	J	274	Total	C	N	O	S	0	0	0
			2015	1352	303	349	11			
2	L	278	Total	C	N	O	S	0	0	0
			2065	1384	313	356	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	277	Total	C	N	O	S	0	0	0
			2060	1381	312	355	12			
2	P	271	Total	C	N	O	S	0	0	0
			2015	1353	302	348	12			

There are 72 discrepancies between the modelled and reference sequences:

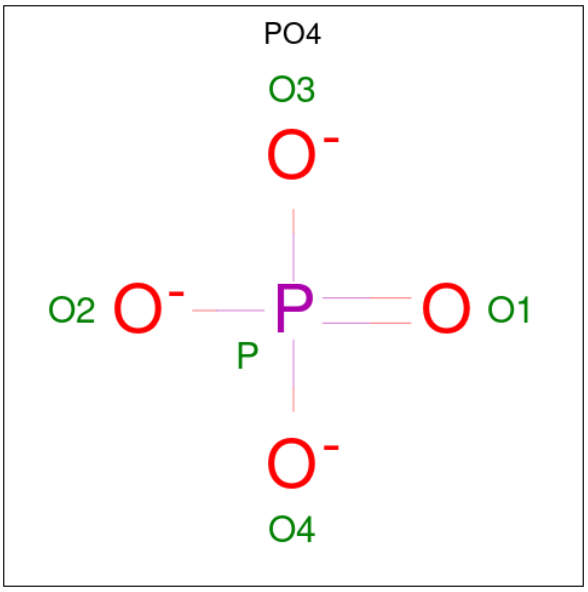
Chain	Residue	Modelled	Actual	Comment	Reference
B	100	SER	PHE	conflict	UNP A0A0H2ZPI2
B	283	GLY	-	expression tag	UNP A0A0H2ZPI2
B	284	SER	-	expression tag	UNP A0A0H2ZPI2
B	285	GLU	-	expression tag	UNP A0A0H2ZPI2
B	286	ASN	-	expression tag	UNP A0A0H2ZPI2
B	287	LEU	-	expression tag	UNP A0A0H2ZPI2
B	288	TYR	-	expression tag	UNP A0A0H2ZPI2
B	289	PHE	-	expression tag	UNP A0A0H2ZPI2
B	290	GLN	-	expression tag	UNP A0A0H2ZPI2
D	100	SER	PHE	conflict	UNP A0A0H2ZPI2
D	283	GLY	-	expression tag	UNP A0A0H2ZPI2
D	284	SER	-	expression tag	UNP A0A0H2ZPI2
D	285	GLU	-	expression tag	UNP A0A0H2ZPI2
D	286	ASN	-	expression tag	UNP A0A0H2ZPI2
D	287	LEU	-	expression tag	UNP A0A0H2ZPI2
D	288	TYR	-	expression tag	UNP A0A0H2ZPI2
D	289	PHE	-	expression tag	UNP A0A0H2ZPI2
D	290	GLN	-	expression tag	UNP A0A0H2ZPI2
F	100	SER	PHE	conflict	UNP A0A0H2ZPI2
F	283	GLY	-	expression tag	UNP A0A0H2ZPI2
F	284	SER	-	expression tag	UNP A0A0H2ZPI2
F	285	GLU	-	expression tag	UNP A0A0H2ZPI2
F	286	ASN	-	expression tag	UNP A0A0H2ZPI2
F	287	LEU	-	expression tag	UNP A0A0H2ZPI2
F	288	TYR	-	expression tag	UNP A0A0H2ZPI2
F	289	PHE	-	expression tag	UNP A0A0H2ZPI2
F	290	GLN	-	expression tag	UNP A0A0H2ZPI2
H	100	SER	PHE	conflict	UNP A0A0H2ZPI2
H	283	GLY	-	expression tag	UNP A0A0H2ZPI2
H	284	SER	-	expression tag	UNP A0A0H2ZPI2
H	285	GLU	-	expression tag	UNP A0A0H2ZPI2
H	286	ASN	-	expression tag	UNP A0A0H2ZPI2
H	287	LEU	-	expression tag	UNP A0A0H2ZPI2
H	288	TYR	-	expression tag	UNP A0A0H2ZPI2

Continued on next page...

Continued from previous page...

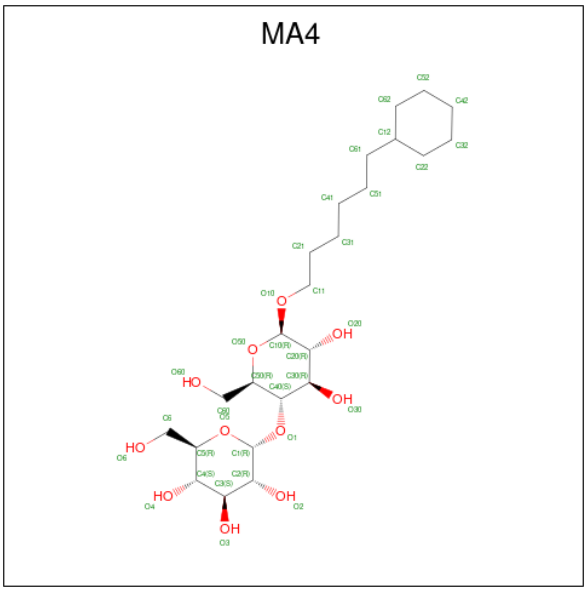
Chain	Residue	Modelled	Actual	Comment	Reference
H	289	PHE	-	expression tag	UNP A0A0H2ZPI2
H	290	GLN	-	expression tag	UNP A0A0H2ZPI2
J	100	SER	PHE	conflict	UNP A0A0H2ZPI2
J	283	GLY	-	expression tag	UNP A0A0H2ZPI2
J	284	SER	-	expression tag	UNP A0A0H2ZPI2
J	285	GLU	-	expression tag	UNP A0A0H2ZPI2
J	286	ASN	-	expression tag	UNP A0A0H2ZPI2
J	287	LEU	-	expression tag	UNP A0A0H2ZPI2
J	288	TYR	-	expression tag	UNP A0A0H2ZPI2
J	289	PHE	-	expression tag	UNP A0A0H2ZPI2
J	290	GLN	-	expression tag	UNP A0A0H2ZPI2
L	100	SER	PHE	conflict	UNP A0A0H2ZPI2
L	283	GLY	-	expression tag	UNP A0A0H2ZPI2
L	284	SER	-	expression tag	UNP A0A0H2ZPI2
L	285	GLU	-	expression tag	UNP A0A0H2ZPI2
L	286	ASN	-	expression tag	UNP A0A0H2ZPI2
L	287	LEU	-	expression tag	UNP A0A0H2ZPI2
L	288	TYR	-	expression tag	UNP A0A0H2ZPI2
L	289	PHE	-	expression tag	UNP A0A0H2ZPI2
L	290	GLN	-	expression tag	UNP A0A0H2ZPI2
N	100	SER	PHE	conflict	UNP A0A0H2ZPI2
N	283	GLY	-	expression tag	UNP A0A0H2ZPI2
N	284	SER	-	expression tag	UNP A0A0H2ZPI2
N	285	GLU	-	expression tag	UNP A0A0H2ZPI2
N	286	ASN	-	expression tag	UNP A0A0H2ZPI2
N	287	LEU	-	expression tag	UNP A0A0H2ZPI2
N	288	TYR	-	expression tag	UNP A0A0H2ZPI2
N	289	PHE	-	expression tag	UNP A0A0H2ZPI2
N	290	GLN	-	expression tag	UNP A0A0H2ZPI2
P	100	SER	PHE	conflict	UNP A0A0H2ZPI2
P	283	GLY	-	expression tag	UNP A0A0H2ZPI2
P	284	SER	-	expression tag	UNP A0A0H2ZPI2
P	285	GLU	-	expression tag	UNP A0A0H2ZPI2
P	286	ASN	-	expression tag	UNP A0A0H2ZPI2
P	287	LEU	-	expression tag	UNP A0A0H2ZPI2
P	288	TYR	-	expression tag	UNP A0A0H2ZPI2
P	289	PHE	-	expression tag	UNP A0A0H2ZPI2
P	290	GLN	-	expression tag	UNP A0A0H2ZPI2

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	G	1	Total O P 5 4 1	0	0
3	I	1	Total O P 5 4 1	0	0
3	K	1	Total O P 5 4 1	0	0
3	M	1	Total O P 5 4 1	0	0
3	O	1	Total O P 5 4 1	0	0

- Molecule 4 is CYCLOHEXYL-HEXYL-BETA-D-MALTOSIDE (three-letter code: MA4) (formula: $C_{24}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 35 24 11	0	0
4	F	1	Total C O 35 24 11	0	0
4	L	1	Total C O 35 24 11	0	0
4	N	1	Total C O 35 24 11	0	0

- Molecule 5 is water.

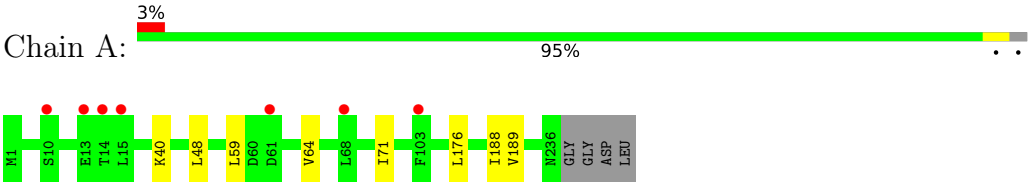
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	3	Total O 3 3	0	0
5	H	1	Total O 1 1	0	0
5	O	3	Total O 3 3	0	0
5	P	1	Total O 1 1	0	0

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.

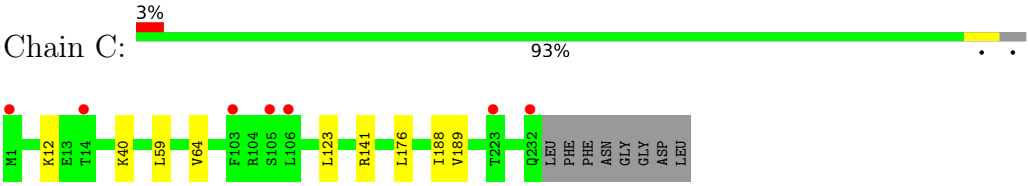
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain A:



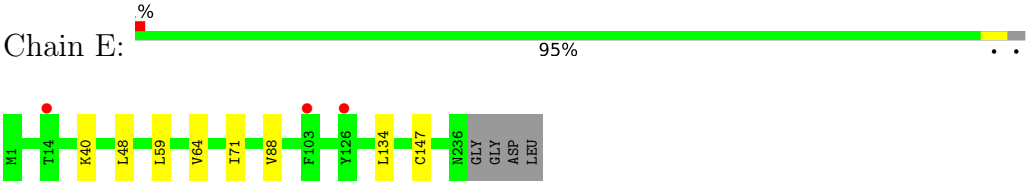
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain C:



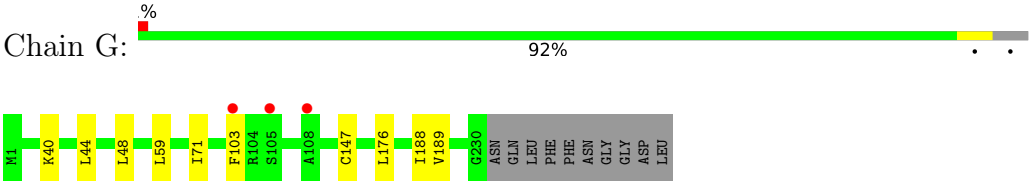
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain E:



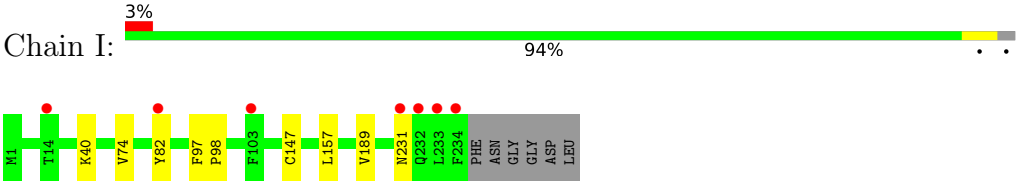
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain G:



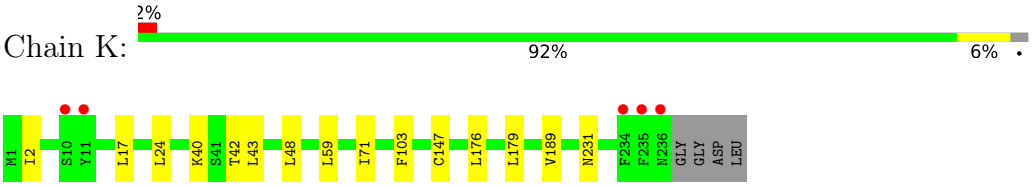
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain I:



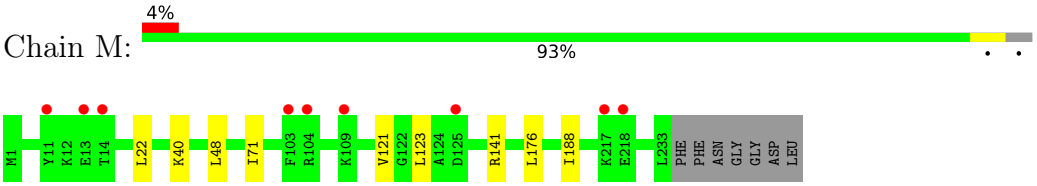
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain K:



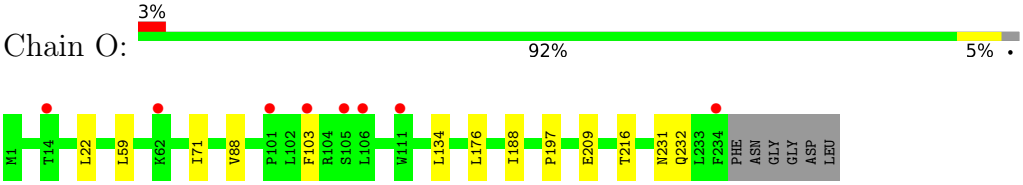
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain M:



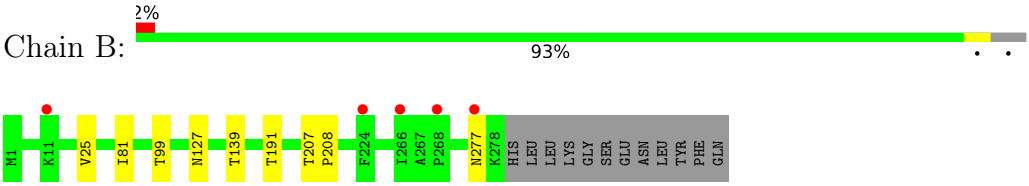
• Molecule 1: Manganese ABC transporter, ATP-binding protein

Chain O:



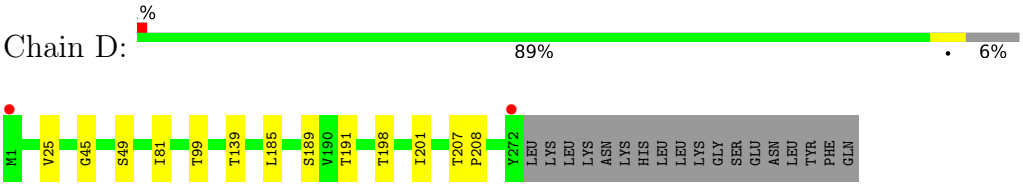
• Molecule 2: Manganese ABC transporter, permease protein

Chain B:



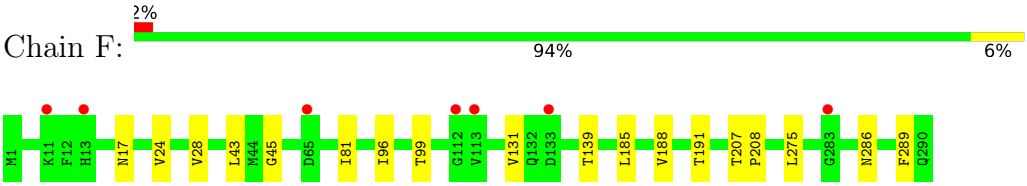
• Molecule 2: Manganese ABC transporter, permease protein

Chain D:



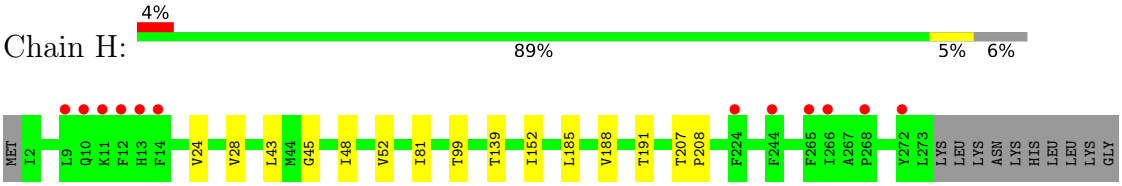
• Molecule 2: Manganese ABC transporter, permease protein

Chain F:



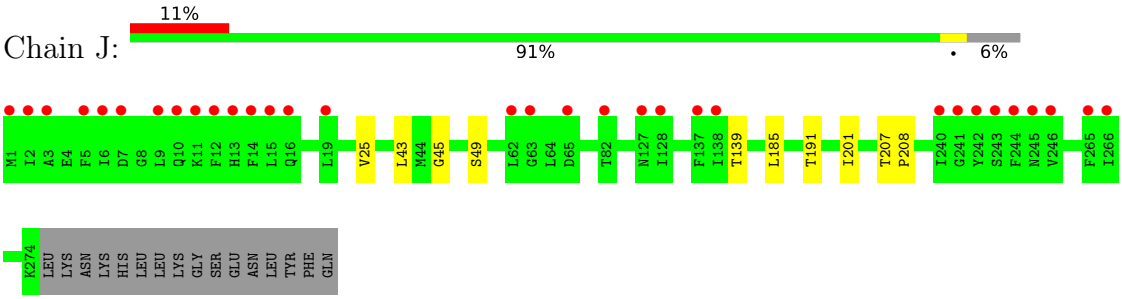
• Molecule 2: Manganese ABC transporter, permease protein

Chain H:



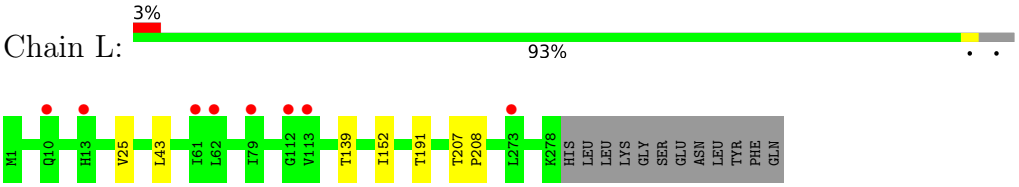
• Molecule 2: Manganese ABC transporter, permease protein

Chain J:



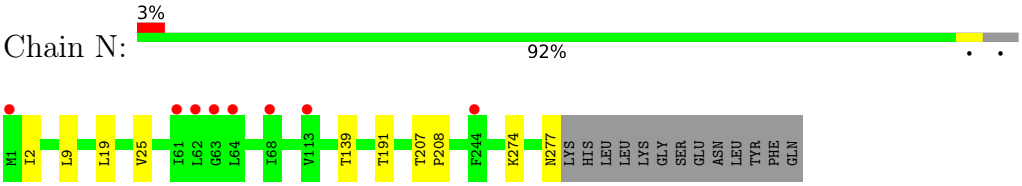
• Molecule 2: Manganese ABC transporter, permease protein

Chain L:



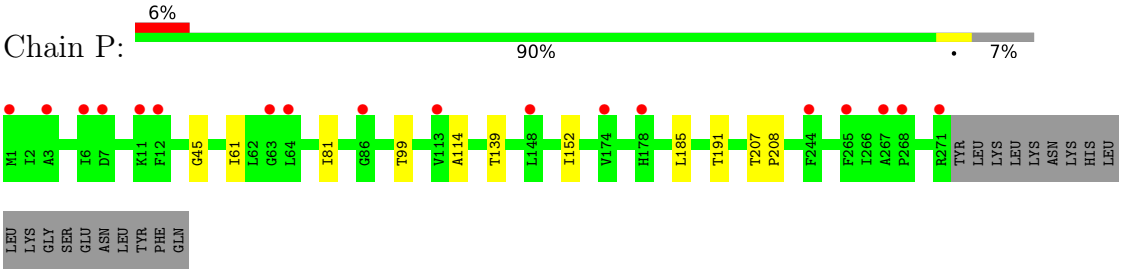
• Molecule 2: Manganese ABC transporter, permease protein

Chain N:



• Molecule 2: Manganese ABC transporter, permease protein

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.55Å 129.56Å 169.62Å 95.35° 92.21° 98.66°	Depositor
Resolution (Å)	49.63 – 2.90 49.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.8 (49.63-2.90) 90.8 (49.63-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.260 , 0.281 0.275 , 0.294	Depositor DCC
R_{free} test set	7870 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	31187	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: PO4, MA4

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	0.25	0/1876	0.41	0/2539
1	C	0.25	0/1828	0.42	0/2476
1	E	0.26	0/1872	0.43	0/2535
1	G	0.26	0/1808	0.42	0/2450
1	I	0.26	0/1865	0.43	0/2523
1	K	0.26	0/1885	0.42	0/2550
1	M	0.25	0/1850	0.42	0/2503
1	O	0.26	0/1846	0.42	0/2500
2	B	0.28	0/2120	0.37	0/2878
2	D	0.27	0/2067	0.38	0/2809
2	F	0.27	0/2215	0.38	0/3007
2	H	0.28	0/2052	0.37	0/2792
2	J	0.28	0/2054	0.37	0/2796
2	L	0.27	0/2104	0.37	0/2859
2	N	0.28	0/2099	0.38	0/2852
2	P	0.28	0/2054	0.37	0/2791
All	All	0.27	0/31595	0.40	0/42860

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	1839	0	1876	5	0
1	C	1793	0	1824	4	0
1	E	1835	0	1865	5	0
1	G	1775	0	1806	6	0
1	I	1831	0	1877	3	0
1	K	1850	0	1892	8	0
1	M	1815	0	1863	4	0
1	O	1810	0	1844	5	0
2	B	2080	0	2206	4	0
2	D	2027	0	2139	9	0
2	F	2173	0	2289	11	0
2	H	2012	0	2115	11	0
2	J	2015	0	2103	6	0
2	L	2065	0	2177	5	0
2	N	2060	0	2175	6	0
2	P	2015	0	2130	6	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	K	5	0	0	1	0
3	M	5	0	0	0	0
3	O	5	0	0	0	0
4	B	35	0	44	0	0
4	F	35	0	44	0	0
4	L	35	0	44	0	0
4	N	35	0	44	0	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	H	1	0	0	0	0
5	O	3	0	0	0	0
5	P	1	0	0	0	0
All	All	31187	0	32357	93	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 1.

All (93) 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)
2:D:139:THR:HG23	2:D:191:THR:HG23	1.72	0.69
2:B:25:VAL:HG22	2:B:191:THR:HG22	1.75	0.68
1:E:59:LEU:HD11	1:E:71:ILE:HD11	1.75	0.68
2:D:189:SER:HA	2:D:201:ILE:HD13	1.79	0.64
2:J:139:THR:HG23	2:J:191:THR:HG23	1.81	0.61
2:B:139:THR:HG23	2:B:191:THR:HG23	1.80	0.61
2:H:139:THR:HG23	2:H:191:THR:HG23	1.85	0.58
2:J:25:VAL:HG22	2:J:191:THR:HG22	1.85	0.58
2:L:139:THR:HG23	2:L:191:THR:HG23	1.86	0.58
2:F:43:LEU:HD13	2:H:43:LEU:HD13	1.86	0.57
2:F:28:VAL:HG12	2:F:188:VAL:HG22	1.87	0.56
2:D:45:GLY:HA2	2:D:185:LEU:HD21	1.86	0.56
2:P:139:THR:HG23	2:P:191:THR:HG23	1.88	0.56
2:J:43:LEU:HD13	2:L:43:LEU:HD13	1.88	0.56
2:N:25:VAL:HG22	2:N:191:THR:HG22	1.89	0.55
2:L:25:VAL:HG22	2:L:191:THR:HG22	1.88	0.55
1:K:59:LEU:HD11	1:K:71:ILE:HD11	1.89	0.54
2:F:139:THR:HG23	2:F:191:THR:CG2	2.39	0.53
2:F:24:VAL:HG11	2:F:139:THR:HG22	1.91	0.52
1:M:176:LEU:HD13	1:M:188:ILE:HD11	1.92	0.51
2:J:45:GLY:HA2	2:J:185:LEU:HD21	1.93	0.51
2:F:81:ILE:HG13	2:F:99:THR:HG21	1.92	0.50
2:P:61:ILE:HG22	2:P:114:ALA:HB3	1.93	0.50
2:F:28:VAL:CG1	2:F:188:VAL:HG22	2.42	0.49
2:D:207:THR:HB	2:D:208:PRO:HD3	1.95	0.49
2:N:139:THR:HG23	2:N:191:THR:HG23	1.93	0.49
2:H:81:ILE:HG13	2:H:99:THR:HG21	1.94	0.49
1:M:48:LEU:HD21	1:M:71:ILE:HG21	1.94	0.48
1:O:197:PRO:HA	1:O:216:THR:HG21	1.95	0.48
1:I:40:LYS:HB3	1:I:189:VAL:HG13	1.95	0.48
2:D:25:VAL:HG22	2:D:191:THR:HG22	1.96	0.47
1:O:88:VAL:CG2	1:O:134:LEU:HD11	2.44	0.47
2:F:275:LEU:HD13	2:F:289:PHE:CE2	2.50	0.47
2:H:45:GLY:HA2	2:H:185:LEU:HD21	1.95	0.47
1:K:40:LYS:HB3	1:K:189:VAL:HG13	1.96	0.47
1:A:176:LEU:HD13	1:A:188:ILE:HD11	1.95	0.47
1:K:176:LEU:HD23	1:K:179:LEU:HD12	1.97	0.46
1:A:59:LEU:HG	1:A:64:VAL:HG22	1.96	0.46
1:A:59:LEU:HD11	1:A:71:ILE:HD11	1.96	0.46
1:C:176:LEU:HD13	1:C:188:ILE:HD11	1.98	0.46
1:K:42:THR:N	3:K:301:PO4:O3	2.46	0.45
1:G:103:PHE:CE1	2:H:152:ILE:HD12	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:THR:HA	2:D:201:ILE:HD11	1.99	0.45
1:G:40:LYS:HB3	1:G:189:VAL:HG13	1.98	0.45
1:A:40:LYS:HB3	1:A:189:VAL:HG13	1.97	0.45
2:F:207:THR:HB	2:F:208:PRO:HD3	1.98	0.45
2:D:49:SER:HB3	2:D:201:ILE:HD12	1.98	0.45
2:H:139:THR:HG23	2:H:191:THR:CG2	2.46	0.45
1:I:74:VAL:HB	1:I:157:LEU:HD23	1.99	0.45
1:E:59:LEU:HG	1:E:64:VAL:HG22	1.98	0.44
2:P:81:ILE:HG13	2:P:99:THR:HG21	2.00	0.44
2:D:81:ILE:CG1	2:D:99:THR:HG21	2.48	0.44
1:G:44:LEU:HD11	1:G:189:VAL:HG23	1.99	0.44
1:C:40:LYS:HB3	1:C:189:VAL:HG13	2.00	0.43
2:N:9:LEU:HD11	2:N:19:LEU:HD22	2.01	0.43
2:F:17:ASN:HB3	2:F:131:VAL:HG23	1.99	0.43
2:H:81:ILE:CG1	2:H:99:THR:HG21	2.49	0.43
1:E:48:LEU:HD21	1:E:71:ILE:HG21	2.00	0.43
2:P:207:THR:HB	2:P:208:PRO:HD3	2.01	0.43
2:H:48:ILE:O	2:H:52:VAL:HG23	2.19	0.43
1:A:48:LEU:HD21	1:A:71:ILE:HG21	2.00	0.42
2:D:81:ILE:HG13	2:D:99:THR:HG21	2.00	0.42
2:H:24:VAL:HG11	2:H:139:THR:HG22	2.00	0.42
2:J:49:SER:HB3	2:J:201:ILE:HD12	2.01	0.42
1:E:88:VAL:HG22	1:E:134:LEU:HD11	2.00	0.42
1:G:176:LEU:HD13	1:G:188:ILE:HD11	2.01	0.42
2:F:45:GLY:HA2	2:F:185:LEU:HD21	2.01	0.42
2:N:274:LYS:HA	2:N:277:ASN:HD22	1.83	0.42
2:F:43:LEU:HG	2:F:96:ILE:HG21	2.01	0.42
2:H:28:VAL:HG12	2:H:188:VAL:HG22	2.00	0.42
1:M:121:VAL:O	1:M:141:ARG:NE	2.52	0.42
1:K:103:PHE:CE1	2:L:152:ILE:HD12	2.55	0.42
2:H:207:THR:HB	2:H:208:PRO:HD3	2.02	0.42
2:P:45:GLY:HA2	2:P:185:LEU:HD21	2.01	0.42
1:E:88:VAL:CG2	1:E:134:LEU:HD11	2.50	0.42
1:G:59:LEU:CD1	1:G:71:ILE:HD11	2.50	0.42
1:M:123:LEU:HD11	1:M:141:ARG:HB2	2.02	0.42
2:B:207:THR:HB	2:B:208:PRO:HD3	2.02	0.42
2:N:2:ILE:HD12	2:N:2:ILE:N	2.35	0.42
1:O:103:PHE:CE1	2:P:152:ILE:HD12	2.55	0.42
1:I:97:PHE:N	1:I:98:PRO:CD	2.83	0.41
1:K:2:ILE:HD12	1:K:24:LEU:HD23	2.01	0.41
1:K:17:LEU:HD21	1:K:43:LEU:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:ILE:HG13	2:B:99:THR:HG21	2.02	0.41
2:L:207:THR:HB	2:L:208:PRO:HD3	2.01	0.41
1:C:59:LEU:HG	1:C:64:VAL:HG22	2.02	0.41
2:J:207:THR:HB	2:J:208:PRO:HD3	2.02	0.41
1:C:123:LEU:HD11	1:C:141:ARG:HB2	2.03	0.41
1:K:48:LEU:CD2	1:K:71:ILE:HD13	2.50	0.41
2:N:207:THR:HB	2:N:208:PRO:HD3	2.02	0.41
1:O:176:LEU:HD13	1:O:188:ILE:HD11	2.02	0.41
1:O:59:LEU:HD22	1:O:71:ILE:HD11	2.02	0.40
1:G:48:LEU:HD21	1:G:71:ILE:HG21	2.02	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	235/240 (98%)	218 (93%)	17 (7%)	0	100	100
1	C	231/240 (96%)	218 (94%)	12 (5%)	1 (0%)	34	66
1	E	235/240 (98%)	221 (94%)	13 (6%)	1 (0%)	34	66
1	G	228/240 (95%)	216 (95%)	12 (5%)	0	100	100
1	I	232/240 (97%)	216 (93%)	15 (6%)	1 (0%)	34	66
1	K	234/240 (98%)	221 (94%)	12 (5%)	1 (0%)	34	66
1	M	232/240 (97%)	218 (94%)	13 (6%)	1 (0%)	34	66
1	O	233/240 (97%)	215 (92%)	15 (6%)	3 (1%)	12	37
2	B	276/290 (95%)	266 (96%)	9 (3%)	1 (0%)	34	66
2	D	270/290 (93%)	261 (97%)	9 (3%)	0	100	100
2	F	288/290 (99%)	281 (98%)	7 (2%)	0	100	100
2	H	270/290 (93%)	265 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	272/290 (94%)	264 (97%)	8 (3%)	0	100	100
2	L	276/290 (95%)	268 (97%)	8 (3%)	0	100	100
2	N	275/290 (95%)	267 (97%)	8 (3%)	0	100	100
2	P	269/290 (93%)	260 (97%)	9 (3%)	0	100	100
All	All	4056/4240 (96%)	3875 (96%)	172 (4%)	9 (0%)	47	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	231	ASN
1	M	40	LYS
1	E	40	LYS
1	K	231	ASN
1	O	232	GLN
1	O	231	ASN
2	B	127	ASN
1	C	12	LYS
1	O	209	GLU

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	199/208 (96%)	199 (100%)	0	100	100
1	C	193/208 (93%)	193 (100%)	0	100	100
1	E	198/208 (95%)	197 (100%)	1 (0%)	88	96
1	G	191/208 (92%)	190 (100%)	1 (0%)	88	96
1	I	199/208 (96%)	197 (99%)	2 (1%)	76	92
1	K	201/208 (97%)	200 (100%)	1 (0%)	88	96
1	M	197/208 (95%)	196 (100%)	1 (0%)	88	96
1	O	195/208 (94%)	194 (100%)	1 (0%)	88	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	221/234 (94%)	220 (100%)	1 (0%)	88 96
2	D	215/234 (92%)	215 (100%)	0	100 100
2	F	230/234 (98%)	229 (100%)	1 (0%)	91 97
2	H	211/234 (90%)	211 (100%)	0	100 100
2	J	210/234 (90%)	210 (100%)	0	100 100
2	L	218/234 (93%)	218 (100%)	0	100 100
2	N	218/234 (93%)	218 (100%)	0	100 100
2	P	214/234 (92%)	214 (100%)	0	100 100
All	All	3310/3536 (94%)	3301 (100%)	9 (0%)	92 98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	277	ASN
1	E	147	CYS
2	F	286	ASN
1	G	147	CYS
1	I	82	TYR
1	I	147	CYS
1	K	147	CYS
1	M	22	LEU
1	O	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	122	HIS
2	B	127	ASN
2	B	277	ASN
1	C	110	HIS
1	C	140	GLN
1	C	174	ASN
2	F	10	GLN
2	F	286	ASN
2	J	245	ASN
1	M	202	GLN
2	N	122	HIS
2	N	127	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	277	ASN
2	P	194	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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	G	301	-	4,4,4	0.94	0	6,6,6	0.46	0
4	MA4	L	301	-	37,37,37	0.44	0	50,50,50	0.63	0
4	MA4	F	301	-	37,37,37	0.46	0	50,50,50	0.67	0
3	PO4	I	301	-	4,4,4	0.90	0	6,6,6	0.51	0
3	PO4	A	301	-	4,4,4	0.95	0	6,6,6	0.40	0
4	MA4	B	301	-	37,37,37	0.47	0	50,50,50	0.95	2 (4%)
3	PO4	O	301	-	4,4,4	0.96	0	6,6,6	0.44	0
3	PO4	K	301	-	4,4,4	0.96	0	6,6,6	0.37	0
3	PO4	C	301	-	4,4,4	0.90	0	6,6,6	0.54	0
4	MA4	N	301	-	37,37,37	0.47	0	50,50,50	0.79	2 (4%)
3	PO4	M	301	-	4,4,4	0.97	0	6,6,6	0.42	0
3	PO4	E	301	-	4,4,4	0.89	0	6,6,6	0.61	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
4	MA4	L	301	-	-	8/18/66/66	0/3/3/3
4	MA4	B	301	-	-	3/18/66/66	0/3/3/3
4	MA4	N	301	-	-	3/18/66/66	0/3/3/3
4	MA4	F	301	-	-	6/18/66/66	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	MA4	C20-C30-C40	3.51	117.70	109.68
4	B	301	MA4	C10-C20-C30	3.43	117.13	110.00
4	N	301	MA4	C1-O5-C5	2.43	118.45	113.69
4	N	301	MA4	C3-C4-C5	2.10	113.98	110.24

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	301	MA4	C4-C5-C6-O6
4	N	301	MA4	O5-C5-C6-O6
4	F	301	MA4	O5-C1-O1-C40
4	F	301	MA4	C50-C40-O1-C1
4	L	301	MA4	O5-C1-O1-C40
4	F	301	MA4	C30-C40-O1-C1
4	B	301	MA4	C21-C31-C41-C51
4	F	301	MA4	C21-C11-O10-C10
4	L	301	MA4	C21-C11-O10-C10
4	N	301	MA4	C21-C31-C41-C51
4	F	301	MA4	C11-C21-C31-C41
4	B	301	MA4	C30-C40-O1-C1
4	L	301	MA4	C30-C40-O1-C1
4	L	301	MA4	C50-C40-O1-C1
4	B	301	MA4	C50-C40-O1-C1
4	L	301	MA4	C22-C12-C61-C51
4	L	301	MA4	C62-C12-C61-C51
4	L	301	MA4	C41-C51-C61-C12
4	F	301	MA4	C41-C51-C61-C12

Continued on next page...

Continued from previous page...

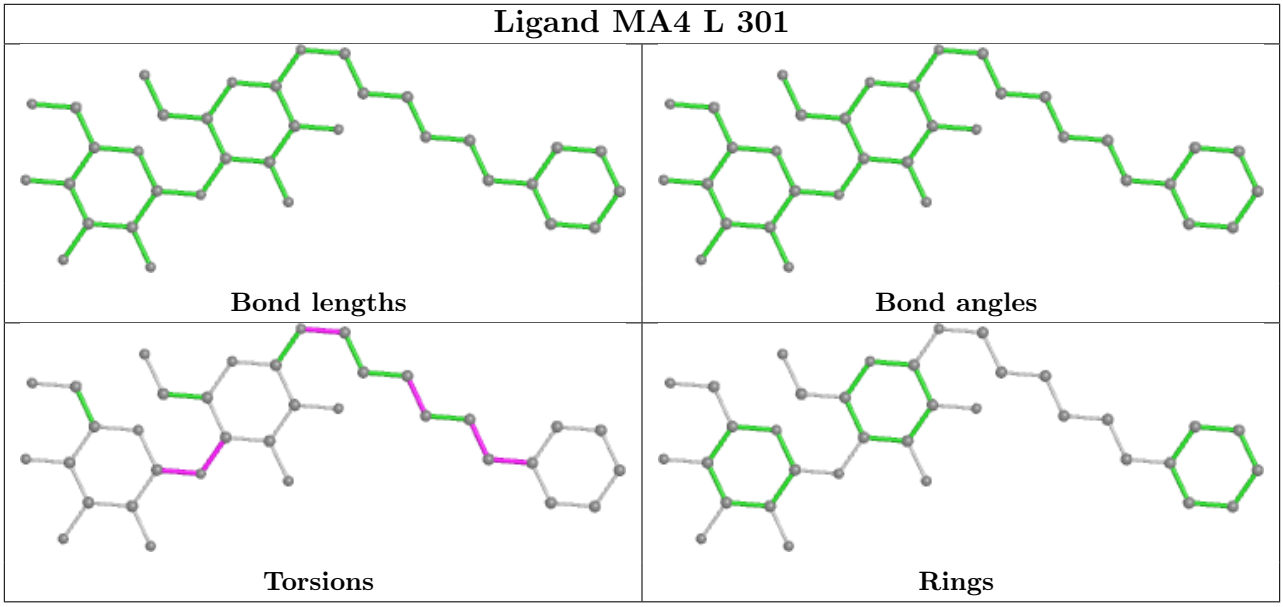
Mol	Chain	Res	Type	Atoms
4	L	301	MA4	C21-C31-C41-C51

There are no ring outliers.

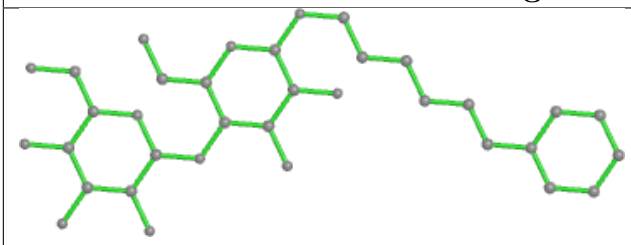
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	301	PO4	1	0

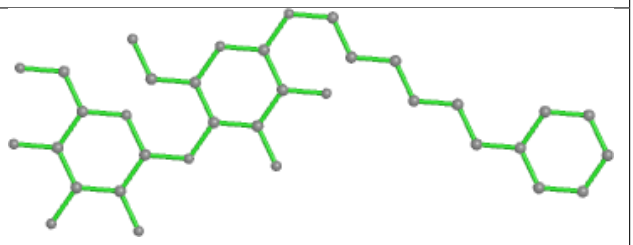
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



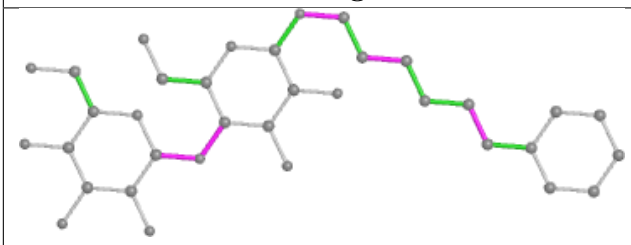
Ligand MA4 F 301



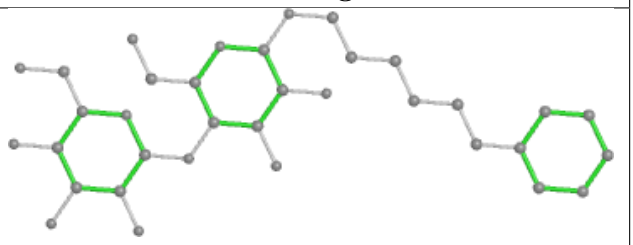
Bond lengths



Bond angles

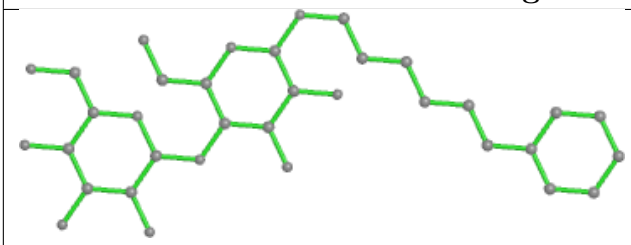


Torsions

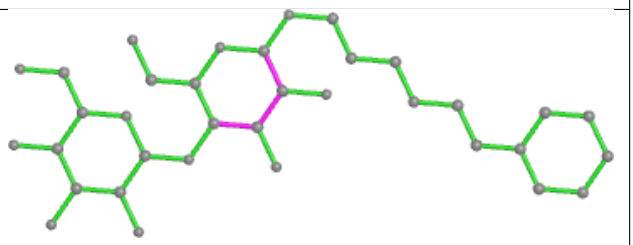


Rings

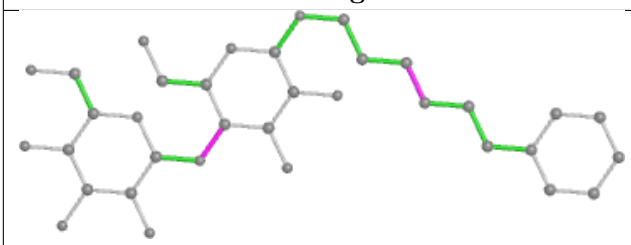
Ligand MA4 B 301



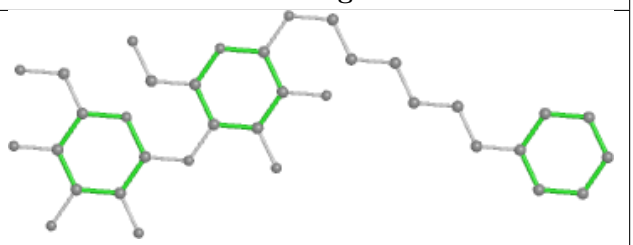
Bond lengths



Bond angles

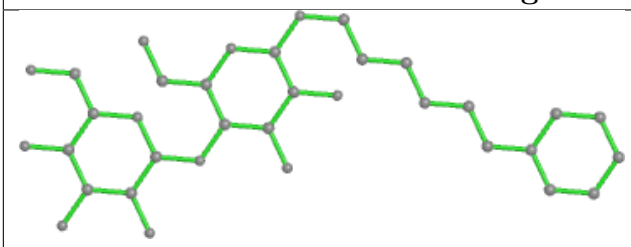


Torsions

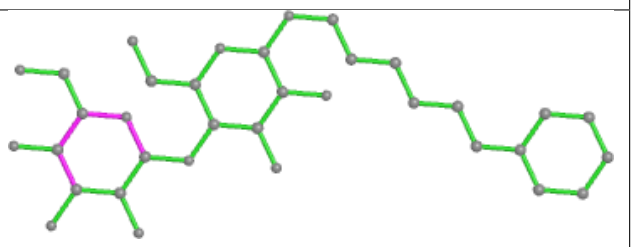


Rings

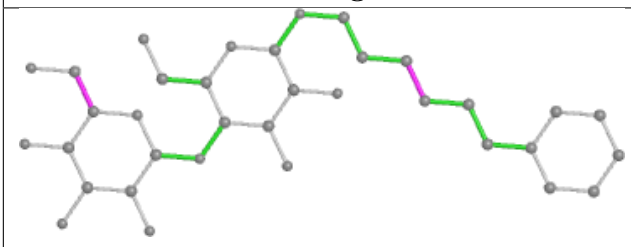
Ligand MA4 N 301



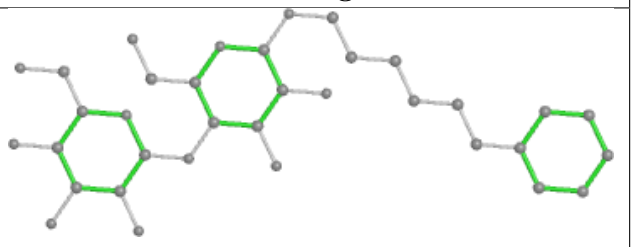
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	236/240 (98%)	0.19	7 (2%)	50	45	34, 40, 53, 55	0
1	C	232/240 (96%)	0.17	7 (3%)	50	45	29, 34, 46, 49	0
1	E	236/240 (98%)	0.01	3 (1%)	77	77	27, 33, 43, 48	0
1	G	230/240 (95%)	0.05	3 (1%)	77	77	24, 33, 41, 45	0
1	I	234/240 (97%)	0.19	7 (2%)	50	45	24, 32, 42, 50	0
1	K	236/240 (98%)	0.12	5 (2%)	63	61	30, 37, 45, 64	0
1	M	233/240 (97%)	0.26	9 (3%)	39	35	31, 42, 51, 57	0
1	O	234/240 (97%)	0.17	8 (3%)	45	40	26, 34, 43, 46	0
2	B	278/290 (95%)	0.14	5 (1%)	68	67	27, 38, 51, 69	0
2	D	272/290 (93%)	0.20	2 (0%)	87	87	30, 39, 51, 69	0
2	F	290/290 (100%)	0.15	7 (2%)	59	56	29, 41, 61, 79	0
2	H	272/290 (93%)	0.39	12 (4%)	34	30	32, 44, 59, 80	0
2	J	274/290 (94%)	0.60	32 (11%)	4	3	29, 45, 66, 84	0
2	L	278/290 (95%)	0.16	8 (2%)	51	47	31, 40, 62, 77	0
2	N	277/290 (95%)	0.18	8 (2%)	51	47	34, 43, 59, 75	0
2	P	271/290 (93%)	0.49	18 (6%)	18	14	32, 48, 59, 107	0
All	All	4083/4240 (96%)	0.22	141 (3%)	44	38	24, 39, 56, 107	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	6	ILE	6.5
2	P	1	MET	5.9
2	J	7	ASP	4.9
1	C	232	GLN	4.7
2	J	14	PHE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	10	GLN	4.6
2	L	61	ILE	4.6
2	J	3	ALA	4.3
2	P	7	ASP	4.2
2	N	61	ILE	4.2
1	A	14	THR	4.1
2	H	268	PRO	4.1
1	A	15	LEU	4.0
2	J	2	ILE	4.0
1	A	10	SER	3.9
2	J	243	SER	3.9
2	P	268	PRO	3.8
2	H	11	LYS	3.8
2	J	9	LEU	3.8
2	N	62	LEU	3.8
2	B	277	ASN	3.8
1	M	109	LYS	3.8
2	P	265	PHE	3.8
1	M	103	PHE	3.7
1	G	103	PHE	3.6
2	P	3	ALA	3.6
2	J	12	PHE	3.5
2	H	265	PHE	3.5
1	K	235	PHE	3.4
1	O	103	PHE	3.4
2	J	13	HIS	3.4
1	A	103	PHE	3.4
2	J	16	GLN	3.4
2	L	273	LEU	3.4
2	H	10	GLN	3.4
1	A	61	ASP	3.3
2	J	128	ILE	3.3
2	F	112	GLY	3.3
1	C	103	PHE	3.2
1	A	13	GLU	3.2
2	J	242	TYR	3.2
2	P	6	ILE	3.2
1	M	218	GLU	3.1
1	I	14	THR	3.1
1	C	223	THR	3.1
2	F	113	VAL	3.0
1	K	236	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	268	PRO	3.0
2	J	246	VAL	3.0
1	C	106	LEU	3.0
1	O	106	LEU	2.9
2	P	63	GLY	2.9
2	D	1	MET	2.9
2	L	62	LEU	2.9
2	H	14	PHE	2.9
2	L	113	VAL	2.9
1	I	231	ASN	2.9
2	J	5	PHE	2.8
2	J	63	GLY	2.8
2	H	13	HIS	2.7
2	L	13	HIS	2.7
2	N	244	PHE	2.7
2	J	11	LYS	2.7
1	I	232	GLN	2.7
1	M	125	ASP	2.7
2	J	265	PHE	2.7
2	F	65	ASP	2.7
1	E	103	PHE	2.6
2	J	245	ASN	2.6
2	L	112	GLY	2.6
1	C	14	THR	2.6
2	P	267	ALA	2.6
2	H	244	PHE	2.6
2	J	15	LEU	2.6
1	G	108	ALA	2.6
2	J	244	PHE	2.6
1	O	111	TRP	2.6
1	I	233	LEU	2.6
2	P	64	LEU	2.6
2	F	13	HIS	2.5
1	I	234	PHE	2.5
2	B	224	PHE	2.5
2	P	86	GLY	2.5
2	N	64	LEU	2.5
2	J	82	THR	2.5
2	J	127	ASN	2.5
1	O	234	PHE	2.5
2	L	79	ILE	2.5
1	O	105	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	68	LEU	2.4
2	J	1	MET	2.4
2	J	62	LEU	2.4
2	J	266	ILE	2.4
1	M	104	ARG	2.4
2	H	9	LEU	2.4
2	N	113	VAL	2.4
1	M	13	GLU	2.4
1	K	10	SER	2.4
2	L	10	GLN	2.3
2	P	113	VAL	2.3
2	J	65	ASP	2.3
2	J	240	ILE	2.3
1	G	105	SER	2.3
2	P	244	PHE	2.3
2	P	148	LEU	2.3
1	M	217	LYS	2.3
1	O	14	THR	2.3
2	H	266	ILE	2.2
2	N	68	ILE	2.2
2	P	12	PHE	2.2
2	F	11	LYS	2.2
2	P	11	LYS	2.2
2	H	272	TYR	2.2
2	F	283	GLY	2.2
2	J	19	LEU	2.2
1	K	234	PHE	2.2
2	B	266	ILE	2.2
1	K	11	TYR	2.2
1	I	82	TYR	2.2
2	J	137	PHE	2.1
1	E	14	THR	2.1
2	P	178	HIS	2.1
1	O	101	PRO	2.1
2	N	63	GLY	2.1
1	O	62	LYS	2.1
2	N	1	MET	2.1
1	M	14	THR	2.1
2	J	241	GLY	2.1
1	M	11[A]	TYR	2.1
2	P	174	VAL	2.1
1	I	103	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	224	PHE	2.1
2	F	133	ASP	2.0
1	E	126	TYR	2.0
2	D	272	TYR	2.0
2	P	271	ARG	2.0
2	H	12	PHE	2.0
2	J	138	ILE	2.0
2	B	11	LYS	2.0
1	C	105	SER	2.0
1	C	1	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

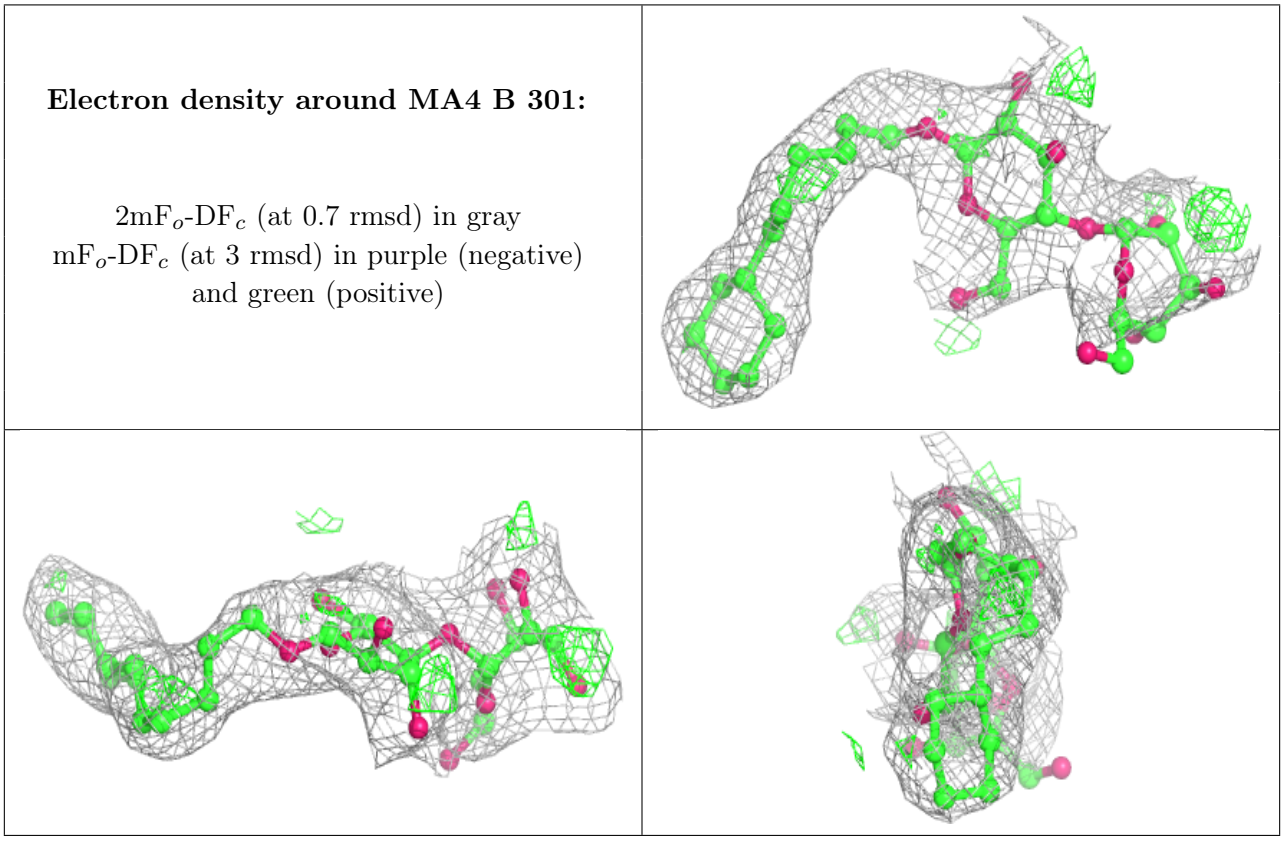
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	MA4	B	301	35/35	0.74	0.31	77,83,86,86	0
3	PO4	K	301	5/5	0.75	0.48	73,74,74,74	0
3	PO4	C	301	5/5	0.80	0.41	70,71,71,72	0
4	MA4	F	301	35/35	0.83	0.28	69,69,72,72	0
4	MA4	N	301	35/35	0.84	0.25	88,92,95,95	0
3	PO4	E	301	5/5	0.85	0.42	54,55,55,55	0
4	MA4	L	301	35/35	0.85	0.21	71,73,75,76	0
3	PO4	I	301	5/5	0.85	0.46	75,76,77,77	0
3	PO4	A	301	5/5	0.87	0.37	66,66,67,67	0
3	PO4	M	301	5/5	0.88	0.44	70,70,70,70	0
3	PO4	O	301	5/5	0.88	0.30	59,60,60,60	0
3	PO4	G	301	5/5	0.89	0.32	60,60,61,61	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.

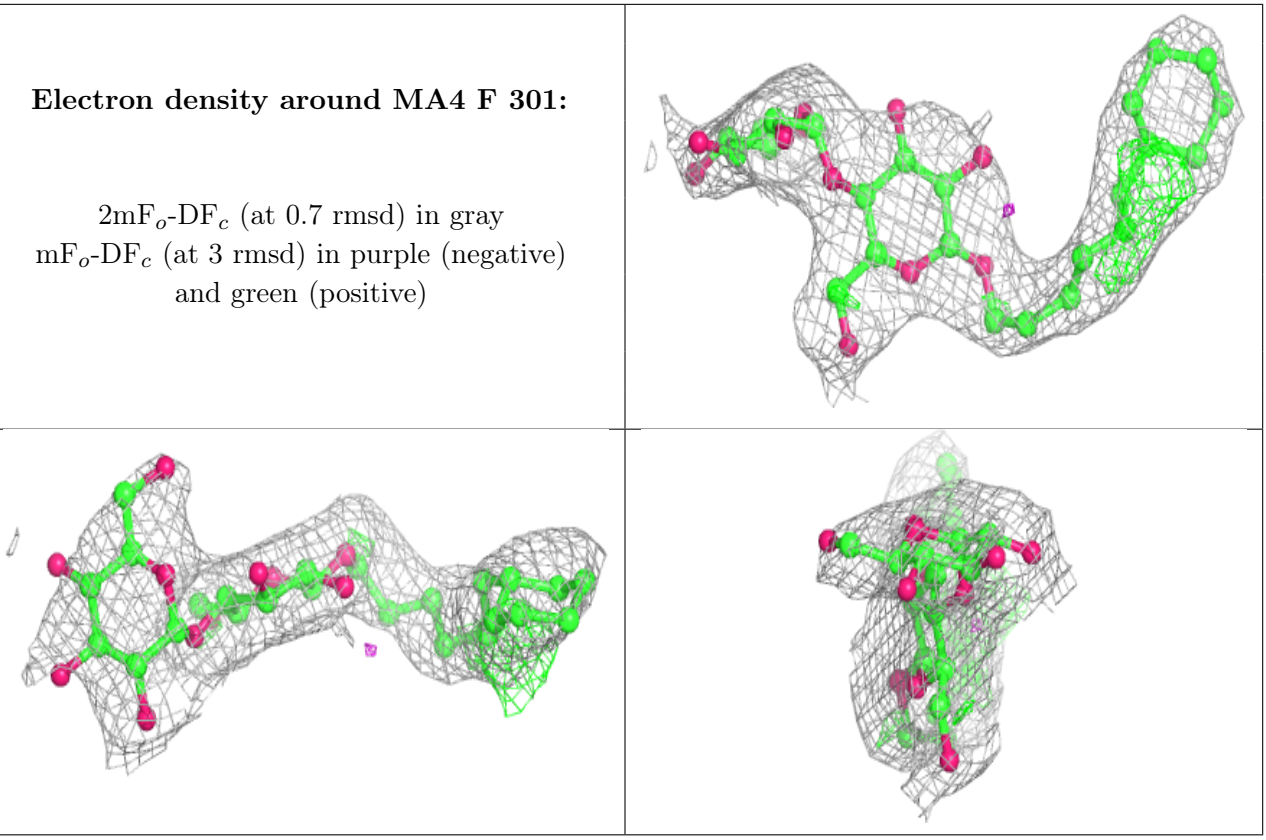
Electron density around MA4 B 301:

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



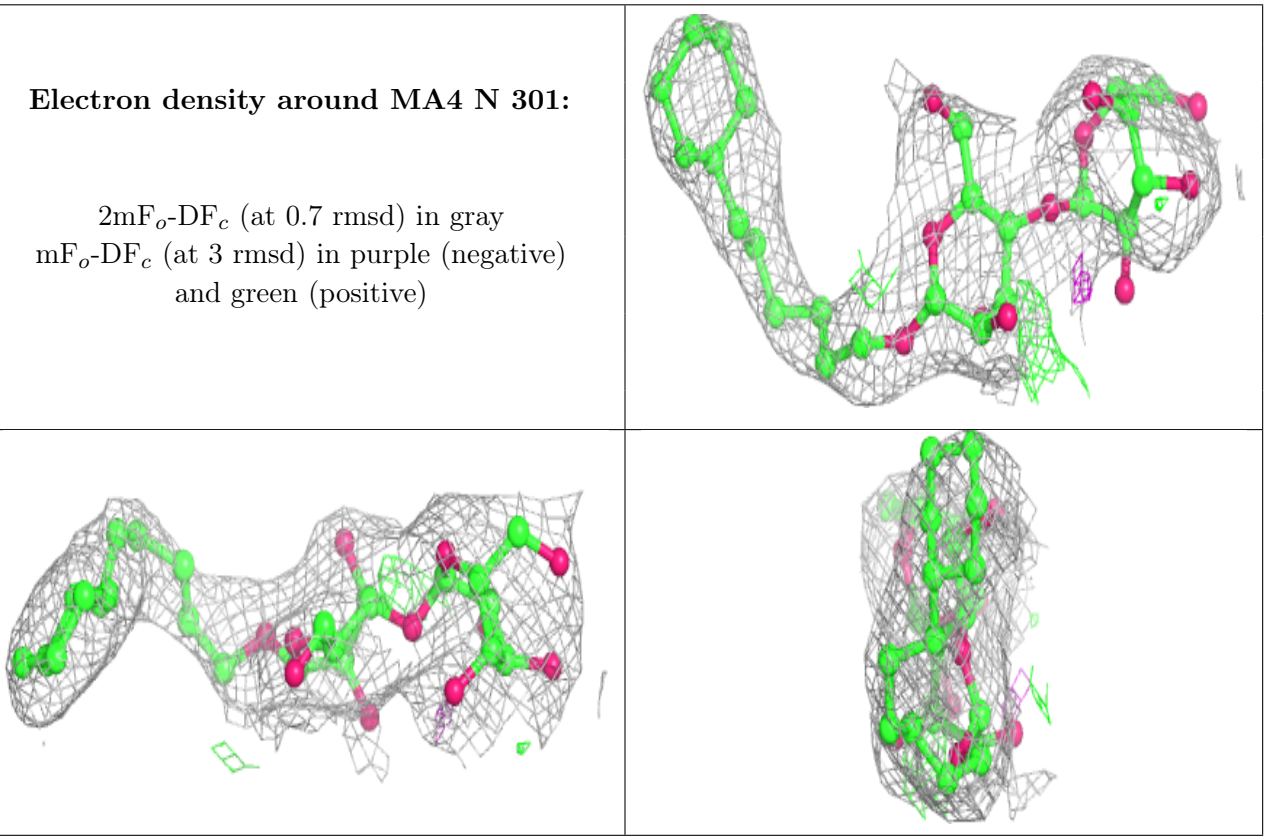
Electron density around MA4 F 301:

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



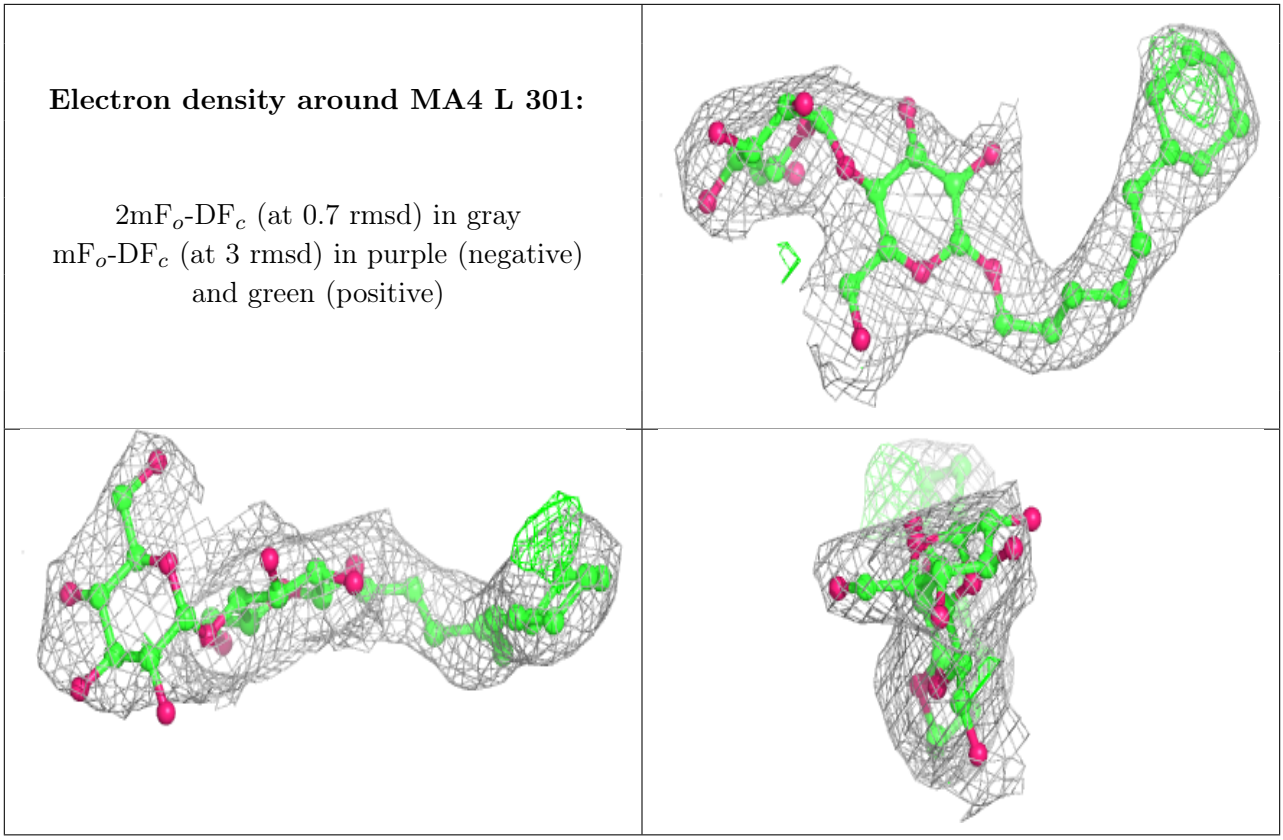
Electron density around MA4 N 301:

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



Electron density around MA4 L 301:

$2mF_o$-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.