



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:00 AM EDT

PDB ID : 6ZG3
Title : the structure of ECF PanT transporter in a complex with a nanobody
Authors : Setyawati, I.; Guskov, A.; Slotboom, D.J.
Deposited on : 2020-06-18
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.37.1
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) : 2.37.1

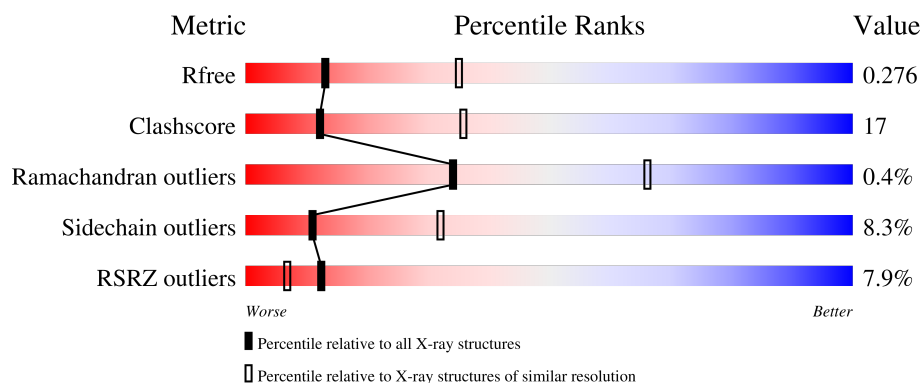
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	300	
1	F	300	
2	B	287	
2	G	287	
3	C	215	

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Mol	Chain	Length	Quality of chain
3	H	215	
4	D	265	
4	I	265	
5	E	136	
5	J	136	

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
6	PEG	D	303	-	-	-	X
7	LMT	C	502	-	-	-	X
7	LMT	D	301	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18233 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 Energy-coupling factor transporter ATP-binding protein EcfA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2147	1354	359	430	4			
1	F	279	Total	C	N	O	S	0	0	0
			2143	1352	358	429	4			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q1GBJ0
A	-16	HIS	-	expression tag	UNP Q1GBJ0
A	-15	HIS	-	expression tag	UNP Q1GBJ0
A	-14	HIS	-	expression tag	UNP Q1GBJ0
A	-13	HIS	-	expression tag	UNP Q1GBJ0
A	-12	HIS	-	expression tag	UNP Q1GBJ0
A	-11	HIS	-	expression tag	UNP Q1GBJ0
A	-10	HIS	-	expression tag	UNP Q1GBJ0
A	-9	HIS	-	expression tag	UNP Q1GBJ0
A	-8	HIS	-	expression tag	UNP Q1GBJ0
A	-7	HIS	-	expression tag	UNP Q1GBJ0
A	-6	GLY	-	expression tag	UNP Q1GBJ0
A	-5	GLU	-	expression tag	UNP Q1GBJ0
A	-4	ASN	-	expression tag	UNP Q1GBJ0
A	-3	LEU	-	expression tag	UNP Q1GBJ0
A	-2	TYR	-	expression tag	UNP Q1GBJ0
A	-1	PHE	-	expression tag	UNP Q1GBJ0
A	0	GLN	-	expression tag	UNP Q1GBJ0
A	1	GLY	-	expression tag	UNP Q1GBJ0
F	-17	MET	-	initiating methionine	UNP Q1GBJ0
F	-16	HIS	-	expression tag	UNP Q1GBJ0
F	-15	HIS	-	expression tag	UNP Q1GBJ0
F	-14	HIS	-	expression tag	UNP Q1GBJ0
F	-13	HIS	-	expression tag	UNP Q1GBJ0
F	-12	HIS	-	expression tag	UNP Q1GBJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	expression tag	UNP Q1GBJ0
F	-10	HIS	-	expression tag	UNP Q1GBJ0
F	-9	HIS	-	expression tag	UNP Q1GBJ0
F	-8	HIS	-	expression tag	UNP Q1GBJ0
F	-7	HIS	-	expression tag	UNP Q1GBJ0
F	-6	GLY	-	expression tag	UNP Q1GBJ0
F	-5	GLU	-	expression tag	UNP Q1GBJ0
F	-4	ASN	-	expression tag	UNP Q1GBJ0
F	-3	LEU	-	expression tag	UNP Q1GBJ0
F	-2	TYR	-	expression tag	UNP Q1GBJ0
F	-1	PHE	-	expression tag	UNP Q1GBJ0
F	0	GLN	-	expression tag	UNP Q1GBJ0
F	1	GLY	-	expression tag	UNP Q1GBJ0

- Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	282	Total	C	N	O	S	0	0	0
			2187	1396	371	412	8			
2	G	283	Total	C	N	O	S	0	0	0
			2195	1401	372	413	9			

- Molecule 3 is a protein called Conserved hypothetical membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	0
			1553	1033	257	262	1			
3	H	207	Total	C	N	O	S	0	0	0
			1553	1033	257	262	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	208	TRP	-	expression tag	UNP Q1GBG0
C	209	SER	-	expression tag	UNP Q1GBG0
C	210	HIS	-	expression tag	UNP Q1GBG0
C	211	PRO	-	expression tag	UNP Q1GBG0
C	212	GLN	-	expression tag	UNP Q1GBG0
C	213	PHE	-	expression tag	UNP Q1GBG0
C	214	GLU	-	expression tag	UNP Q1GBG0
C	215	LYS	-	expression tag	UNP Q1GBG0
H	208	TRP	-	expression tag	UNP Q1GBG0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	209	SER	-	expression tag	UNP Q1GBG0
H	210	HIS	-	expression tag	UNP Q1GBG0
H	211	PRO	-	expression tag	UNP Q1GBG0
H	212	GLN	-	expression tag	UNP Q1GBG0
H	213	PHE	-	expression tag	UNP Q1GBG0
H	214	GLU	-	expression tag	UNP Q1GBG0
H	215	LYS	-	expression tag	UNP Q1GBG0

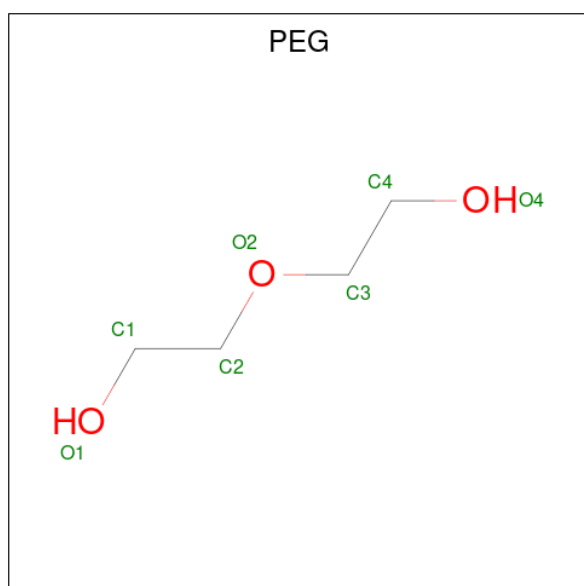
- Molecule 4 is a protein called Putative cobalt ABC transporter, permease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	260	Total	C	N	O	S	0	1	0
			2105	1406	337	348	14			
4	I	260	Total	C	N	O	S	0	0	0
			2093	1397	336	346	14			

- Molecule 5 is a protein called CA14381 nanobody.

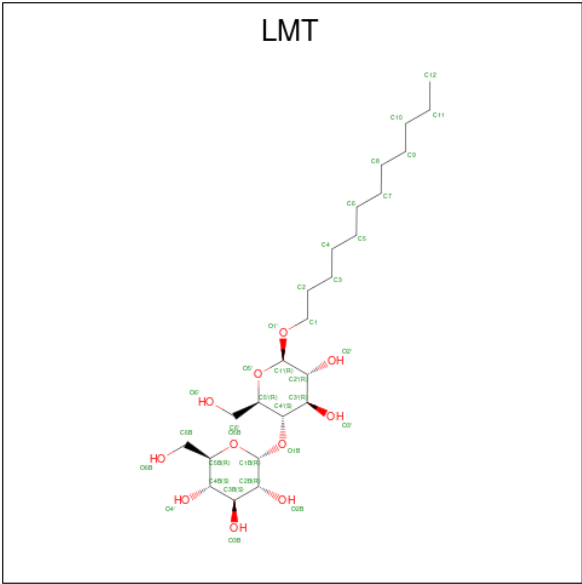
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	126	Total	C	N	O	S	0	0	0
			964	603	164	192	5			
5	J	125	Total	C	N	O	S	0	0	0
			955	598	162	190	5			

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		
6	E	1	Total	C	O	0	0
			7	4	3		
6	I	1	Total	C	O	0	0
			7	4	3		
6	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



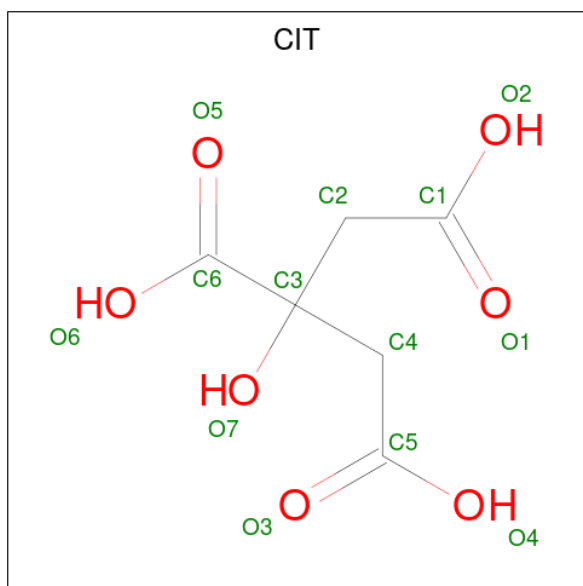
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			32	21	11		

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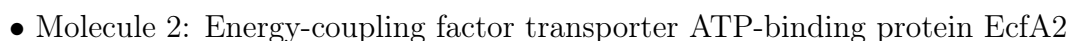
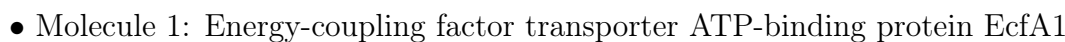
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			35	24	11		
7	D	1	Total	C	O	0	0
			35	24	11		
7	G	1	Total	C	O	0	0
			35	24	11		
7	H	1	Total	C	O	0	0
			35	24	11		
7	H	1	Total	C	O	0	0
			35	24	11		
7	I	1	Total	C	O	0	0
			35	24	11		

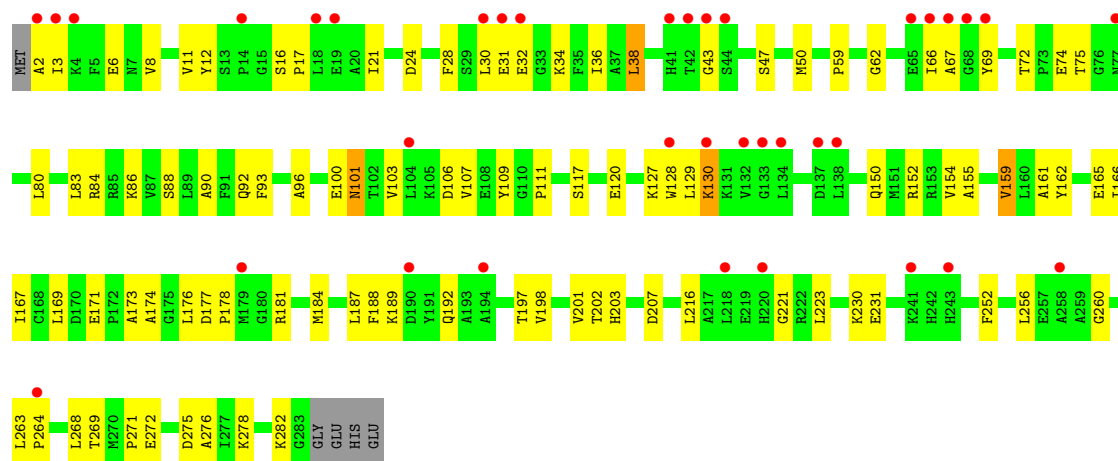
- Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



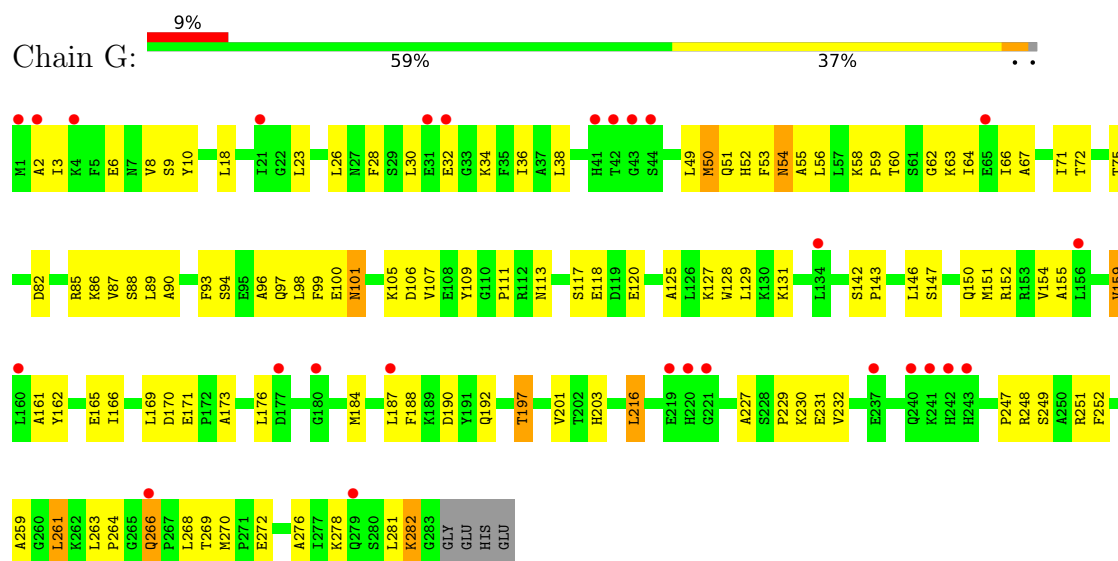
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	6	7		
8	H	1	Total	C	O	0	0
			13	6	7		

- Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA1

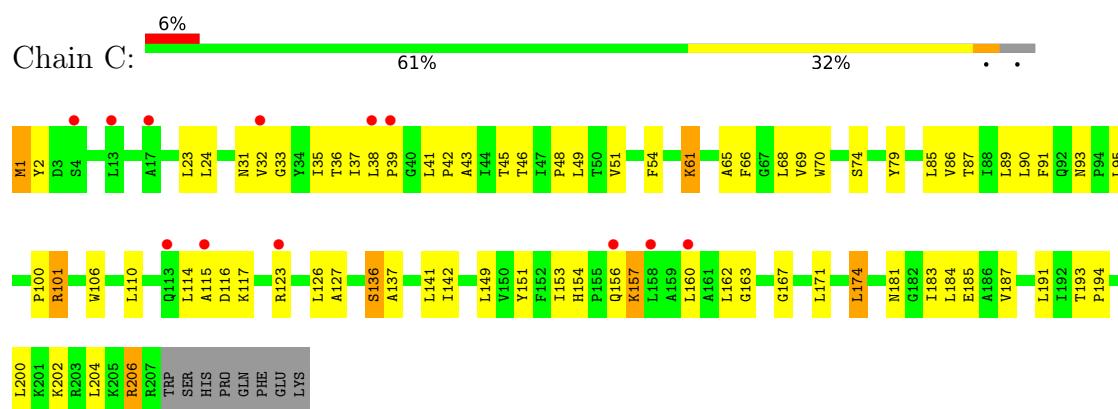




• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA2

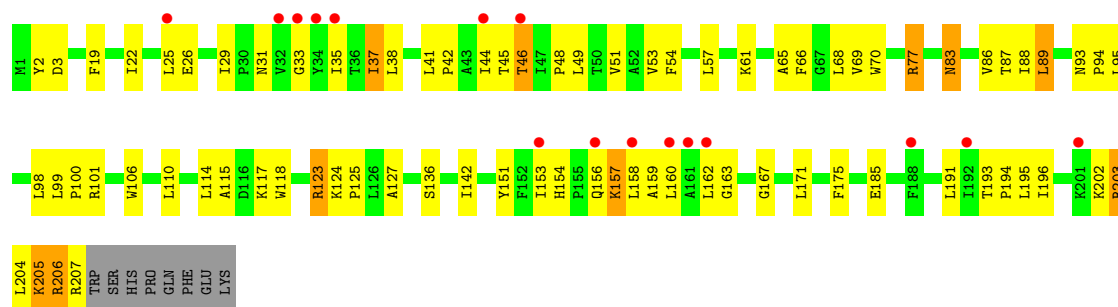


• Molecule 3: Conserved hypothetical membrane protein

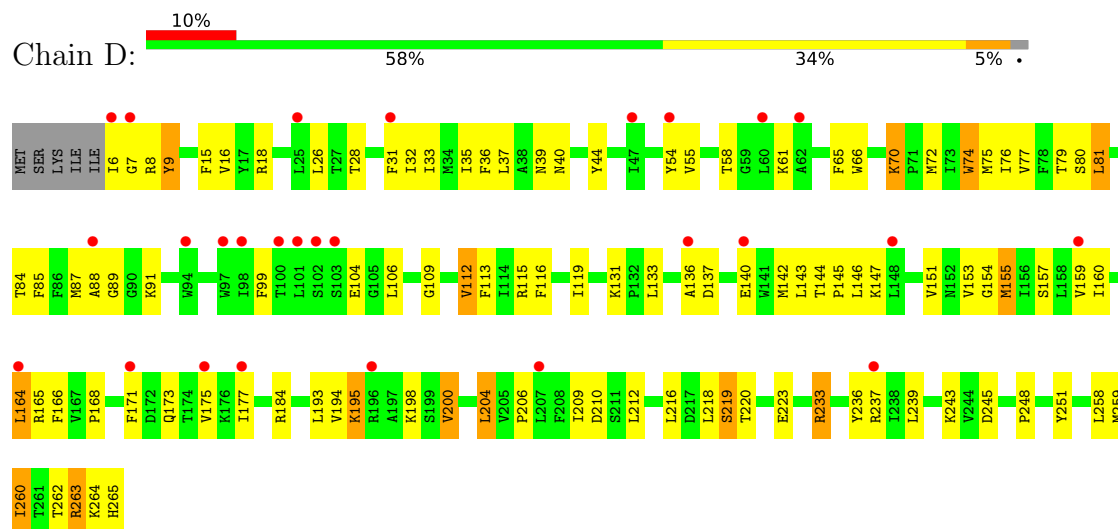


• Molecule 3: Conserved hypothetical membrane protein

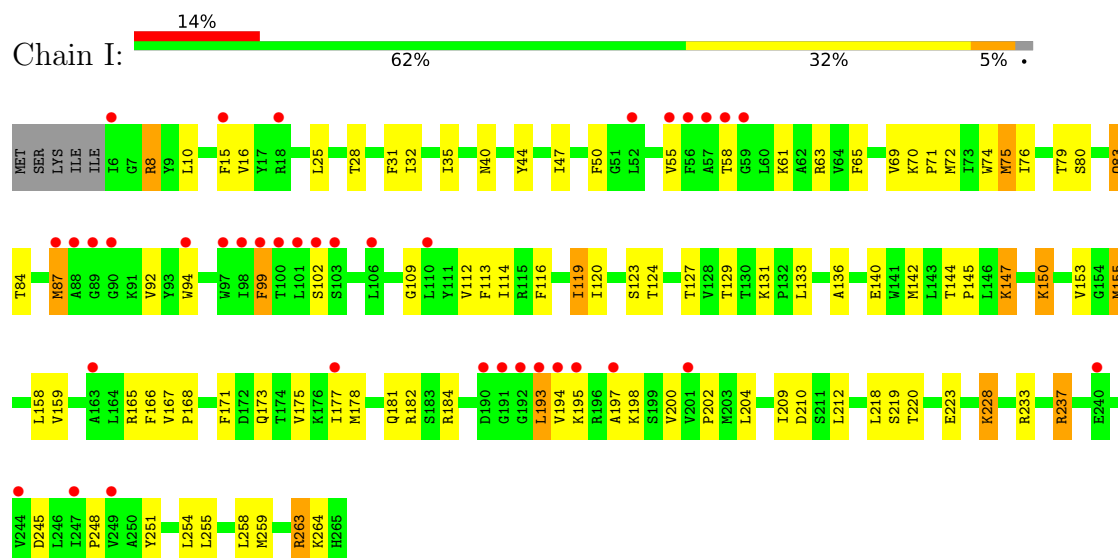




- Molecule 4: Putative cobalt ABC transporter, permease protein

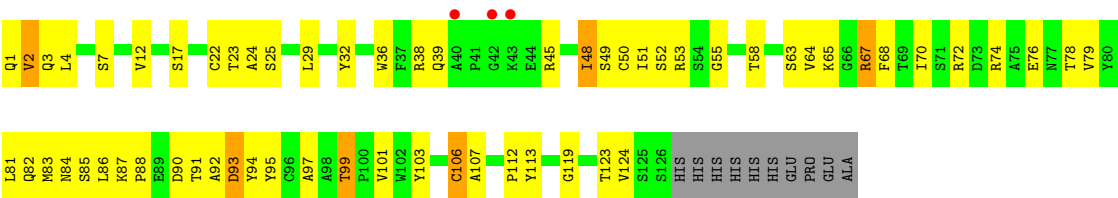


- Molecule 4: Putative cobalt ABC transporter, permease protein

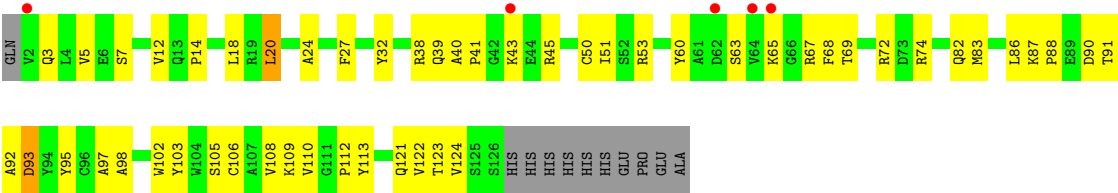


- Molecule 5: CA14381 nanobody





● Molecule 5: CA14381 nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	97.29Å 110.47Å 110.50Å 89.00° 102.27° 102.24°	Depositor
Resolution (Å)	48.83 – 2.80 48.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (48.83-2.80) 96.3 (48.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.242 , 0.276 0.244 , 0.276	Depositor DCC
R_{free} test set	5214 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.378 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18233	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, PEG, CIT

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	0.50	0/2180	0.73	1/2959 (0.0%)
1	F	0.50	0/2176	0.70	0/2954
2	B	0.42	0/2233	0.65	0/3014
2	G	0.42	0/2241	0.65	0/3024
3	C	0.46	0/1584	0.73	0/2164
3	H	0.45	0/1584	0.71	0/2164
4	D	0.50	0/2160	0.68	1/2934 (0.0%)
4	I	0.49	0/2147	0.69	2/2916 (0.1%)
5	E	0.59	1/987 (0.1%)	0.75	1/1342 (0.1%)
5	J	0.59	1/978 (0.1%)	0.73	0/1330
All	All	0.48	2/18270 (0.0%)	0.70	5/24801 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	50	CYS	CB-SG	-6.92	1.70	1.82
5	E	106	CYS	CB-SG	-6.11	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	81	LEU	CA-CB-CG	8.09	133.90	115.30
5	E	106	CYS	CA-CB-SG	-6.20	102.85	114.00
1	A	222	LEU	CA-CB-CG	-5.41	102.86	115.30
4	I	193	LEU	CB-CG-CD1	-5.30	101.99	111.00
4	I	193	LEU	CA-CB-CG	5.30	127.48	115.30

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	2147	0	2159	80	0
1	F	2143	0	2153	71	0
2	B	2187	0	2190	70	0
2	G	2195	0	2202	98	0
3	C	1553	0	1697	64	0
3	H	1553	0	1697	73	0
4	D	2105	0	2200	69	0
4	I	2093	0	2192	69	0
5	E	964	0	913	48	0
5	J	955	0	902	31	0
6	A	7	0	10	1	0
6	B	7	0	10	0	0
6	C	21	0	30	2	0
6	D	14	0	20	0	0
6	E	7	0	10	0	0
6	I	7	0	10	0	0
6	J	7	0	10	1	0
7	C	67	0	83	4	0
7	D	35	0	46	4	0
7	G	35	0	46	5	0
7	H	70	0	92	7	0
7	I	35	0	46	2	0
8	C	13	0	5	1	0
8	H	13	0	5	1	0
All	All	18233	0	18728	630	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 17.

All (630) 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:F:12:THR:HG22	1:F:25:ASP:H	1.20	1.03
2:G:6:GLU:O	2:G:62:GLY:HA3	1.68	0.94
1:A:12:THR:HG22	1:A:25:ASP:H	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:248:ARG:HH11	2:G:251:ARG:HH11	1.18	0.88
5:J:67:ARG:NH2	5:J:90:ASP:OD2	2.08	0.87
3:C:151:TYR:HB3	3:C:157:LYS:HZ1	1.42	0.84
4:D:133:LEU:HD21	4:D:237:ARG:HG3	1.59	0.83
3:C:115:ALA:HB2	3:C:127:ALA:HB3	1.59	0.83
1:A:274:SER:HA	1:F:277:GLN:HE22	1.43	0.81
2:B:264:PRO:HD2	2:B:276:ALA:HB1	1.62	0.81
4:D:40:ASN:HD21	4:D:263:ARG:HA	1.49	0.77
1:A:112:ASN:OD1	4:I:233:ARG:NH1	2.17	0.77
1:A:161:LYS:NZ	5:E:112:PRO:O	2.18	0.77
2:G:127:LYS:HE2	2:G:131:LYS:HE2	1.65	0.77
1:A:77:ASP:OD1	1:A:77:ASP:N	2.11	0.76
5:E:51:ILE:HG12	5:E:58:THR:HG22	1.68	0.76
5:E:67:ARG:NH2	5:E:90:ASP:OD2	2.18	0.76
1:F:262:PRO:HD2	1:F:265:ILE:HD12	1.65	0.76
2:B:107:VAL:HG21	2:B:129:LEU:HD21	1.67	0.75
1:A:106:VAL:HG13	1:A:156:GLY:HA2	1.69	0.74
3:H:42:PRO:HD3	3:H:86:VAL:HG21	1.69	0.74
1:A:171:THR:HB	1:A:179:LYS:HG2	1.69	0.74
4:D:80:SER:HA	4:D:112:VAL:HG21	1.69	0.73
3:C:151:TYR:HB3	3:C:157:LYS:NZ	2.02	0.73
1:F:12:THR:HG22	1:F:25:ASP:N	2.01	0.73
1:F:77:ASP:N	1:F:77:ASP:OD1	2.19	0.72
1:F:145:SER:O	1:F:149:LYS:HG3	1.88	0.72
3:C:38:LEU:HB3	3:C:41:LEU:HD13	1.72	0.72
4:D:16:VAL:HG21	4:D:58:THR:HG22	1.73	0.71
4:D:233:ARG:NH1	1:F:112:ASN:OD1	2.25	0.70
1:F:171:THR:HB	1:F:179:LYS:HG2	1.73	0.70
2:B:34:LYS:HA	2:B:192:GLN:HE21	1.57	0.70
2:B:3:ILE:HB	2:B:30:LEU:HB2	1.73	0.70
4:I:263:ARG:HH11	4:I:263:ARG:HB3	1.56	0.69
7:H:601:LMT:H21	7:H:601:LMT:O2'	1.91	0.69
7:C:501:LMT:H82	7:D:301:LMT:H22	1.74	0.68
2:G:30:LEU:HD22	2:G:36:ILE:HG12	1.75	0.68
3:C:157:LYS:HE2	3:C:171:LEU:HD21	1.76	0.68
2:G:3:ILE:HD11	2:G:166:ILE:HD13	1.75	0.68
3:H:83:ASN:OD1	3:H:83:ASN:N	2.26	0.68
1:A:214:LEU:HG	1:A:224:GLN:HG3	1.73	0.68
2:G:264:PRO:HD2	2:G:276:ALA:HB1	1.76	0.68
3:H:41:LEU:HB3	3:H:42:PRO:HD2	1.76	0.68
3:C:42:PRO:O	3:C:181:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:O	1:A:43:GLY:N	2.26	0.67
3:C:157:LYS:HD3	3:C:160:LEU:HD12	1.77	0.67
1:A:222:LEU:HD23	1:A:240:ILE:HD11	1.75	0.67
4:D:200:VAL:HG13	4:D:204:LEU:HG	1.75	0.67
2:G:173:ALA:HA	2:G:176:LEU:HD12	1.75	0.66
1:F:97:PHE:CE1	1:F:141:PRO:HG3	2.31	0.66
1:F:199:SER:OG	1:F:206:GLU:OE2	2.13	0.66
5:E:23:THR:HG23	5:E:78:THR:HG22	1.77	0.66
2:B:2:ALA:N	2:B:32:GLU:OE1	2.28	0.66
4:D:248:PRO:O	4:D:251:TYR:HB3	1.97	0.65
5:E:106:CYS:SG	5:E:107:ALA:N	2.69	0.65
2:B:90:ALA:HB3	2:B:169:LEU:HD23	1.78	0.65
2:G:6:GLU:HB2	2:G:63:LYS:H	1.62	0.65
2:G:230:LYS:NZ	2:G:272:GLU:OE1	2.27	0.65
1:A:199:SER:OG	1:A:206:GLU:OE1	2.09	0.65
1:A:5:ILE:HD11	1:A:196:THR:HG21	1.79	0.64
1:A:188:LYS:HE3	6:A:301:PEG:H12	1.79	0.64
5:E:2:VAL:O	5:E:4:LEU:N	2.31	0.64
4:D:66:TRP:NE1	4:D:70:LYS:HD3	2.12	0.64
1:A:30:ILE:HG21	1:A:198:ILE:HD11	1.80	0.64
2:B:6:GLU:O	2:B:62:GLY:HA3	1.98	0.64
2:B:30:LEU:HD22	2:B:36:ILE:HD13	1.79	0.64
4:I:150:LYS:H	4:I:150:LYS:HD2	1.62	0.64
2:G:3:ILE:HG23	2:G:66:ILE:HG12	1.79	0.63
2:B:72:THR:N	2:B:75:THR:OG1	2.32	0.63
2:G:107:VAL:HG21	2:G:129:LEU:HD21	1.81	0.63
1:A:166:ILE:HG12	1:A:198:ILE:HB	1.80	0.63
1:F:113:ARG:HE	1:F:160:VAL:HG11	1.62	0.63
2:B:3:ILE:HG23	2:B:66:ILE:HG12	1.79	0.63
1:F:5:ILE:HD11	1:F:196:THR:HG21	1.80	0.63
5:J:51:ILE:HD13	5:J:72:ARG:HG3	1.79	0.63
3:H:89:LEU:HD22	3:H:159:ALA:HB1	1.80	0.62
3:H:115:ALA:HB2	3:H:127:ALA:HB3	1.81	0.62
2:G:109:TYR:O	2:G:113:ASN:ND2	2.31	0.62
1:A:14:THR:HG22	1:A:21:PRO:HA	1.81	0.62
1:F:84:GLU:HG2	1:F:113:ARG:NH1	2.14	0.62
3:H:26:GLU:OE2	3:H:46:THR:OG1	2.17	0.62
3:C:54:PHE:CE2	3:C:66:PHE:HB2	2.34	0.62
2:B:3:ILE:HD11	2:B:166:ILE:HD13	1.82	0.62
2:B:69:TYR:HD2	2:B:83:LEU:HB2	1.65	0.62
3:C:79:TYR:HE1	4:D:36:PHE:HZ	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:THR:CG2	1:F:25:ASP:H	2.05	0.62
3:C:100:PRO:HG3	3:C:142:ILE:HG22	1.80	0.62
3:H:202:LYS:O	3:H:205:LYS:HD2	1.98	0.62
5:E:36:TRP:O	5:E:48:ILE:HG13	2.00	0.61
3:H:95:LEU:HD12	7:H:603:LMT:H22	1.83	0.61
3:H:204:LEU:HD12	4:I:212:LEU:HD21	1.81	0.61
2:B:177:ASP:HB2	2:B:178:PRO:HD2	1.81	0.61
4:I:69:VAL:HG22	4:I:120:ILE:HG21	1.83	0.61
1:A:6:ILE:HG12	1:A:69:VAL:HG22	1.83	0.61
2:B:171:GLU:OE1	2:B:203:HIS:ND1	2.34	0.61
4:D:84:THR:HG23	4:D:109:GLY:HA3	1.83	0.61
2:G:3:ILE:HB	2:G:30:LEU:HB2	1.83	0.60
2:B:256:LEU:HD12	2:B:263:LEU:HD11	1.81	0.60
2:G:142:SER:CB	3:H:202:LYS:HD2	2.32	0.60
3:H:196:ILE:HD11	4:I:204:LEU:HB3	1.83	0.60
1:A:133:MET:HE2	1:A:136:TYR:HD2	1.66	0.60
4:D:263:ARG:HG2	4:D:263:ARG:HH11	1.67	0.60
4:I:133:LEU:HD21	4:I:237:ARG:HG2	1.82	0.60
5:E:76:GLU:O	5:E:78:THR:HG23	2.01	0.59
5:J:91:THR:OG1	5:J:123:THR:HA	2.02	0.59
2:G:171:GLU:OE1	2:G:203:HIS:ND1	2.35	0.59
3:C:37:ILE:HG23	3:C:38:LEU:HG	1.85	0.59
3:C:153:ILE:HD11	7:C:502:LMT:H5'	1.85	0.59
4:I:72:MET:HB3	4:I:76:ILE:HD11	1.83	0.59
2:G:72:THR:N	2:G:75:THR:OG1	2.35	0.59
4:I:76:ILE:HD12	4:I:116:PHE:CG	2.37	0.59
5:E:51:ILE:HG21	5:E:72:ARG:HG3	1.85	0.59
1:F:22:ALA:O	1:F:23:LEU:HD12	2.02	0.59
1:F:111:GLU:HG3	1:F:120:MET:HE1	1.85	0.59
2:G:117:SER:H	2:G:120:GLU:HB2	1.67	0.58
4:I:80:SER:HA	4:I:112:VAL:HG21	1.85	0.58
4:D:154:GLY:O	4:D:157:SER:OG	2.21	0.58
5:E:32:TYR:O	5:E:72:ARG:NH2	2.24	0.58
3:H:114:LEU:O	3:H:117:LYS:N	2.36	0.58
1:A:183:LEU:HD11	1:A:206:GLU:HG3	1.86	0.58
4:D:74:TRP:HA	4:D:74:TRP:CE3	2.39	0.58
3:H:94:PRO:HG2	7:H:603:LMT:O3'	2.03	0.58
2:B:88:SER:OG	2:B:159:VAL:HG12	2.03	0.58
5:J:39:GLN:HB2	5:J:45:ARG:HB3	1.85	0.58
4:I:155:MET:O	4:I:159:VAL:HG23	2.02	0.58
3:C:1:MET:SD	3:C:1:MET:N	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:10:TYR:O	2:G:23:LEU:N	2.30	0.57
2:G:100:GLU:OE1	7:G:901:LMT:O2'	2.23	0.57
4:I:120:ILE:O	4:I:124:THR:HG23	2.04	0.57
2:B:106:ASP:OD1	4:D:184:ARG:NH2	2.37	0.57
3:C:79:TYR:CE1	4:D:36:PHE:HZ	2.20	0.57
5:E:36:TRP:NE1	5:E:81:LEU:HB2	2.19	0.57
1:A:97:PHE:CE1	1:A:141:PRO:HG3	2.40	0.57
1:A:150:GLN:HG3	1:A:174:LEU:HD11	1.85	0.57
4:D:177:ILE:HD13	4:D:206:PRO:HB3	1.85	0.57
5:J:60:TYR:HB2	5:J:65:LYS:HD2	1.87	0.57
2:G:38:LEU:HB2	2:G:201:VAL:HG22	1.87	0.57
3:H:54:PHE:CE1	3:H:66:PHE:HB2	2.40	0.57
4:D:6:ILE:HD12	4:D:168:PRO:HG3	1.85	0.57
2:G:261:LEU:HB3	2:G:263:LEU:HD13	1.86	0.57
4:I:119:ILE:O	4:I:123:SER:HB2	2.05	0.57
2:G:67:ALA:HB1	2:G:86:LYS:HD2	1.87	0.57
4:D:84:THR:CG2	4:D:109:GLY:HA3	2.34	0.57
1:F:97:PHE:CD1	1:F:141:PRO:HG3	2.40	0.57
5:E:39:GLN:OE1	5:E:45:ARG:NH1	2.38	0.56
5:E:93:ASP:HB3	5:E:95:TYR:CE1	2.40	0.56
2:G:8:VAL:HG13	2:G:59:PRO:HB3	1.86	0.56
4:I:178:MET:O	4:I:182:ARG:HG3	2.05	0.56
4:D:76:ILE:HD12	4:D:116:PHE:CG	2.40	0.56
4:D:263:ARG:O	4:D:265:HIS:N	2.38	0.56
3:C:206:ARG:HD3	3:C:206:ARG:H	1.69	0.56
3:C:89:LEU:HD21	3:C:160:LEU:HD11	1.88	0.56
2:G:6:GLU:O	2:G:62:GLY:CA	2.49	0.56
1:F:161:LYS:HE2	5:J:112:PRO:O	2.05	0.56
1:A:54:ASN:OD1	1:A:56:LEU:HG	2.05	0.55
1:A:119:GLU:O	1:A:123:ILE:HG13	2.05	0.55
1:F:102:VAL:HG21	1:F:136:TYR:O	2.06	0.55
3:H:191:LEU:O	3:H:194:PRO:HD2	2.06	0.55
2:B:8:VAL:HG13	2:B:59:PRO:HB3	1.86	0.55
2:B:101:ASN:OD1	2:B:101:ASN:N	2.28	0.55
2:G:105:LYS:HZ3	7:G:901:LMT:H3'	1.72	0.55
4:I:72:MET:C	4:I:76:ILE:HG12	2.26	0.55
5:E:68:PHE:HA	5:E:82:GLN:O	2.07	0.55
2:G:55:ALA:O	2:G:58:LYS:NZ	2.33	0.55
3:H:31:ASN:OD1	3:H:31:ASN:N	2.40	0.55
3:H:49:LEU:O	3:H:53:VAL:HG23	2.07	0.55
3:C:1:MET:SD	1:F:62:LEU:HD13	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:LYS:HE2	6:C:504:PEG:H12	1.89	0.55
2:B:117:SER:H	2:B:120:GLU:HB2	1.71	0.55
2:B:171:GLU:OE2	2:B:202:THR:HA	2.06	0.55
2:G:88:SER:OG	2:G:159:VAL:HG12	2.07	0.55
2:B:181:ARG:NH1	2:B:207:ASP:OD2	2.40	0.54
3:H:45:THR:OG1	3:H:48:PRO:HD3	2.07	0.54
3:C:191:LEU:O	3:C:194:PRO:HD2	2.07	0.54
4:I:255:LEU:HD11	4:I:259:MET:HE2	1.89	0.54
2:G:128:TRP:HZ3	2:G:187:LEU:HD11	1.72	0.54
3:H:154:HIS:O	3:H:156:GLN:N	2.41	0.54
4:I:245:ASP:O	4:I:248:PRO:HD2	2.07	0.54
1:A:36:THR:HB	1:A:212:GLN:HB3	1.88	0.54
2:B:230:LYS:NZ	2:B:272:GLU:OE1	2.35	0.54
2:G:18:LEU:HD21	5:J:123:THR:HG22	1.87	0.54
1:A:262:PRO:HD2	1:A:265:ILE:HD12	1.89	0.54
1:A:279:ASN:OD1	2:G:281:LEU:HA	2.08	0.54
2:B:252:PHE:CZ	1:F:271:LEU:HD23	2.41	0.54
2:G:166:ILE:HG12	2:G:197:THR:CG2	2.37	0.54
1:F:244:ILE:HD11	1:F:249:ARG:HD2	1.90	0.54
2:B:275:ASP:OD1	1:F:257:ARG:NE	2.35	0.54
2:G:98:LEU:HD23	2:G:143:PRO:HB3	1.90	0.54
4:I:99:PHE:N	4:I:99:PHE:CD1	2.75	0.54
1:A:13:PHE:O	1:A:22:ALA:N	2.39	0.53
4:D:72:MET:HB3	4:D:76:ILE:HD11	1.89	0.53
4:D:72:MET:C	4:D:76:ILE:HG12	2.28	0.53
4:I:109:GLY:O	4:I:112:VAL:HG22	2.08	0.53
3:C:74:SER:OG	8:C:503:CIT:O3	2.23	0.53
3:H:37:ILE:HB	3:H:38:LEU:HD22	1.90	0.53
1:A:14:THR:HG22	1:A:21:PRO:CA	2.38	0.53
7:G:901:LMT:H5B	7:G:901:LMT:H6D	1.89	0.53
5:J:108:VAL:O	5:J:109:LYS:HD2	2.09	0.53
5:E:17:SER:HB2	5:E:83:MET:O	2.09	0.53
2:G:66:ILE:HG22	2:G:87:VAL:HG21	1.90	0.53
3:H:77:ARG:HH11	3:H:77:ARG:HB3	1.74	0.53
4:I:142:MET:O	4:I:145:PRO:HD2	2.09	0.53
3:C:51:VAL:HG21	3:C:70:TRP:CE3	2.43	0.53
3:H:157:LYS:HB3	3:H:157:LYS:NZ	2.23	0.53
2:B:28:PHE:HB3	2:B:223:LEU:HD21	1.91	0.53
1:F:113:ARG:HG2	1:F:113:ARG:HH11	1.73	0.53
2:G:165:GLU:HG3	2:G:166:ILE:HG13	1.91	0.53
1:A:17:ASP:OD1	1:A:17:ASP:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:PRO:HG3	3:C:86:VAL:HG21	1.91	0.52
4:D:259:MET:O	4:D:263:ARG:HG3	2.08	0.52
7:I:301:LMT:H21	7:I:301:LMT:O2'	2.10	0.52
2:B:90:ALA:CB	2:B:169:LEU:HD23	2.40	0.52
1:F:214:LEU:HG	1:F:224:GLN:HG3	1.91	0.52
2:G:90:ALA:HB3	2:G:169:LEU:HD23	1.91	0.52
5:J:32:TYR:HB3	5:J:98:ALA:HB1	1.91	0.52
1:A:133:MET:HA	1:A:133:MET:CE	2.39	0.52
2:B:152:ARG:HD2	2:B:176:LEU:HD11	1.90	0.52
4:D:143:LEU:HD11	7:D:301:LMT:H41	1.90	0.52
3:H:87:THR:HG22	8:H:602:CIT:O6	2.09	0.52
1:A:271:LEU:HD23	2:G:252:PHE:CZ	2.45	0.52
2:B:93:PHE:HA	2:B:152:ARG:NH2	2.24	0.52
3:C:42:PRO:HD3	3:C:86:VAL:HG21	1.92	0.52
5:J:3:GLN:HG3	5:J:5:VAL:HG23	1.90	0.52
5:E:39:GLN:HB2	5:E:45:ARG:HG3	1.92	0.52
2:G:107:VAL:HB	2:G:125:ALA:HB1	1.92	0.52
5:J:102:TRP:CE3	5:J:106:CYS:HA	2.45	0.52
5:J:53:ARG:O	5:J:74:ARG:NH2	2.43	0.52
3:C:45:THR:OG1	3:C:48:PRO:HD3	2.10	0.52
5:E:99:THR:HG22	5:E:113:TYR:CD2	2.44	0.52
2:G:282:LYS:H	2:G:282:LYS:HD3	1.74	0.52
3:H:151:TYR:HB3	3:H:157:LYS:NZ	2.25	0.52
4:D:39:ASN:OD1	4:D:40:ASN:ND2	2.43	0.51
4:D:136:ALA:O	4:D:140:GLU:HG3	2.09	0.51
4:I:55:VAL:HG13	4:I:65:PHE:CE2	2.45	0.51
2:B:167:ILE:CG2	2:B:198:VAL:HG22	2.39	0.51
1:F:17:ASP:OD1	1:F:17:ASP:N	2.43	0.51
1:F:240:ILE:HD11	1:F:242:LEU:HD12	1.92	0.51
2:G:101:ASN:OD1	2:G:101:ASN:N	2.41	0.51
3:H:123:ARG:HE	3:H:123:ARG:HA	1.75	0.51
2:G:52:HIS:HB3	2:G:64:ILE:HD13	1.93	0.51
4:I:166:PHE:HE2	4:I:218:LEU:HD11	1.75	0.51
1:F:119:GLU:O	1:F:123:ILE:HG13	2.10	0.51
2:B:80:LEU:HD13	2:B:84:ARG:NH2	2.25	0.51
3:C:206:ARG:NH1	4:D:216:LEU:HD13	2.26	0.51
2:G:38:LEU:HD11	2:G:49:LEU:HD23	1.93	0.51
3:H:157:LYS:C	3:H:159:ALA:H	2.12	0.51
3:H:88:ILE:HD12	4:I:79:THR:HG21	1.93	0.51
4:D:32:ILE:HG13	4:D:33:ILE:N	2.25	0.51
4:I:144:THR:HB	4:I:147:LYS:HZ1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:248:ARG:NH1	2:G:251:ARG:HH11	1.98	0.51
1:A:279:ASN:HD22	2:G:261:LEU:HG	1.76	0.50
2:B:178:PRO:HG3	1:F:204:LEU:CD2	2.41	0.50
1:F:14:THR:HB	1:F:21:PRO:HA	1.93	0.50
1:A:79:VAL:O	1:A:83:ARG:HG3	2.12	0.50
1:A:279:ASN:ND2	2:G:261:LEU:HG	2.26	0.50
5:E:52:SER:O	5:E:55:GLY:N	2.39	0.50
1:F:115:VAL:HG12	1:F:120:MET:HG3	1.92	0.50
1:A:5:ILE:HG12	1:A:32:ARG:HA	1.92	0.50
4:D:77:VAL:HA	4:D:80:SER:OG	2.12	0.50
5:E:17:SER:HB2	5:E:84:ASN:HA	1.94	0.50
1:F:145:SER:OG	1:F:148:GLN:HG3	2.11	0.50
3:C:37:ILE:HD13	4:D:193:LEU:HD11	1.93	0.50
4:D:44:TYR:OH	4:D:115:ARG:NH1	2.45	0.50
5:E:64:VAL:HA	5:E:67:ARG:NH1	2.26	0.50
2:G:82:ASP:O	2:G:85:ARG:HG2	2.11	0.50
3:H:163:GLY:O	3:H:167:GLY:N	2.29	0.50
4:I:136:ALA:O	4:I:140:GLU:HG3	2.11	0.50
1:A:43:GLY:O	1:A:45:GLY:N	2.44	0.50
1:A:201:THR:OG1	1:A:202:HIS:N	2.44	0.50
2:B:24:ASP:N	2:B:221:GLY:O	2.39	0.50
3:C:154:HIS:O	3:C:156:GLN:N	2.45	0.50
1:F:239:ARG:C	1:F:239:ARG:HD3	2.32	0.50
7:I:301:LMT:O6B	7:I:301:LMT:O4'	2.22	0.50
2:G:9:SER:O	2:G:60:THR:OG1	2.25	0.49
2:G:117:SER:OG	2:G:118:GLU:N	2.45	0.49
5:E:88:PRO:HA	5:E:124:VAL:HG13	1.94	0.49
2:G:2:ALA:N	2:G:32:GLU:HG2	2.28	0.49
3:H:205:LYS:HG2	3:H:206:ARG:HD2	1.94	0.49
3:C:70:TRP:CD2	3:C:101:ARG:HG3	2.48	0.49
2:G:96:ALA:CB	4:I:177:ILE:HD11	2.42	0.49
3:H:35:ILE:HB	3:H:44:ILE:HD11	1.94	0.49
3:H:37:ILE:CD1	4:I:193:LEU:HD11	2.43	0.49
3:H:100:PRO:HB3	3:H:142:ILE:HG22	1.95	0.49
2:G:155:ALA:O	2:G:159:VAL:HG23	2.12	0.49
4:D:81:LEU:HA	4:D:84:THR:OG1	2.12	0.49
4:D:173:GLN:HG2	4:D:210:ASP:OD2	2.13	0.49
1:F:31:GLU:O	1:F:34:SER:OG	2.18	0.49
3:H:69:VAL:HG22	7:H:601:LMT:H101	1.95	0.49
5:E:12:VAL:O	5:E:124:VAL:HA	2.12	0.49
1:A:114:ALA:O	5:E:53:ARG:NH2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:TRP:HZ3	2:B:187:LEU:HD11	1.78	0.49
5:E:83:MET:HB3	5:E:86:LEU:HD21	1.94	0.49
4:I:32:ILE:HG12	4:I:119:ILE:HD13	1.93	0.49
4:I:219:SER:O	4:I:223:GLU:HG3	2.12	0.49
5:J:38:ARG:HG3	5:J:92:ALA:HB3	1.94	0.49
5:J:93:ASP:HB3	5:J:95:TYR:CE1	2.48	0.49
2:B:67:ALA:HB1	2:B:86:LYS:HD2	1.93	0.48
4:D:18:ARG:NH1	5:E:25:SER:HB2	2.28	0.48
2:B:11:VAL:HG23	2:B:12:TYR:O	2.13	0.48
1:F:158:LEU:HD13	1:F:189:ILE:HG23	1.95	0.48
3:H:44:ILE:HG22	3:H:185:GLU:HB2	1.95	0.48
5:J:12:VAL:O	5:J:124:VAL:HA	2.13	0.48
1:A:75:GLY:O	1:A:79:VAL:HG23	2.12	0.48
1:A:175:ASP:O	1:A:178:GLY:N	2.46	0.48
3:H:151:TYR:HB3	3:H:157:LYS:HZ3	1.78	0.48
4:I:171:PHE:O	4:I:175:VAL:HG23	2.13	0.48
5:E:36:TRP:CD1	5:E:81:LEU:HB2	2.48	0.48
3:H:159:ALA:O	3:H:160:LEU:HD23	2.13	0.48
1:A:203:ASP:HB3	1:A:206:GLU:HB2	1.95	0.48
2:B:100:GLU:HB2	2:B:106:ASP:HB2	1.95	0.48
2:B:128:TRP:CD1	2:B:161:ALA:HA	2.48	0.48
4:D:55:VAL:HG13	4:D:65:PHE:CE2	2.48	0.48
2:G:96:ALA:HB1	4:I:177:ILE:HD11	1.94	0.48
2:G:117:SER:N	2:G:120:GLU:HB2	2.28	0.48
2:G:100:GLU:HB2	2:G:106:ASP:HB2	1.96	0.48
4:D:146:LEU:HD13	7:D:301:LMT:H4'	1.95	0.48
5:E:51:ILE:HG13	5:E:70:ILE:HG23	1.95	0.48
1:A:113:ARG:HD3	5:E:101:VAL:O	2.14	0.48
2:B:150:GLN:O	2:B:154:VAL:HG23	2.13	0.48
5:E:86:LEU:HD23	5:E:86:LEU:HA	1.61	0.48
2:G:229:PRO:HA	2:G:232:VAL:HG12	1.96	0.48
3:H:89:LEU:CD2	3:H:159:ALA:HB1	2.42	0.48
4:D:194:VAL:HG23	4:D:195:LYS:H	1.79	0.48
5:E:90:ASP:O	5:E:94:TYR:OH	2.21	0.48
1:F:70:ASP:HB3	1:F:85:LYS:HD3	1.96	0.48
2:G:147:SER:O	2:G:151:MET:HG3	2.14	0.48
5:J:67:ARG:HH21	5:J:87:LYS:HG3	1.78	0.48
2:B:31:GLU:OE1	2:B:31:GLU:N	2.42	0.47
3:C:86:VAL:HG13	3:C:174:LEU:HD13	1.95	0.47
3:C:204:LEU:HD23	3:C:204:LEU:O	2.14	0.47
1:F:185:LEU:O	1:F:189:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:28:PHE:HE2	2:G:30:LEU:HG	1.77	0.47
1:A:164:VAL:HG21	1:A:198:ILE:HD13	1.96	0.47
1:A:185:LEU:O	1:A:189:ILE:HG13	2.14	0.47
1:A:231:PHE:N	1:A:232:PRO:HD2	2.30	0.47
2:B:28:PHE:HE2	2:B:30:LEU:HG	1.79	0.47
4:D:166:PHE:HE2	4:D:218:LEU:HD11	1.78	0.47
3:H:157:LYS:HB3	3:H:157:LYS:HZ3	1.78	0.47
3:H:162:LEU:HD23	4:I:87:MET:HA	1.96	0.47
4:I:194:VAL:HG23	4:I:195:LYS:H	1.78	0.47
2:G:128:TRP:CD1	2:G:161:ALA:HA	2.48	0.47
3:H:19:PHE:HE2	3:H:57:LEU:HD12	1.79	0.47
1:A:64:LYS:HA	1:A:64:LYS:HD3	1.59	0.47
4:I:80:SER:O	4:I:84:THR:HG23	2.14	0.47
3:H:154:HIS:C	3:H:156:GLN:H	2.16	0.47
4:D:74:TRP:HA	4:D:74:TRP:HE3	1.76	0.47
2:G:93:PHE:HA	2:G:152:ARG:NH2	2.30	0.47
3:H:118:TRP:CZ3	3:H:127:ALA:HB2	2.49	0.47
4:I:76:ILE:HD12	4:I:116:PHE:CD2	2.48	0.47
5:E:38:ARG:HG3	5:E:92:ALA:HB3	1.96	0.47
2:G:99:PHE:CZ	4:I:202:PRO:HG3	2.50	0.47
4:I:44:TYR:HD2	4:I:114:ILE:HD12	1.80	0.47
4:I:177:ILE:HD13	4:I:177:ILE:HA	1.74	0.47
5:J:68:PHE:HA	5:J:82:GLN:O	2.15	0.47
5:J:86:LEU:HA	5:J:86:LEU:HD23	1.64	0.47
5:E:45:ARG:HD2	1:F:135:ASP:OD2	2.14	0.47
4:D:236:TYR:HD1	1:F:120:MET:HE2	1.78	0.47
4:I:8:ARG:HD2	4:I:8:ARG:HA	1.41	0.47
5:J:20:LEU:HD11	5:J:122:VAL:HG21	1.97	0.47
2:G:8:VAL:O	2:G:26:LEU:HB2	2.15	0.46
3:H:33:GLY:O	3:H:35:ILE:HG12	2.15	0.46
1:A:102:VAL:HG21	1:A:136:TYR:O	2.15	0.46
1:A:165:ILE:O	1:A:197:VAL:HA	2.15	0.46
2:G:86:LYS:HD3	2:G:165:GLU:OE1	2.14	0.46
3:H:106:TRP:CZ2	3:H:110:LEU:HD11	2.50	0.46
2:B:96:ALA:HB1	4:D:177:ILE:HD11	1.98	0.46
4:D:155:MET:O	4:D:159:VAL:HG23	2.14	0.46
1:F:69:VAL:HG11	1:F:86:VAL:CG2	2.46	0.46
5:J:97:ALA:HB1	5:J:113:TYR:HB3	1.97	0.46
5:E:23:THR:HG22	5:E:24:ALA:O	2.16	0.46
1:A:257:ARG:HB3	2:G:278:LYS:HD3	1.97	0.46
4:D:177:ILE:HD13	4:D:206:PRO:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:65:ALA:CB	7:H:601:LMT:H32	2.45	0.46
3:H:171:LEU:HG	3:H:175:PHE:CE1	2.51	0.46
3:C:65:ALA:CB	7:C:501:LMT:H22	2.46	0.46
1:F:106:VAL:HG13	1:F:156:GLY:HA2	1.98	0.46
7:G:901:LMT:H11	7:G:901:LMT:H42	1.67	0.46
3:H:160:LEU:HD22	4:I:83:GLN:HA	1.97	0.46
1:A:144:LEU:O	1:A:149:LYS:NZ	2.46	0.46
3:C:85:LEU:HD11	3:C:160:LEU:HD21	1.98	0.46
3:C:184:LEU:HD23	3:C:184:LEU:HA	1.71	0.46
4:D:194:VAL:HG23	4:D:195:LYS:N	2.31	0.46
5:E:97:ALA:HB1	5:E:113:TYR:HB3	1.96	0.46
4:I:75:MET:O	4:I:75:MET:HG3	2.15	0.46
5:J:83:MET:HE2	5:J:86:LEU:HD21	1.98	0.46
2:B:127:LYS:O	2:B:130:LYS:HG3	2.15	0.46
2:B:278:LYS:HD3	1:F:259:ILE:HD11	1.97	0.46
2:G:100:GLU:HG3	2:G:106:ASP:HA	1.97	0.46
3:H:22:ILE:O	3:H:26:GLU:HG3	2.16	0.46
1:F:74:LEU:HD22	1:F:82:VAL:HG11	1.97	0.45
4:D:37:LEU:HB3	4:D:263:ARG:NH1	2.31	0.45
4:D:85:PHE:CB	4:D:89:GLY:HA2	2.46	0.45
5:E:65:LYS:HB2	5:E:65:LYS:HE3	1.75	0.45
3:C:85:LEU:O	3:C:89:LEU:HD13	2.16	0.45
2:G:50:MET:HE2	2:G:50:MET:HB2	1.79	0.45
1:A:79:VAL:HG21	3:H:2:TYR:HB3	1.98	0.45
2:G:66:ILE:CG2	2:G:87:VAL:HG21	2.46	0.45
3:H:157:LYS:HG3	3:H:159:ALA:HB3	1.98	0.45
4:I:173:GLN:HG2	4:I:210:ASP:OD2	2.16	0.45
1:A:5:ILE:HG23	1:A:32:ARG:CZ	2.47	0.45
4:D:219:SER:O	4:D:223:GLU:HG3	2.17	0.45
4:I:228:LYS:HE2	4:I:228:LYS:HB3	1.68	0.45
1:A:126:GLN:NE2	1:F:126:GLN:HG3	2.31	0.45
4:I:197:ALA:O	4:I:200:VAL:HG22	2.17	0.45
1:A:12:THR:CG2	1:A:25:ASP:H	2.17	0.45
3:C:61:LYS:HG2	6:C:504:PEG:H12	1.98	0.45
4:D:80:SER:O	4:D:84:THR:HG23	2.16	0.45
1:F:54:ASN:OD1	1:F:56:LEU:HG	2.16	0.45
1:F:174:LEU:HA	1:F:174:LEU:HD23	1.67	0.45
5:E:48:ILE:HG13	5:E:48:ILE:H	1.64	0.45
5:E:68:PHE:CD1	5:E:68:PHE:N	2.83	0.45
1:A:14:THR:HG23	1:A:60:ASP:OD2	2.17	0.45
2:B:230:LYS:HA	2:B:268:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:144:THR:N	4:D:145:PRO:HD2	2.32	0.45
4:D:218:LEU:HA	4:D:218:LEU:HD23	1.73	0.45
3:H:42:PRO:CD	3:H:86:VAL:HG21	2.44	0.45
4:I:31:PHE:O	4:I:35:ILE:HG13	2.17	0.45
4:I:177:ILE:O	4:I:181:GLN:HG2	2.17	0.45
1:A:13:PHE:CZ	1:A:57:LEU:HD13	2.51	0.45
3:C:31:ASN:ND2	3:C:46:THR:OG1	2.50	0.45
4:I:99:PHE:HD2	4:I:102:SER:HG	1.63	0.45
1:A:244:ILE:HD11	1:A:249:ARG:HD3	1.98	0.44
1:F:81:GLU:HG3	5:J:105:SER:HB3	1.99	0.44
2:G:26:LEU:HA	2:G:26:LEU:HD23	1.71	0.44
3:H:68:LEU:HD12	3:H:98:LEU:HD22	1.99	0.44
2:G:53:PHE:HA	2:G:66:ILE:CD1	2.48	0.44
3:H:65:ALA:O	3:H:69:VAL:HG23	2.17	0.44
3:H:157:LYS:H	3:H:157:LYS:HG2	1.53	0.44
2:B:100:GLU:HG3	2:B:106:ASP:HA	1.98	0.44
2:G:106:ASP:CG	4:I:184:ARG:HH22	2.20	0.44
4:I:50:PHE:CE1	4:I:258:LEU:HD12	2.52	0.44
4:I:150:LYS:H	4:I:150:LYS:CD	2.30	0.44
4:D:147:LYS:HG3	4:D:153:VAL:HG12	2.00	0.44
2:G:38:LEU:HB3	2:G:201:VAL:HG13	1.99	0.44
4:I:194:VAL:HG23	4:I:195:LYS:N	2.33	0.44
1:A:131:VAL:HG12	1:A:185:LEU:HD21	2.00	0.44
1:A:160:VAL:O	1:A:160:VAL:CG1	2.66	0.44
2:B:28:PHE:CE2	2:B:216:LEU:HD11	2.52	0.44
4:D:258:LEU:O	4:D:262:THR:HG22	2.17	0.44
2:G:50:MET:HE1	2:G:170:ASP:HB2	1.99	0.44
1:A:12:THR:HG22	1:A:25:ASP:N	2.18	0.44
2:G:142:SER:HB3	3:H:202:LYS:HD2	1.99	0.44
4:I:72:MET:O	4:I:76:ILE:HG12	2.18	0.44
4:I:147:LYS:HE3	4:I:153:VAL:CG2	2.48	0.44
1:F:41:HIS:CD2	1:F:42:ASN:H	2.35	0.44
2:G:51:GLN:HB3	2:G:56:LEU:HB2	2.00	0.44
2:G:129:LEU:HD23	2:G:129:LEU:HA	1.83	0.44
4:I:50:PHE:CZ	4:I:254:LEU:HB3	2.52	0.44
6:J:201:PEG:H41	6:J:201:PEG:H22	1.75	0.44
3:C:23:LEU:HD21	3:C:70:TRP:HA	2.00	0.44
1:F:41:HIS:CG	1:F:42:ASN:H	2.35	0.44
2:G:94:SER:O	2:G:97:GLN:HG3	2.18	0.44
3:H:203:ARG:HD2	3:H:203:ARG:HA	1.65	0.44
2:B:92:GLN:HG3	2:B:171:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:LEU:HD23	3:C:24:LEU:HA	1.77	0.43
5:E:91:THR:HG23	5:E:123:THR:HA	1.98	0.43
5:E:91:THR:OG1	5:E:124:VAL:HG12	2.18	0.43
1:F:14:THR:HG22	1:F:60:ASP:OD2	2.18	0.43
3:H:25:LEU:O	3:H:29:ILE:HB	2.18	0.43
5:J:45:ARG:HG3	5:J:110:VAL:HG21	1.99	0.43
1:A:35:TRP:CD1	1:A:35:TRP:C	2.91	0.43
1:A:158:LEU:HD13	1:A:189:ILE:HG23	2.00	0.43
2:B:86:LYS:HD3	2:B:165:GLU:OE1	2.18	0.43
2:B:184:MET:HG3	2:B:188:PHE:CE2	2.52	0.43
4:D:171:PHE:O	4:D:175:VAL:HG23	2.18	0.43
2:G:10:TYR:H	2:G:23:LEU:HB2	1.82	0.43
2:G:90:ALA:CB	2:G:169:LEU:HD23	2.48	0.43
3:H:204:LEU:HD23	3:H:204:LEU:O	2.18	0.43
4:I:147:LYS:HE3	4:I:153:VAL:HG22	2.00	0.43
1:A:70:ASP:HB3	1:A:85:LYS:HD3	1.99	0.43
2:B:72:THR:N	2:B:75:THR:HG1	2.14	0.43
2:B:109:TYR:HD2	4:D:184:ARG:HD3	1.84	0.43
2:B:278:LYS:HD3	1:F:259:ILE:CG1	2.49	0.43
1:A:97:PHE:CE1	1:A:105:ASP:HB2	2.53	0.43
2:B:155:ALA:O	2:B:159:VAL:HG23	2.19	0.43
3:C:89:LEU:HD11	3:C:160:LEU:HD21	2.01	0.43
3:C:204:LEU:HD12	4:D:212:LEU:HD21	2.00	0.43
5:E:49:SER:O	5:E:50:CYS:HB3	2.18	0.43
1:F:14:THR:CB	1:F:21:PRO:HA	2.49	0.43
2:G:247:PRO:HG2	2:G:268:LEU:HD22	2.00	0.43
4:I:32:ILE:HD11	4:I:119:ILE:HG23	2.00	0.43
2:B:166:ILE:HG12	2:B:197:THR:CG2	2.49	0.43
3:C:126:LEU:HA	3:C:126:LEU:HD23	1.75	0.43
4:I:158:LEU:HA	4:I:158:LEU:HD23	1.70	0.43
1:A:46:LYS:HB2	1:A:200:ILE:HG23	2.00	0.43
2:B:173:ALA:HA	2:B:176:LEU:HD13	2.01	0.43
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.86	0.43
3:C:87:THR:HA	3:C:91:PHE:HD2	1.84	0.43
3:C:171:LEU:HD23	3:C:171:LEU:HA	1.76	0.43
5:J:51:ILE:CD1	5:J:72:ARG:HG3	2.45	0.43
1:A:69:VAL:HG11	1:A:86:VAL:CG2	2.49	0.43
5:J:43:LYS:HB3	5:J:43:LYS:HE2	1.88	0.43
1:A:9:ASP:HB2	1:A:66:SER:O	2.18	0.43
1:A:145:SER:O	1:A:149:LYS:HG3	2.19	0.43
2:B:152:ARG:NH1	2:B:174:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:VAL:HG21	3:H:70:TRP:CE3	2.53	0.43
1:A:48:THR:HG22	1:A:52:LEU:HD12	2.00	0.43
1:A:215:VAL:O	1:A:221:LEU:HD12	2.19	0.43
3:C:31:ASN:OD1	3:C:31:ASN:N	2.51	0.43
4:D:137:ASP:HB3	4:D:239:LEU:HD11	2.01	0.43
1:F:54:ASN:OD1	1:F:54:ASN:C	2.57	0.43
1:F:74:LEU:HD12	1:F:75:GLY:N	2.34	0.43
2:G:34:LYS:HA	2:G:192:GLN:HE21	1.84	0.43
4:I:32:ILE:HA	4:I:35:ILE:HD12	2.01	0.43
2:B:103:VAL:O	2:B:107:VAL:HG23	2.19	0.43
4:D:260:ILE:HD12	4:D:260:ILE:HA	1.69	0.43
1:F:278:LEU:O	1:F:279:ASN:HB2	2.18	0.43
2:G:105:LYS:HZ1	7:G:901:LMT:H21	1.83	0.43
3:H:153:ILE:HG22	3:H:154:HIS:CD2	2.54	0.43
3:H:160:LEU:HD12	3:H:162:LEU:HD11	2.01	0.43
4:I:25:LEU:HD12	4:I:25:LEU:HA	1.74	0.43
4:I:144:THR:OG1	4:I:145:PRO:HD3	2.19	0.43
1:F:79:VAL:O	1:F:83:ARG:HG3	2.18	0.42
4:D:31:PHE:CE1	4:D:35:ILE:HD11	2.54	0.42
2:G:28:PHE:CE2	2:G:216:LEU:HD21	2.54	0.42
2:G:72:THR:N	2:G:75:THR:HG1	2.16	0.42
3:H:151:TYR:CE1	3:H:157:LYS:HA	2.53	0.42
3:C:136:SER:OG	3:C:185:GLU:HB3	2.18	0.42
4:D:40:ASN:ND2	4:D:263:ARG:HA	2.24	0.42
4:D:72:MET:HB3	4:D:76:ILE:CD1	2.49	0.42
1:F:136:TYR:HB3	1:F:139:SER:HB2	2.01	0.42
1:A:133:MET:HE1	1:A:148:GLN:HE21	1.84	0.42
3:C:41:LEU:HB3	3:C:42:PRO:CD	2.49	0.42
4:D:66:TRP:O	4:D:70:LYS:HG2	2.20	0.42
5:E:53:ARG:HB2	5:E:103:TYR:HA	2.01	0.42
1:F:84:GLU:HG2	1:F:113:ARG:HH12	1.82	0.42
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.83	0.42
4:D:245:ASP:O	4:D:248:PRO:HD2	2.19	0.42
7:D:301:LMT:H1B	7:D:301:LMT:H3'	1.60	0.42
1:F:64:LYS:HA	1:F:64:LYS:HD3	1.83	0.42
1:F:144:LEU:HA	1:F:144:LEU:HD12	1.81	0.42
2:G:50:MET:HE2	2:G:201:VAL:HG21	2.02	0.42
5:J:53:ARG:HB2	5:J:103:TYR:HA	2.02	0.42
2:B:28:PHE:HB3	2:B:223:LEU:CD2	2.48	0.42
3:C:114:LEU:O	3:C:117:LYS:N	2.52	0.42
5:E:36:TRP:CG	5:E:81:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:209:ILE:HD13	4:I:209:ILE:HA	1.94	0.42
3:C:49:LEU:HD12	3:C:193:THR:OG1	2.19	0.42
2:G:230:LYS:HD2	2:G:266:GLN:OE1	2.19	0.42
3:H:49:LEU:HD12	3:H:193:THR:OG1	2.19	0.42
4:D:7:GLY:O	4:D:9:TYR:N	2.52	0.42
1:F:74:LEU:HD13	1:F:82:VAL:HG21	2.02	0.42
3:H:106:TRP:CE2	3:H:110:LEU:HD11	2.55	0.42
3:C:162:LEU:HD23	3:C:162:LEU:HA	1.77	0.42
3:C:183:ILE:O	3:C:187:VAL:HG13	2.20	0.42
4:D:160:ILE:O	4:D:164:LEU:HD13	2.19	0.42
1:F:273:GLN:O	1:F:276:TRP:HB3	2.20	0.42
4:I:16:VAL:HG21	4:I:58:THR:HG22	2.01	0.42
2:B:38:LEU:HB2	2:B:201:VAL:HG22	2.02	0.42
4:D:85:PHE:HB3	4:D:89:GLY:HA2	2.02	0.42
5:E:94:TYR:O	5:E:119:GLY:HA2	2.20	0.42
2:G:111:PRO:HD3	2:G:162:TYR:HD1	1.85	0.42
3:H:38:LEU:HB3	3:H:41:LEU:HD13	2.02	0.42
3:H:93:ASN:HD21	7:H:603:LMT:H32	1.84	0.42
5:J:14:PRO:HB3	5:J:88:PRO:HD3	2.02	0.42
1:A:259:ILE:HD11	2:G:278:LYS:HA	2.01	0.41
2:B:38:LEU:HD12	2:B:216:LEU:HB2	2.01	0.41
3:C:33:GLY:O	3:C:35:ILE:HG12	2.20	0.41
3:C:123:ARG:O	3:C:126:LEU:HB2	2.20	0.41
3:C:137:ALA:O	3:C:141:LEU:HG	2.20	0.41
3:C:153:ILE:HG22	3:C:154:HIS:CD2	2.55	0.41
1:F:131:VAL:HG12	1:F:185:LEU:HD21	2.02	0.41
1:F:222:LEU:HD22	1:F:240:ILE:HG21	2.02	0.41
2:G:249:SER:OG	2:G:270:MET:HG2	2.20	0.41
3:H:171:LEU:HD12	3:H:171:LEU:HA	1.80	0.41
1:A:19:PRO:HG2	1:A:20:ARG:HG2	2.01	0.41
1:A:276:TRP:CE3	2:G:259:ALA:HB1	2.55	0.41
4:D:66:TRP:HE1	4:D:70:LYS:HD3	1.85	0.41
1:F:278:LEU:HA	1:F:278:LEU:HD23	1.71	0.41
4:I:248:PRO:O	4:I:251:TYR:HB3	2.20	0.41
1:A:135:ASP:HB3	5:J:45:ARG:NH1	2.35	0.41
5:E:67:ARG:HH21	5:E:87:LYS:HG3	1.84	0.41
2:B:269:THR:HG22	2:B:272:GLU:CG	2.50	0.41
3:C:37:ILE:HD12	3:C:37:ILE:HA	1.91	0.41
2:G:59:PRO:HD3	2:G:64:ILE:HD12	2.02	0.41
2:G:166:ILE:HG12	2:G:197:THR:HG23	2.01	0.41
2:G:184:MET:HG3	2:G:188:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:THR:HG22	3:C:43:ALA:CB	2.50	0.41
4:D:109:GLY:O	4:D:112:VAL:HG23	2.20	0.41
1:F:41:HIS:CG	1:F:42:ASN:N	2.88	0.41
1:F:120:MET:HE3	1:F:120:MET:HB3	1.91	0.41
1:F:158:LEU:HD13	1:F:189:ILE:HD12	2.01	0.41
2:B:269:THR:HG23	2:B:271:PRO:HD2	2.03	0.41
2:B:21:ILE:CD1	2:B:43:GLY:HA2	2.51	0.41
2:B:111:PRO:HD3	2:B:162:TYR:HD1	1.86	0.41
3:C:65:ALA:O	3:C:69:VAL:HG23	2.21	0.41
3:C:200:LEU:HD23	4:D:209:ILE:HD13	2.03	0.41
5:E:4:LEU:HD22	5:E:22:CYS:SG	2.60	0.41
5:E:45:ARG:NH2	5:E:95:TYR:CE2	2.89	0.41
2:G:18:LEU:HG	5:J:121:GLN:CD	2.40	0.41
3:C:42:PRO:CD	3:C:86:VAL:HG21	2.50	0.41
2:G:54:ASN:HB2	2:G:89:LEU:HD13	2.02	0.41
4:I:70:LYS:N	4:I:71:PRO:HD2	2.35	0.41
1:A:237:LEU:HB3	1:A:242:LEU:HB2	2.03	0.41
2:B:16:SER:HB3	2:B:17:PRO:HD2	2.02	0.41
2:B:269:THR:HG22	2:B:272:GLU:HG3	2.02	0.41
5:E:67:ARG:HG2	5:E:85:SER:HB2	2.03	0.41
1:F:166:ILE:HA	1:F:198:ILE:O	2.21	0.41
2:G:52:HIS:HB3	2:G:64:ILE:CD1	2.50	0.41
2:G:227:ALA:CB	2:G:231:GLU:HG2	2.51	0.41
3:H:35:ILE:O	3:H:44:ILE:HG13	2.21	0.41
3:H:99:LEU:N	3:H:100:PRO:HD2	2.35	0.41
3:H:124:LYS:HB2	3:H:125:PRO:HD3	2.02	0.41
3:H:158:LEU:HD23	3:H:158:LEU:HA	1.79	0.41
7:H:603:LMT:H12	7:H:603:LMT:H41	1.91	0.41
5:E:29:LEU:HD13	5:E:79:VAL:HG23	2.03	0.41
4:I:167:VAL:N	4:I:168:PRO:CD	2.84	0.41
3:C:106:TRP:CE2	3:C:110:LEU:HD11	2.55	0.40
1:F:122:LYS:HE3	1:F:122:LYS:HB3	1.80	0.40
3:H:204:LEU:HD12	4:I:212:LEU:HD11	2.03	0.40
5:J:40:ALA:HB1	5:J:41:PRO:HD2	2.03	0.40
1:A:232:PRO:O	1:A:234:VAL:HG23	2.21	0.40
2:B:269:THR:CG2	2:B:272:GLU:H	2.34	0.40
3:C:36:THR:HG22	3:C:43:ALA:HB2	2.03	0.40
2:G:150:GLN:O	2:G:154:VAL:HG23	2.21	0.40
1:A:193:ASN:HB2	1:A:195:LEU:HG	2.03	0.40
3:C:163:GLY:O	3:C:167:GLY:N	2.38	0.40
4:D:26:LEU:CD2	4:D:142:MET:HE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:144:THR:HA	4:I:153:VAL:HG11	2.04	0.40
4:I:258:LEU:HD23	4:I:258:LEU:HA	1.74	0.40
1:A:117:ARG:N	1:A:118:PRO:HD2	2.37	0.40
2:B:117:SER:N	2:B:120:GLU:HB2	2.35	0.40
3:C:149:LEU:HD21	7:C:502:LMT:H11	2.03	0.40
2:G:63:LYS:HG2	2:G:72:THR:HG22	2.04	0.40
2:G:99:PHE:CE2	4:I:202:PRO:HG3	2.57	0.40
5:J:24:ALA:HB1	5:J:27:PHE:CE1	2.56	0.40
3:C:93:ASN:OD1	3:C:95:LEU:HB2	2.22	0.40
1:F:251:LYS:HZ3	1:F:251:LYS:HB2	1.87	0.40
2:G:64:ILE:HB	2:G:71:ILE:HB	2.03	0.40
3:H:70:TRP:CD2	3:H:101:ARG:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/300 (93%)	264 (95%)	12 (4%)	2 (1%)	22	53
1	F	277/300 (92%)	264 (95%)	12 (4%)	1 (0%)	34	66
2	B	280/287 (98%)	269 (96%)	10 (4%)	1 (0%)	34	66
2	G	281/287 (98%)	274 (98%)	7 (2%)	0	100	100
3	C	205/215 (95%)	198 (97%)	6 (3%)	1 (0%)	29	61
3	H	205/215 (95%)	199 (97%)	6 (3%)	0	100	100
4	D	259/265 (98%)	245 (95%)	11 (4%)	3 (1%)	13	39
4	I	258/265 (97%)	242 (94%)	15 (6%)	1 (0%)	34	66
5	E	124/136 (91%)	118 (95%)	5 (4%)	1 (1%)	19	49
5	J	123/136 (90%)	119 (97%)	4 (3%)	0	100	100
All	All	2290/2406 (95%)	2192 (96%)	88 (4%)	10 (0%)	34	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	SER
5	E	3	GLN
1	F	44	SER
2	B	260	GLY
4	D	8	ARG
4	D	264	LYS
1	A	42	ASN
4	D	88	ALA
4	I	94	TRP
3	C	39	PRO

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	240/259 (93%)	223 (93%)	17 (7%)	14	39
1	F	240/259 (93%)	223 (93%)	17 (7%)	14	39
2	B	230/234 (98%)	220 (96%)	10 (4%)	29	62
2	G	231/234 (99%)	219 (95%)	12 (5%)	23	55
3	C	162/170 (95%)	149 (92%)	13 (8%)	12	34
3	H	162/170 (95%)	147 (91%)	15 (9%)	9	26
4	D	229/233 (98%)	196 (86%)	33 (14%)	3	10
4	I	228/233 (98%)	199 (87%)	29 (13%)	4	14
5	E	103/112 (92%)	94 (91%)	9 (9%)	10	30
5	J	102/112 (91%)	96 (94%)	6 (6%)	19	49
All	All	1927/2016 (96%)	1766 (92%)	161 (8%)	11	31

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	36	THR

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Mol	Chain	Res	Type
1	A	46	LYS
1	A	54	ASN
1	A	64	LYS
1	A	65	SER
1	A	77	ASP
1	A	97	PHE
1	A	98	VAL
1	A	122	LYS
1	A	135	ASP
1	A	144	LEU
1	A	145	SER
1	A	164	VAL
1	A	175	ASP
1	A	200	ILE
1	A	206	GLU
2	B	38	LEU
2	B	47	SER
2	B	50	MET
2	B	74	GLU
2	B	101	ASN
2	B	130	LYS
2	B	159	VAL
2	B	189	LYS
2	B	231	GLU
2	B	282	LYS
3	C	1	MET
3	C	2	TYR
3	C	32	VAL
3	C	61	LYS
3	C	68	LEU
3	C	90	LEU
3	C	101	ARG
3	C	116	ASP
3	C	136	SER
3	C	157	LYS
3	C	174	LEU
3	C	202	LYS
3	C	206	ARG
4	D	9	TYR
4	D	15	PHE
4	D	28	THR
4	D	54[A]	TYR

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Mol	Chain	Res	Type
4	D	54[B]	TYR
4	D	61	LYS
4	D	70	LYS
4	D	74	TRP
4	D	75	MET
4	D	79	THR
4	D	87	MET
4	D	91	LYS
4	D	99	PHE
4	D	104	GLU
4	D	106	LEU
4	D	112	VAL
4	D	113	PHE
4	D	119	ILE
4	D	131	LYS
4	D	151	VAL
4	D	155	MET
4	D	164	LEU
4	D	165	ARG
4	D	195	LYS
4	D	198	LYS
4	D	200	VAL
4	D	204	LEU
4	D	219	SER
4	D	220	THR
4	D	233	ARG
4	D	243	LYS
4	D	260	ILE
4	D	263	ARG
5	E	1	GLN
5	E	2	VAL
5	E	7	SER
5	E	48	ILE
5	E	63	SER
5	E	67	ARG
5	E	74	ARG
5	E	93	ASP
5	E	99	THR
1	F	8	PHE
1	F	36	THR
1	F	44	SER
1	F	46	LYS

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Mol	Chain	Res	Type
1	F	54	ASN
1	F	64	LYS
1	F	66	SER
1	F	77	ASP
1	F	94	ASP
1	F	97	PHE
1	F	144	LEU
1	F	145	SER
1	F	164	VAL
1	F	175	ASP
1	F	228	GLU
1	F	239	ARG
1	F	251	LYS
2	G	50	MET
2	G	54	ASN
2	G	101	ASN
2	G	146	LEU
2	G	159	VAL
2	G	190	ASP
2	G	197	THR
2	G	216	LEU
2	G	261	LEU
2	G	266	GLN
2	G	269	THR
2	G	282	LYS
3	H	3	ASP
3	H	37	ILE
3	H	46	THR
3	H	61	LYS
3	H	77	ARG
3	H	83	ASN
3	H	89	LEU
3	H	123	ARG
3	H	136	SER
3	H	157	LYS
3	H	195	LEU
3	H	203	ARG
3	H	205	LYS
3	H	206	ARG
3	H	207	ARG
4	I	8	ARG
4	I	10	LEU

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Mol	Chain	Res	Type
4	I	15	PHE
4	I	28	THR
4	I	40	ASN
4	I	47	ILE
4	I	61	LYS
4	I	63	ARG
4	I	74	TRP
4	I	75	MET
4	I	83	GLN
4	I	87	MET
4	I	92	VAL
4	I	99	PHE
4	I	113	PHE
4	I	119	ILE
4	I	127	THR
4	I	129	THR
4	I	131	LYS
4	I	147	LYS
4	I	150	LYS
4	I	155	MET
4	I	165	ARG
4	I	198	LYS
4	I	220	THR
4	I	228	LYS
4	I	237	ARG
4	I	263	ARG
4	I	264	LYS
5	J	7	SER
5	J	18	LEU
5	J	20	LEU
5	J	63	SER
5	J	69	THR
5	J	93	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	40	ASN
1	F	41	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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	LMT	D	301	-	36,36,36	1.14	3 (8%)	47,47,47	1.15	5 (10%)
6	PEG	J	201	-	6,6,6	0.50	0	5,5,5	0.52	0
6	PEG	C	505	-	6,6,6	0.50	0	5,5,5	0.26	0
7	LMT	H	601	-	36,36,36	1.07	1 (2%)	47,47,47	1.24	8 (17%)
6	PEG	B	301	-	6,6,6	0.51	0	5,5,5	0.38	0
7	LMT	H	603	-	36,36,36	1.05	3 (8%)	47,47,47	1.86	13 (27%)
6	PEG	A	301	-	6,6,6	0.57	0	5,5,5	0.40	0
6	PEG	E	201	-	6,6,6	0.49	0	5,5,5	0.40	0
6	PEG	C	506	-	6,6,6	0.51	0	5,5,5	0.38	0
6	PEG	C	504	-	6,6,6	0.51	0	5,5,5	0.24	0
6	PEG	D	302	-	6,6,6	0.50	0	5,5,5	0.29	0
7	LMT	C	502	-	36,36,36	1.09	4 (11%)	47,47,47	1.09	3 (6%)
6	PEG	I	302	-	6,6,6	0.49	0	5,5,5	0.35	0
7	LMT	G	901	-	36,36,36	1.09	4 (11%)	47,47,47	1.29	6 (12%)
7	LMT	C	501	-	33,33,36	1.11	2 (6%)	44,44,47	1.10	4 (9%)
8	CIT	H	602	-	12,12,12	1.06	0	17,17,17	1.88	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CIT	C	503	-	12,12,12	1.13	0	17,17,17	1.47	2 (11%)
6	PEG	D	303	-	6,6,6	0.64	0	5,5,5	0.67	0
7	LMT	I	301	-	36,36,36	1.10	2 (5%)	47,47,47	1.59	10 (21%)

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	LMT	D	301	-	-	11/21/61/61	0/2/2/2
6	PEG	J	201	-	-	2/4/4/4	-
6	PEG	C	505	-	-	2/4/4/4	-
7	LMT	H	601	-	-	14/21/61/61	0/2/2/2
6	PEG	B	301	-	-	3/4/4/4	-
7	LMT	H	603	-	-	9/21/61/61	0/2/2/2
6	PEG	A	301	-	-	1/4/4/4	-
6	PEG	E	201	-	-	0/4/4/4	-
6	PEG	C	506	-	-	1/4/4/4	-
6	PEG	C	504	-	-	3/4/4/4	-
6	PEG	D	302	-	-	2/4/4/4	-
7	LMT	C	502	-	-	11/21/61/61	0/2/2/2
6	PEG	I	302	-	-	3/4/4/4	-
7	LMT	G	901	-	-	14/21/61/61	0/2/2/2
7	LMT	C	501	-	-	8/18/58/61	0/2/2/2
8	CIT	H	602	-	-	11/16/16/16	-
8	CIT	C	503	-	-	12/16/16/16	-
6	PEG	D	303	-	-	2/4/4/4	-
7	LMT	I	301	-	-	16/21/61/61	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	301	LMT	C4'-C5'	2.77	1.60	1.52
7	C	501	LMT	O3'-C3'	-2.52	1.37	1.43
7	H	603	LMT	O3'-C3'	-2.51	1.37	1.43
7	D	301	LMT	O3'-C3'	-2.47	1.37	1.43
7	I	301	LMT	C1B-C2B	2.39	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	301	LMT	C1B-C2B	2.32	1.59	1.52
7	C	502	LMT	C3'-C2'	2.30	1.58	1.52
7	H	603	LMT	O5'-C1'	2.28	1.47	1.41
7	C	502	LMT	O2B-C2B	-2.26	1.37	1.43
7	G	901	LMT	O3'-C3'	-2.26	1.37	1.43
7	C	502	LMT	O3'-C3'	-2.25	1.37	1.43
7	G	901	LMT	C3B-C2B	2.24	1.58	1.52
7	H	603	LMT	O2B-C2B	-2.22	1.37	1.43
7	G	901	LMT	C4'-C5'	2.20	1.58	1.52
7	D	301	LMT	C4B-C3B	2.11	1.57	1.52
7	H	601	LMT	O3B-C3B	-2.10	1.38	1.43
7	G	901	LMT	C4B-C3B	2.09	1.57	1.52
7	C	502	LMT	O4'-C4B	-2.03	1.38	1.43
7	C	501	LMT	C4B-C5B	2.00	1.57	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	603	LMT	O5B-C5B-C4B	5.60	119.86	109.69
7	H	603	LMT	C3'-C4'-C5'	-5.22	98.95	110.93
7	I	301	LMT	O1'-C1'-C2'	4.09	114.69	108.30
8	C	503	CIT	O6-C6-C3	4.03	120.05	113.05
8	H	602	CIT	O6-C6-C3	3.97	119.94	113.05
7	G	901	LMT	O1'-C1'-C2'	3.75	114.15	108.30
7	I	301	LMT	O5'-C5'-C4'	3.73	117.61	109.75
7	I	301	LMT	O5'-C1'-C2'	-3.70	102.51	110.35
7	I	301	LMT	O1B-C1B-C2B	3.39	116.89	108.10
7	H	603	LMT	C1B-O5B-C5B	3.26	120.09	113.69
8	H	602	CIT	C2-C3-C6	-3.22	103.19	110.11
7	G	901	LMT	O5'-C5'-C4'	3.15	116.40	109.75
7	G	901	LMT	C1'-C2'-C3'	-3.09	103.55	110.00
7	C	502	LMT	C2'-C3'-C4'	3.07	116.70	109.68
7	C	501	LMT	C3'-C4'-C5'	-3.06	103.92	110.93
7	H	603	LMT	O1B-C4'-C3'	3.04	115.38	107.28
7	H	603	LMT	O1B-C4'-C5'	3.03	117.74	109.45
7	H	603	LMT	C1B-O1B-C4'	-2.92	110.75	117.96
7	D	301	LMT	O5B-C5B-C4B	2.82	114.82	109.69
7	H	601	LMT	O5'-C5'-C6'	2.78	113.35	106.44
7	I	301	LMT	C1B-O1B-C4'	2.78	124.84	117.96
7	G	901	LMT	O5'-C1'-C2'	-2.72	104.60	110.35
7	D	301	LMT	O5B-C1B-C2B	2.70	116.06	110.35
7	H	601	LMT	O5'-C5'-C4'	2.66	115.36	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	603	LMT	O5B-C1B-C2B	2.65	115.97	110.35
7	I	301	LMT	C1B-C2B-C3B	2.65	115.51	110.00
8	H	602	CIT	O4-C5-C4	2.60	122.70	114.35
7	I	301	LMT	C1'-C2'-C3'	-2.56	104.66	110.00
7	I	301	LMT	O5B-C5B-C6B	2.53	112.72	106.44
8	H	602	CIT	O2-C1-C2	2.50	122.39	114.35
7	C	502	LMT	C1'-O5'-C5'	-2.49	108.79	113.69
7	G	901	LMT	C4B-C3B-C2B	2.49	115.17	110.82
7	H	601	LMT	O1B-C1B-C2B	2.49	114.55	108.10
7	D	301	LMT	O1B-C1B-C2B	2.48	114.52	108.10
7	H	601	LMT	C1-O1'-C1'	2.44	117.89	113.84
7	H	603	LMT	C4B-C3B-C2B	-2.43	106.58	110.82
7	C	501	LMT	O5B-C5B-C4B	2.41	114.07	109.69
7	C	501	LMT	C4-C3-C2	-2.40	102.24	114.42
7	H	603	LMT	C1-O1'-C1'	2.37	117.77	113.84
7	D	301	LMT	O5B-C5B-C6B	2.36	112.31	106.44
7	H	603	LMT	O5'-C5'-C6'	2.31	112.17	106.44
7	I	301	LMT	C3B-C4B-C5B	-2.30	106.13	110.24
7	H	601	LMT	C1'-O5'-C5'	2.28	118.17	113.69
8	C	503	CIT	O4-C5-C4	2.19	121.38	114.35
7	H	603	LMT	O1B-C1B-C2B	2.14	113.65	108.10
7	I	301	LMT	C1-O1'-C1'	2.09	117.30	113.84
7	C	502	LMT	C1'-C2'-C3'	2.07	114.31	110.00
7	C	501	LMT	O1'-C1'-C2'	2.07	111.53	108.30
7	H	601	LMT	O1'-C1'-C2'	2.06	111.53	108.30
7	H	603	LMT	C6B-C5B-C4B	-2.06	108.17	113.00
7	D	301	LMT	O1B-C4'-C3'	2.05	112.74	107.28
7	H	601	LMT	C2'-C3'-C4'	2.05	114.36	109.68
8	H	602	CIT	O1-C1-C2	-2.04	116.97	122.94
7	H	601	LMT	O5B-C5B-C6B	2.02	111.47	106.44
7	H	603	LMT	C2'-C3'-C4'	-2.02	105.07	109.68
7	G	901	LMT	C1B-C2B-C3B	2.01	114.19	110.00

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	501	LMT	O5'-C1'-O1'-C1
7	D	301	LMT	C2-C1-O1'-C1'
7	G	901	LMT	C2'-C1'-O1'-C1
7	G	901	LMT	O5'-C1'-O1'-C1
7	G	901	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
7	H	601	LMT	C2'-C1'-O1'-C1
7	H	601	LMT	O5'-C1'-O1'-C1
7	I	301	LMT	C2'-C1'-O1'-C1
7	I	301	LMT	O5'-C1'-O1'-C1
7	I	301	LMT	C2-C1-O1'-C1'
8	C	503	CIT	C1-C2-C3-O7
8	C	503	CIT	C1-C2-C3-C4
8	C	503	CIT	C1-C2-C3-C6
8	C	503	CIT	C2-C3-C4-C5
8	C	503	CIT	O7-C3-C4-C5
8	C	503	CIT	C6-C3-C4-C5
8	C	503	CIT	C2-C3-C6-O5
8	C	503	CIT	C2-C3-C6-O6
8	C	503	CIT	O7-C3-C6-O5
8	C	503	CIT	O7-C3-C6-O6
8	H	602	CIT	C1-C2-C3-O7
8	H	602	CIT	C1-C2-C3-C4
8	H	602	CIT	C1-C2-C3-C6
8	H	602	CIT	C2-C3-C6-O5
8	H	602	CIT	C2-C3-C6-O6
8	H	602	CIT	O7-C3-C6-O5
8	H	602	CIT	O7-C3-C6-O6
7	I	301	LMT	O5B-C1B-O1B-C4'
7	D	301	LMT	C3'-C4'-O1B-C1B
7	I	301	LMT	C2B-C1B-O1B-C4'
7	I	301	LMT	O5'-C5'-C6'-O6'
7	H	603	LMT	C4B-C5B-C6B-O6B
6	J	201	PEG	C4-C3-O2-C2
7	H	601	LMT	C3'-C4'-O1B-C1B
7	H	603	LMT	O5B-C5B-C6B-O6B
7	D	301	LMT	O5'-C5'-C6'-O6'
7	H	601	LMT	O5B-C5B-C6B-O6B
7	I	301	LMT	C4'-C5'-C6'-O6'
7	D	301	LMT	C4'-C5'-C6'-O6'
7	G	901	LMT	O5B-C5B-C6B-O6B
7	H	603	LMT	C4'-C5'-C6'-O6'
7	D	301	LMT	C4B-C5B-C6B-O6B
6	C	506	PEG	C1-C2-O2-C3
7	I	301	LMT	C5'-C4'-O1B-C1B
7	G	901	LMT	C4B-C5B-C6B-O6B
7	I	301	LMT	C3'-C4'-O1B-C1B
7	H	601	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
7	C	502	LMT	O5B-C5B-C6B-O6B
7	D	301	LMT	O1'-C1-C2-C3
6	C	505	PEG	O1-C1-C2-O2
7	D	301	LMT	O5B-C5B-C6B-O6B
7	C	502	LMT	O1'-C1-C2-C3
7	I	301	LMT	O1'-C1-C2-C3
7	H	603	LMT	O1'-C1-C2-C3
7	H	603	LMT	O5'-C5'-C6'-O6'
6	I	302	PEG	O1-C1-C2-O2
6	I	302	PEG	O2-C3-C4-O4
7	C	502	LMT	C11-C10-C9-C8
7	H	601	LMT	C6-C7-C8-C9
7	C	501	LMT	O5B-C5B-C6B-O6B
7	C	502	LMT	C6-C7-C8-C9
7	H	603	LMT	C11-C10-C9-C8
6	A	301	PEG	O2-C3-C4-O4
6	B	301	PEG	O2-C3-C4-O4
7	G	901	LMT	C5-C6-C7-C8
7	H	603	LMT	C3-C4-C5-C6
7	D	301	LMT	C3-C4-C5-C6
7	I	301	LMT	O5B-C5B-C6B-O6B
7	H	601	LMT	C5-C6-C7-C8
7	I	301	LMT	C9-C10-C11-C12
7	C	502	LMT	C4'-C5'-C6'-O6'
7	G	901	LMT	C7-C8-C9-C10
7	C	501	LMT	C5-C6-C7-C8
7	G	901	LMT	O1'-C1-C2-C3
7	C	501	LMT	C2'-C1'-O1'-C1
6	C	504	PEG	O1-C1-C2-O2
7	I	301	LMT	C3-C4-C5-C6
7	C	502	LMT	C7-C8-C9-C10
7	C	502	LMT	C2-C3-C4-C5
6	C	504	PEG	O2-C3-C4-O4
7	G	901	LMT	C9-C10-C11-C12
7	C	502	LMT	C1-C2-C3-C4
7	C	502	LMT	C5-C6-C7-C8
6	C	505	PEG	O2-C3-C4-O4
7	H	603	LMT	C1-C2-C3-C4
7	H	601	LMT	C4'-C5'-C6'-O6'
7	H	601	LMT	C5'-C4'-O1B-C1B
7	H	601	LMT	C2-C1-O1'-C1'
7	C	501	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
6	B	301	PEG	C4-C3-O2-C2
7	D	301	LMT	C1-C2-C3-C4
7	G	901	LMT	C2-C3-C4-C5
7	G	901	LMT	O5B-C1B-O1B-C4'
7	G	901	LMT	C4'-C5'-C6'-O6'
7	C	501	LMT	O1'-C1-C2-C3
7	C	502	LMT	C4B-C5B-C6B-O6B
6	D	303	PEG	O2-C3-C4-O4
6	D	302	PEG	C4-C3-O2-C2
7	H	601	LMT	O1'-C1-C2-C3
6	C	504	PEG	C1-C2-O2-C3
7	H	601	LMT	C1-C2-C3-C4
7	D	301	LMT	C7-C8-C9-C10
6	B	301	PEG	O1-C1-C2-O2
7	I	301	LMT	C1-C2-C3-C4
6	I	302	PEG	C4-C3-O2-C2
7	C	502	LMT	O5'-C5'-C6'-O6'
6	J	201	PEG	C1-C2-O2-C3
6	D	302	PEG	C1-C2-O2-C3
7	G	901	LMT	C1-C2-C3-C4
7	I	301	LMT	C7-C8-C9-C10
8	H	602	CIT	C3-C4-C5-O4
7	G	901	LMT	C2B-C1B-O1B-C4'
7	H	603	LMT	C4-C5-C6-C7
8	H	602	CIT	C3-C4-C5-O3
7	I	301	LMT	C2-C3-C4-C5
6	D	303	PEG	C1-C2-O2-C3
7	H	601	LMT	C9-C10-C11-C12
7	D	301	LMT	C2-C3-C4-C5
8	C	503	CIT	C3-C4-C5-O3
8	H	602	CIT	O1-C1-C2-C3
8	C	503	CIT	C3-C4-C5-O4
8	H	602	CIT	O2-C1-C2-C3
7	H	601	LMT	C4-C5-C6-C7
7	C	501	LMT	C4-C5-C6-C7
7	C	501	LMT	C3'-C4'-O1B-C1B

There are no ring outliers.

12 monomers are involved in 27 short contacts:

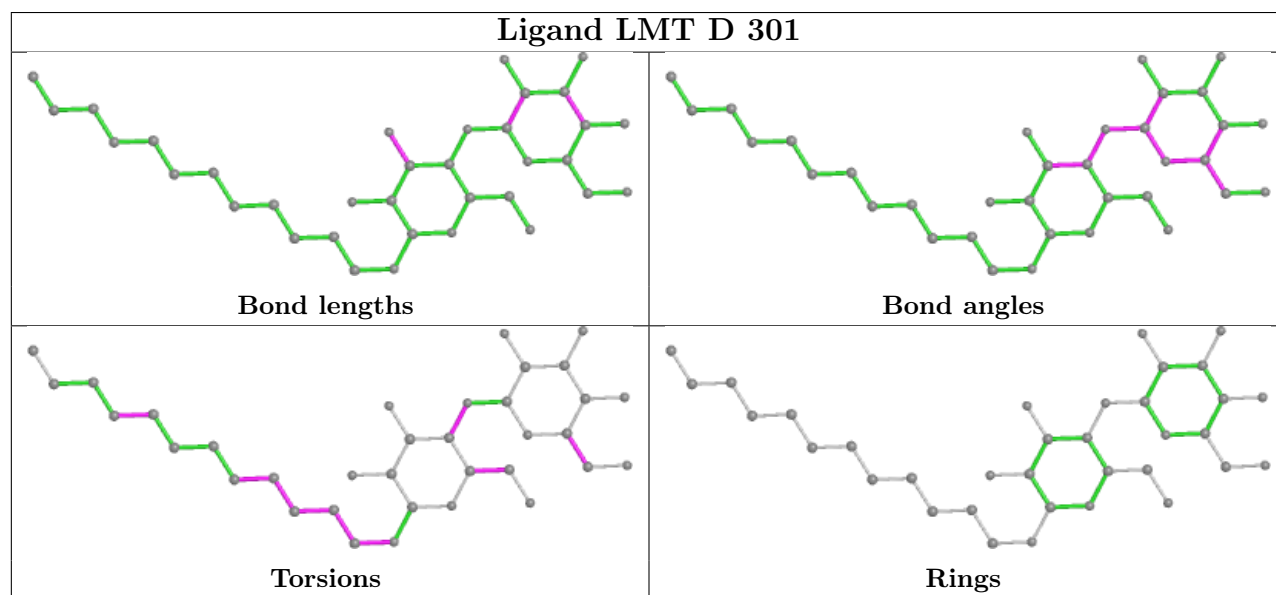
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	301	LMT	4	0

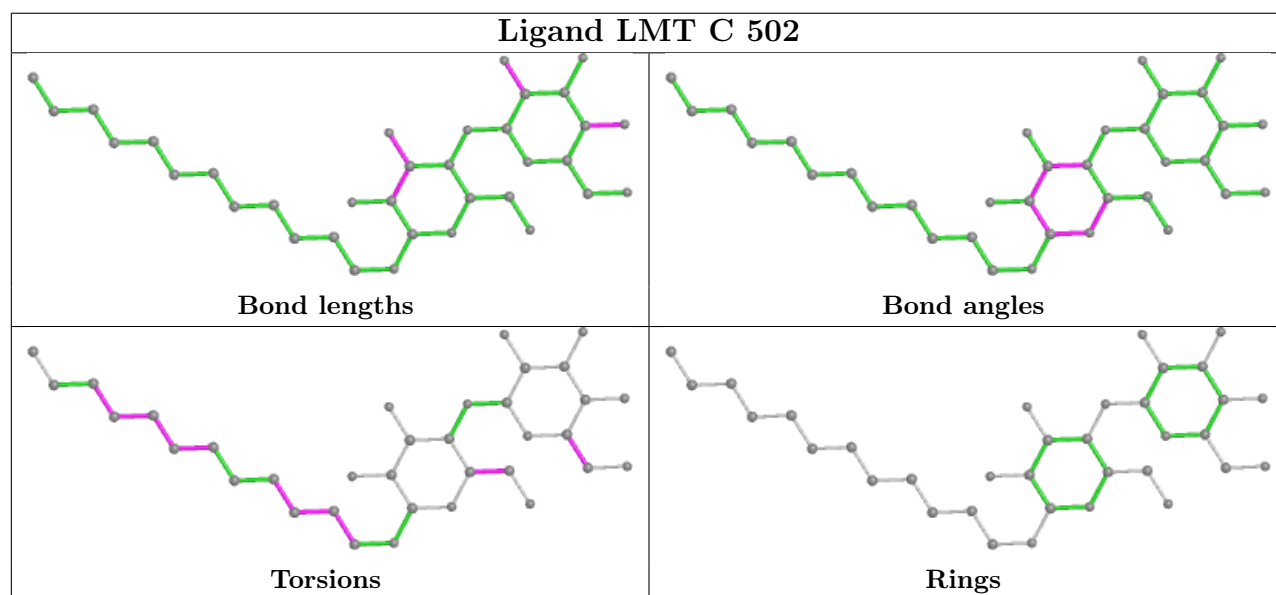
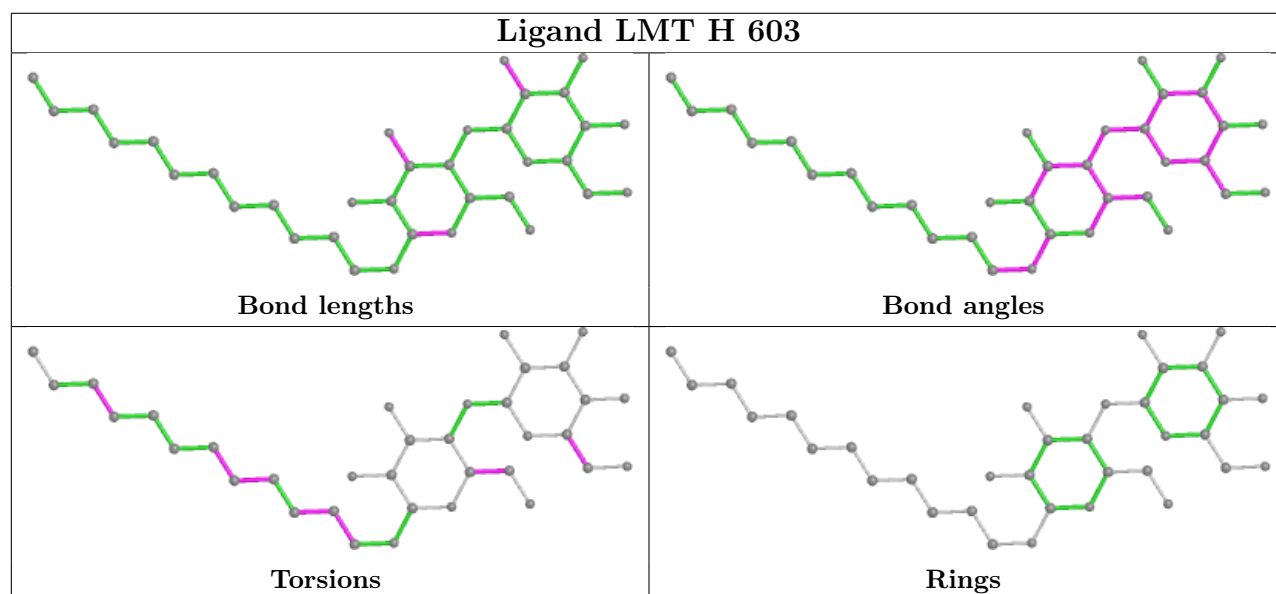
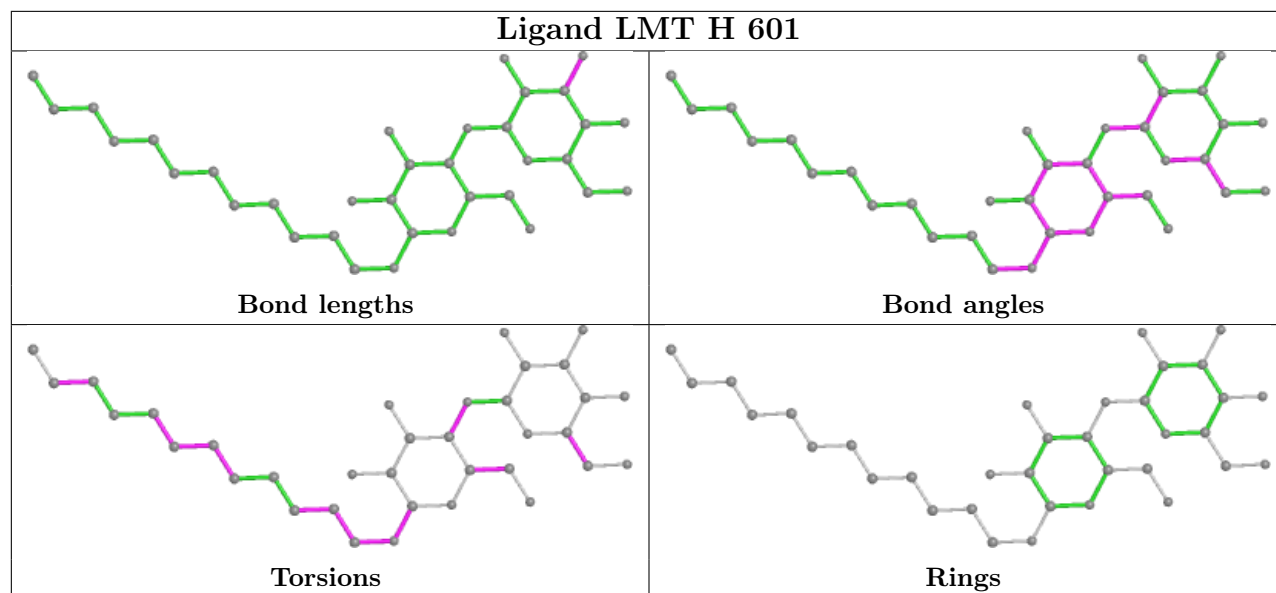
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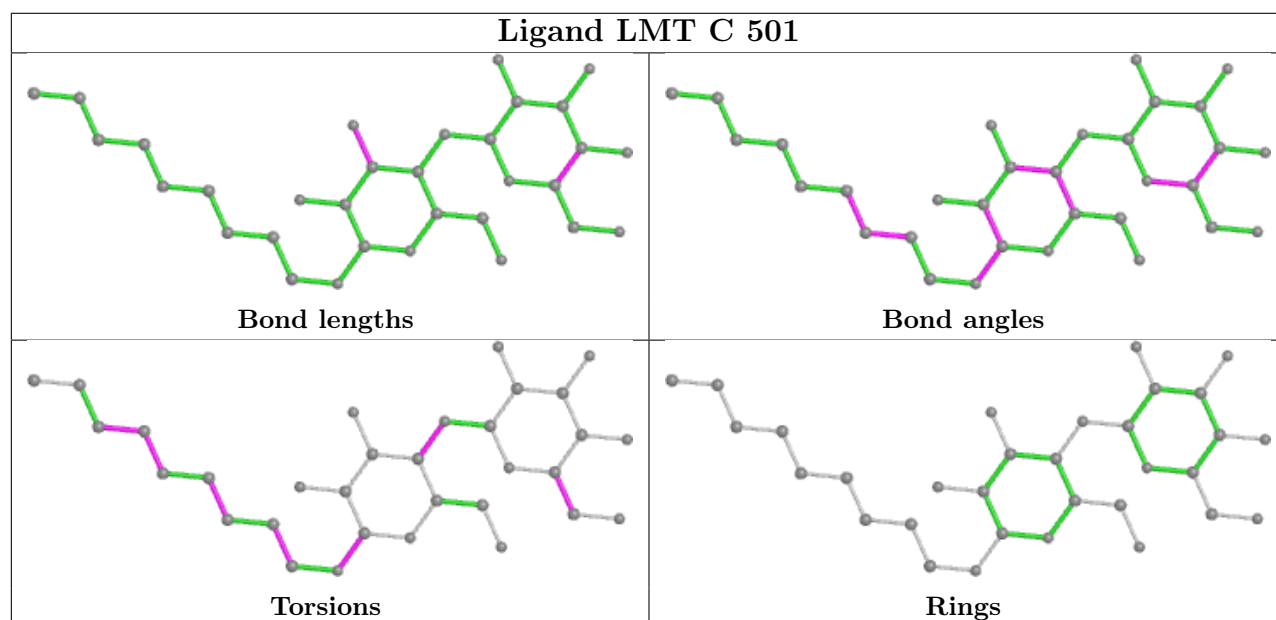
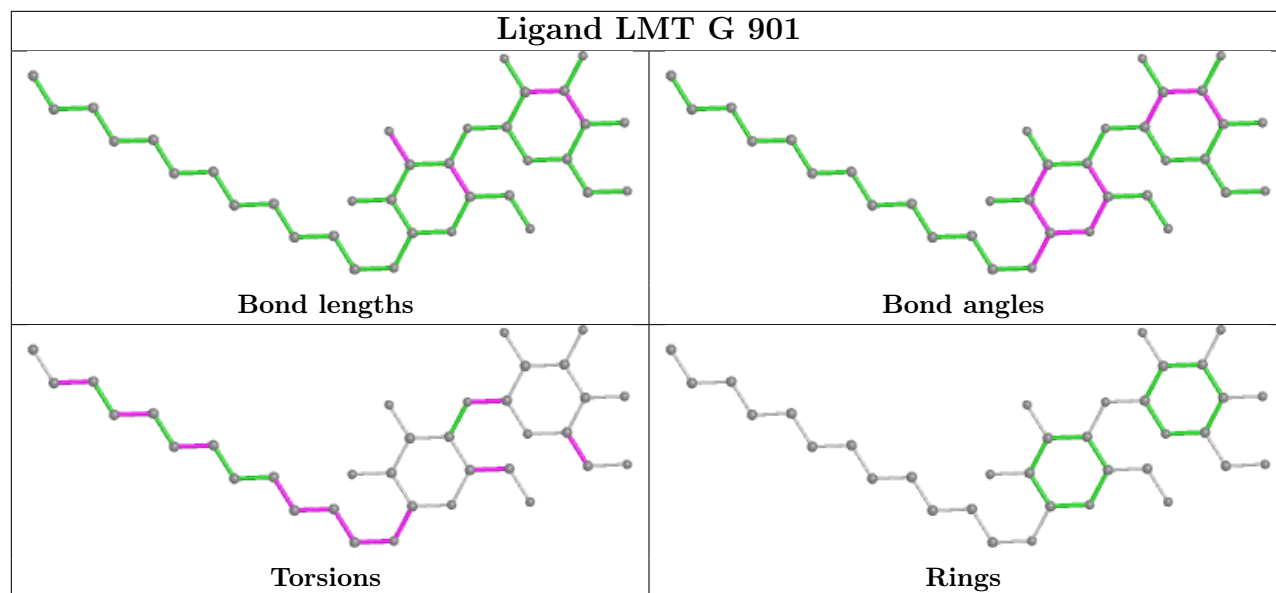
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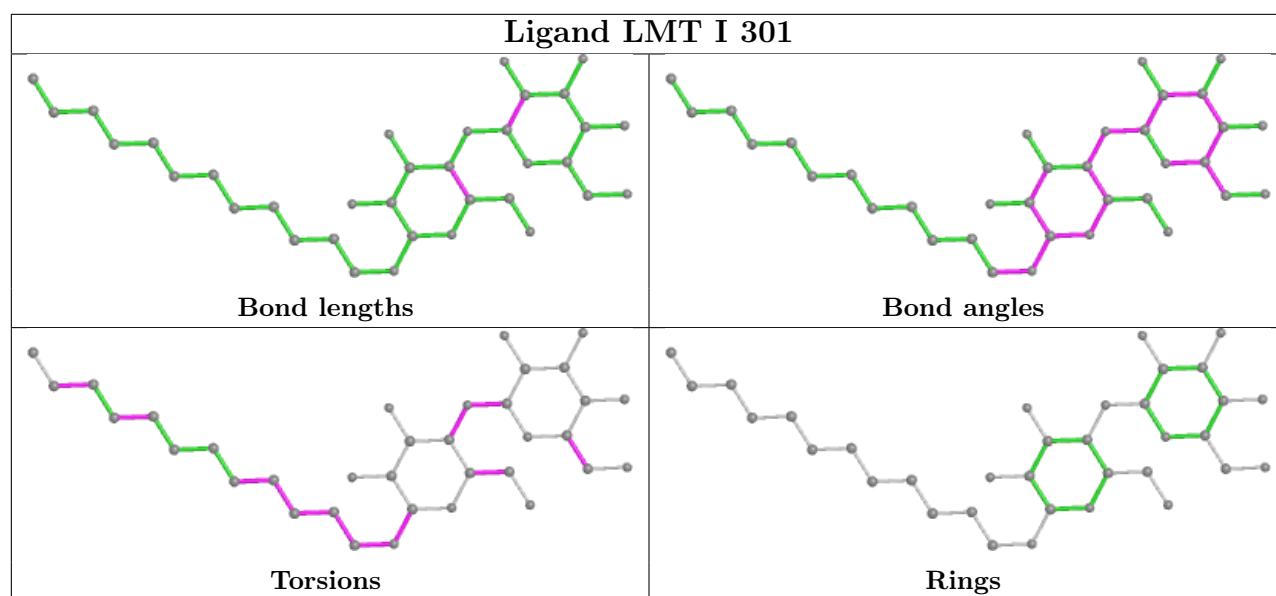
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	201	PEG	1	0
7	H	601	LMT	3	0
7	H	603	LMT	4	0
6	A	301	PEG	1	0
6	C	504	PEG	2	0
7	C	502	LMT	2	0
7	G	901	LMT	5	0
7	C	501	LMT	2	0
8	H	602	CIT	1	0
8	C	503	CIT	1	0
7	I	301	LMT	2	0

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	280/300 (93%)	-0.06	7 (2%) 57 47	58, 88, 140, 209	0
1	F	279/300 (93%)	0.12	12 (4%) 35 25	61, 88, 137, 222	0
2	B	282/287 (98%)	0.47	36 (12%) 3 2	77, 117, 164, 217	0
2	G	283/287 (98%)	0.38	27 (9%) 8 4	82, 117, 163, 226	0
3	C	207/215 (96%)	0.09	12 (5%) 23 15	73, 96, 166, 260	0
3	H	207/215 (96%)	0.35	16 (7%) 13 7	71, 102, 175, 227	0
4	D	260/265 (98%)	0.49	27 (10%) 6 3	70, 118, 198, 257	0
4	I	260/265 (98%)	0.68	37 (14%) 2 1	66, 112, 187, 234	0
5	E	126/136 (92%)	-0.11	3 (2%) 59 49	63, 87, 124, 156	0
5	J	125/136 (91%)	0.00	5 (4%) 38 28	65, 89, 120, 138	0
All	All	2309/2406 (95%)	0.28	182 (7%) 12 7	58, 104, 168, 260	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1	MET	20.3
3	H	33	GLY	12.0
2	B	2	ALA	11.1
4	I	100	THR	9.8
4	I	102	SER	9.0
4	I	191	GLY	8.9
4	I	99	PHE	8.8
4	D	6	ILE	8.8
4	I	192	GLY	8.1
2	G	32	GLU	8.1
2	B	31	GLU	7.9
3	H	161	ALA	7.6
4	I	87	MET	7.5

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Mol	Chain	Res	Type	RSRZ
2	B	258	ALA	7.5
3	H	32	VAL	7.2
4	I	97	TRP	6.9
4	I	58	THR	6.9
2	B	32	GLU	6.6
3	C	32	VAL	6.6
2	G	237	GLU	6.5
4	D	100	THR	6.3
1	F	177	GLU	6.3
2	B	41	HIS	6.1
4	I	98	ILE	5.9
2	G	21	ILE	5.7
3	H	160	LEU	5.6
4	I	197	ALA	5.5
4	D	140	GLU	5.3
3	H	44	ILE	5.3
3	H	162	LEU	5.3
1	F	276	TRP	5.3
2	G	240	GLN	5.3
2	B	264	PRO	5.2
4	I	190	ASP	5.2
5	J	2	VAL	5.2
2	B	67	ALA	5.2
2	B	42	THR	5.0
4	D	97	TRP	4.9
4	I	15	PHE	4.9
3	C	160	LEU	4.7
4	I	56	PHE	4.7
3	C	158	LEU	4.7
4	I	193	LEU	4.6
2	G	241	LYS	4.5
2	G	41	HIS	4.5
4	D	164	LEU	4.4
4	I	59	GLY	4.4
2	B	30	LEU	4.3
1	F	231	PHE	4.2
4	I	194	VAL	4.2
4	D	98	ILE	4.2
4	D	101	LEU	4.1
2	G	243	HIS	4.1
2	B	66	ILE	4.1
2	B	241	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	19	GLU	4.1
2	B	220	HIS	4.1
5	J	65	LYS	4.1
4	D	7	GLY	4.1
4	I	18	ARG	4.0
2	B	194	ALA	4.0
2	B	243	HIS	4.0
5	E	42	GLY	3.8
2	G	134	LEU	3.8
3	C	39	PRO	3.8
4	I	89	GLY	3.7
4	I	101	LEU	3.7
1	A	121	LEU	3.6
4	D	159	VAL	3.6
1	A	41	HIS	3.6
4	I	103	SER	3.5
2	G	220	HIS	3.5
4	D	175	VAL	3.5
4	D	60	LEU	3.5
3	H	188	PHE	3.5
2	B	18	LEU	3.4
4	I	106	LEU	3.4
4	I	195	LYS	3.3
1	F	181	GLN	3.3
5	E	43	LYS	3.2
2	G	42	THR	3.2
3	C	17	ALA	3.2
1	F	175	ASP	3.2
1	A	240	ILE	3.1
3	H	201	LYS	3.1
2	G	180	GLY	3.1
3	H	153	ILE	3.1
4	I	88	ALA	3.1
4	I	244	VAL	3.1
3	H	35	ILE	3.1
2	G	44	SER	3.1
3	H	156	GLN	3.1
2	B	104	LEU	3.1
1	A	160	VAL	3.0
2	B	65	GLU	3.0
2	B	179	MET	3.0
2	B	130	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
3	H	46	THR	2.9
4	D	102	SER	2.9
2	G	4	LYS	2.9
5	J	62	ASP	2.9
3	C	4	SER	2.9
2	B	69	TYR	2.9
3	H	192	ILE	2.9
4	I	52	LEU	2.9
4	I	55	VAL	2.8
2	B	218	LEU	2.8
4	D	207	LEU	2.8
4	D	177	ILE	2.8
3	C	38	LEU	2.7
1	F	20	ARG	2.7
2	G	2	ALA	2.7
1	F	17	ASP	2.6
4	D	62	ALA	2.6
4	I	201	VAL	2.6
4	D	148	LEU	2.6
1	F	280	SER	2.6
4	I	94	TRP	2.6
2	G	242	HIS	2.6
4	D	237	ARG	2.6
2	B	190	ASP	2.6
4	I	110	LEU	2.5
4	D	25	LEU	2.5
4	D	136	ALA	2.5
5	J	64	VAL	2.5
3	H	34	TYR	2.5
2	B	68	GLY	2.5
2	B	77	ASN	2.5
1	A	248	TYR	2.5
1	A	22	ALA	2.5
2	B	132	VAL	2.5
2	G	187	LEU	2.5
1	F	19	PRO	2.5
2	B	134	LEU	2.5
4	I	6	ILE	2.5
4	I	247	ILE	2.5
4	I	90	GLY	2.4
1	A	95	ASN	2.4
2	G	177	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	160	LEU	2.4
3	C	13	LEU	2.4
1	F	265	ILE	2.4
1	F	233	LYS	2.4
2	G	31	GLU	2.4
4	D	88	ALA	2.4
2	G	266	GLN	2.4
3	H	25	LEU	2.4
3	C	123	ARG	2.3
2	G	279	GLN	2.3
2	B	137	ASP	2.3
4	I	240	GLU	2.3
2	G	156	LEU	2.3
2	G	43	GLY	2.3
2	B	138	LEU	2.3
2	B	44	SER	2.3
2	G	65	GLU	2.2
4	D	31	PHE	2.2
2	G	221	GLY	2.2
2	B	3	ILE	2.2
2	B	128	TRP	2.2
4	I	57	ALA	2.2
5	J	43	LYS	2.2
5	E	40	ALA	2.2
4	D	171	PHE	2.2
1	F	246	PHE	2.1
3	H	158	LEU	2.1
3	C	115	ALA	2.1
4	D	47	ILE	2.1
4	D	103	SER	2.1
4	I	249	VAL	2.1
4	D	54[A]	TYR	2.1
4	I	177	ILE	2.1
2	B	133	GLY	2.1
2	G	219	GLU	2.1
3	C	113	GLN	2.0
2	B	43	GLY	2.0
2	B	14	PRO	2.0
3	C	156	GLN	2.0
2	B	4	LYS	2.0
4	I	163	ALA	2.0
4	D	196	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	94	TRP	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.

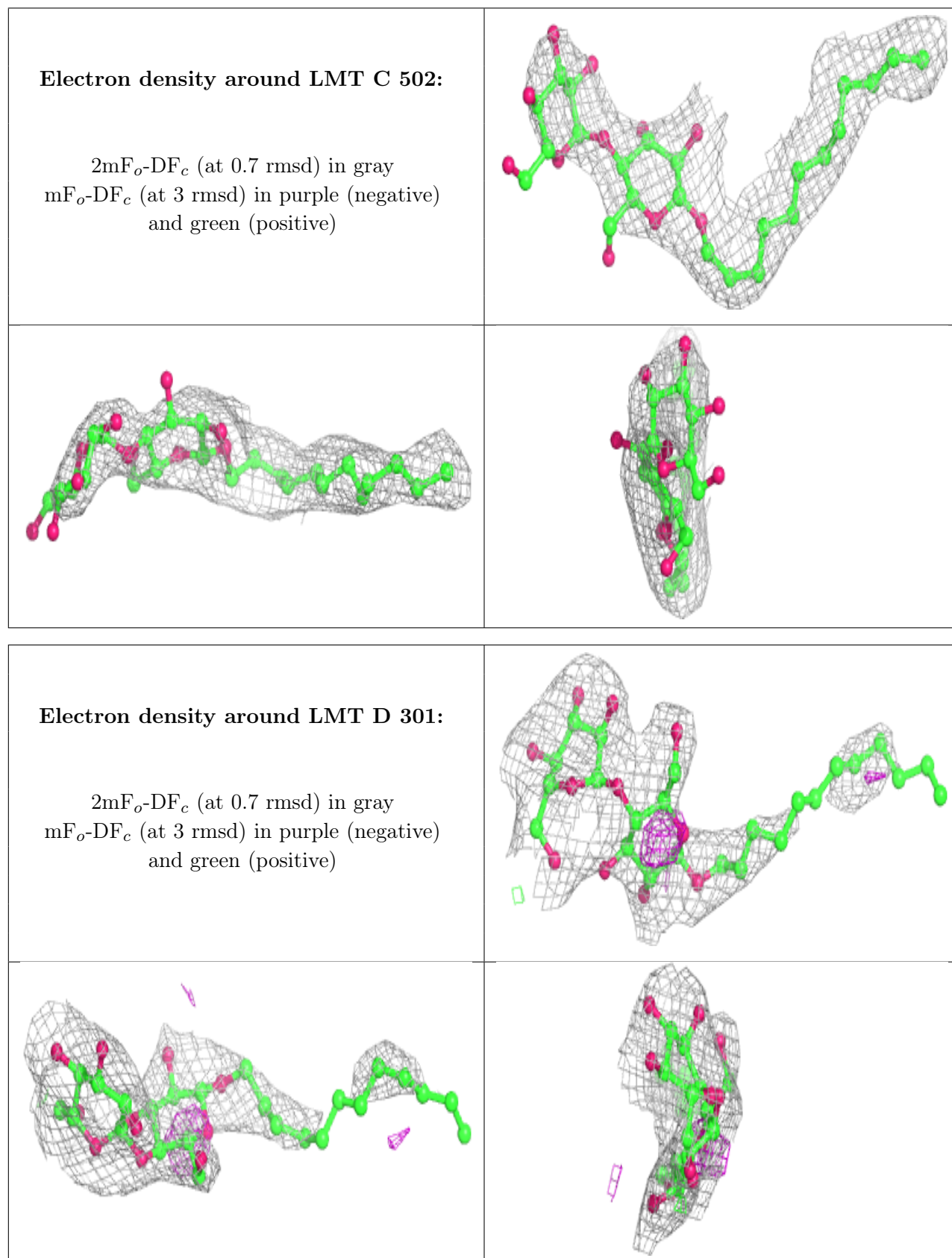
6.4 Ligands [i](#)

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, 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
7	LMT	C	502	35/35	0.64	0.43	96,140,160,170	0
6	PEG	A	301	7/7	0.72	0.21	97,98,105,110	0
7	LMT	D	301	35/35	0.72	0.45	108,129,143,147	0
7	LMT	G	901	35/35	0.73	0.26	115,149,157,159	0
7	LMT	I	301	35/35	0.74	0.36	82,139,173,175	0
6	PEG	D	303	7/7	0.77	0.67	98,100,115,124	0
7	LMT	H	601	35/35	0.79	0.20	82,131,172,172	0
6	PEG	C	504	7/7	0.80	0.11	104,116,122,124	0
7	LMT	C	501	32/35	0.82	0.19	81,136,165,168	0
8	CIT	C	503	13/13	0.83	0.13	132,141,149,191	0
6	PEG	I	302	7/7	0.84	0.50	88,103,110,111	0
7	LMT	H	603	35/35	0.84	0.26	97,137,156,161	0
6	PEG	C	506	7/7	0.85	0.32	101,106,117,122	0
8	CIT	H	602	13/13	0.86	0.13	111,122,134,137	0
6	PEG	E	201	7/7	0.88	0.17	71,82,92,93	0
6	PEG	B	301	7/7	0.90	0.41	102,114,119,121	0
6	PEG	C	505	7/7	0.91	0.11	114,116,125,127	0
6	PEG	D	302	7/7	0.92	0.10	119,125,130,130	0
6	PEG	J	201	7/7	0.95	0.23	72,79,82,84	0

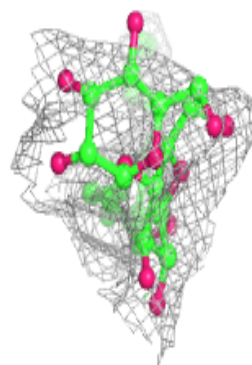
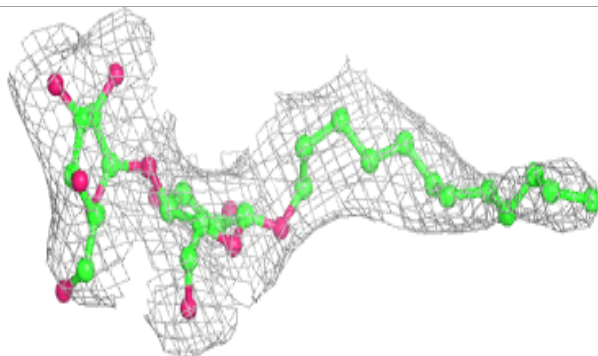
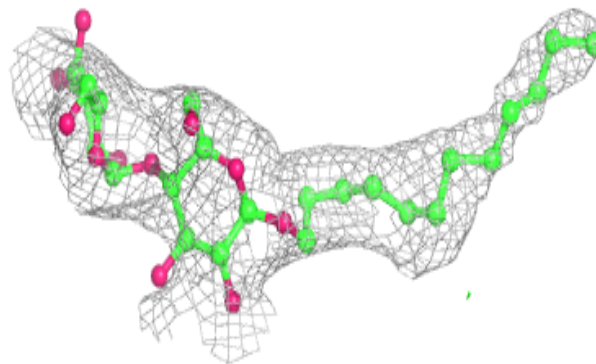
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

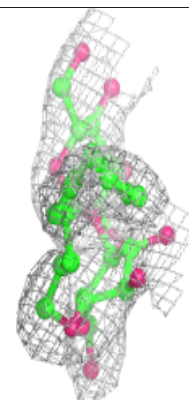
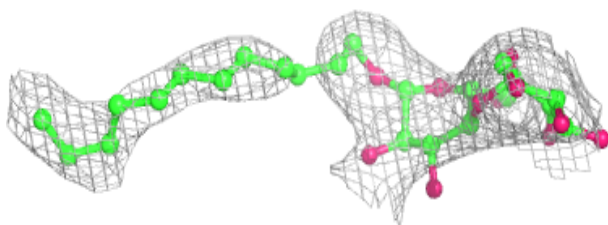
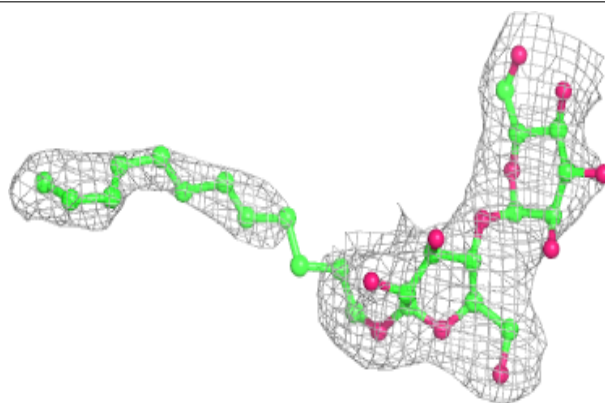


Electron density around LMT G 901:

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

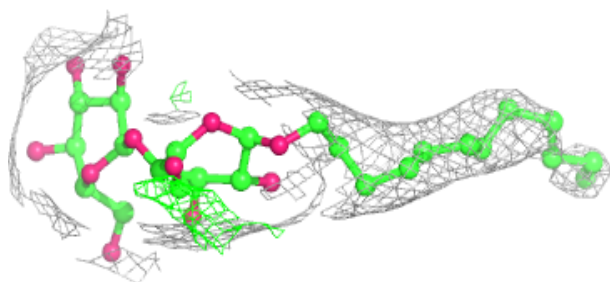
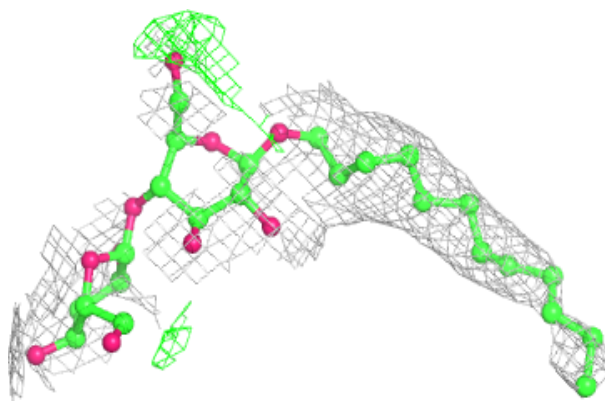
**Electron density around LMT I 301:**

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

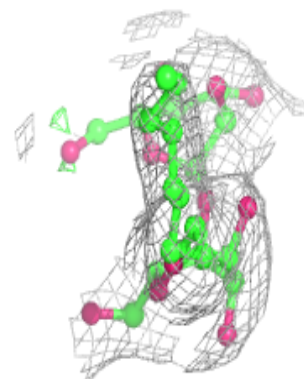
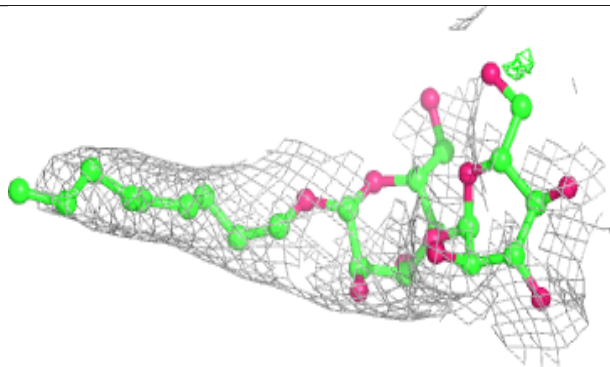


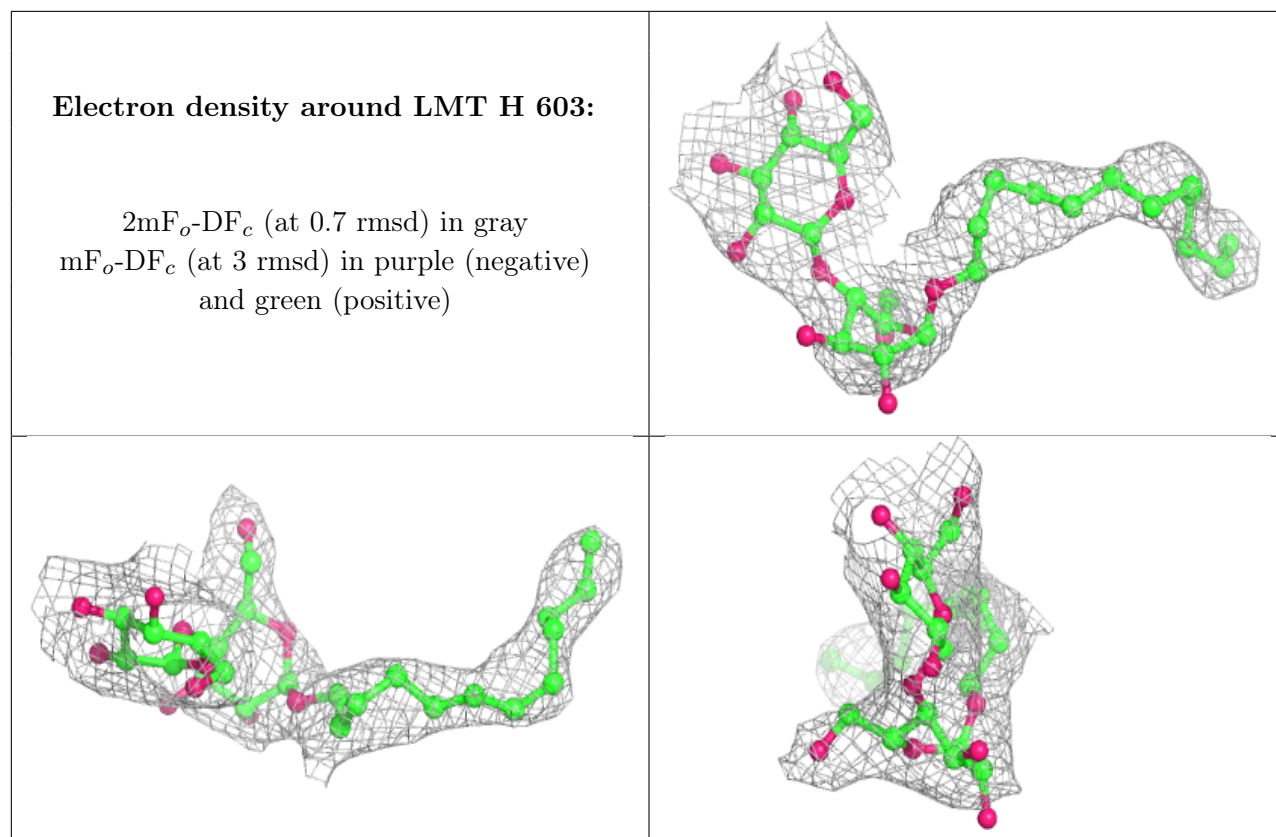
Electron density around LMT H 601:

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

**Electron density around LMT C 501:**

$2mF_o-DF_c$ (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.