Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 11:50 am GMT

PDB ID	:	6SLN
Title	:	Structure of the RagAB peptide transporter
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Deposited on	:	2019-08-20
Resolution	:	2.61 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:

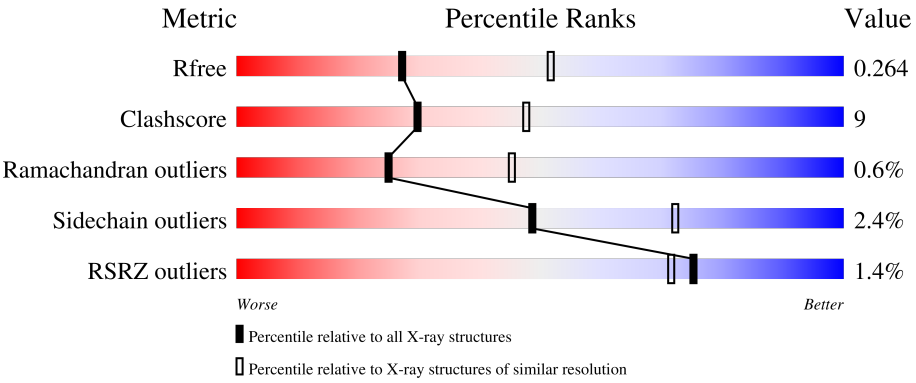
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	997	2% 68% 21% • 9%
1	B	997	% 68% 22% • 10%
2	C	488	77% 21% •
2	D	488	% 82% 17% •
3	P	13	15% 38% 46% 15%

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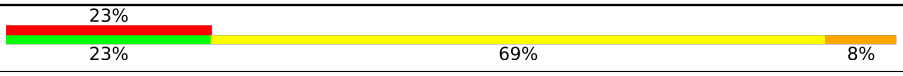
Mol	Chain	Length	Quality of chain
3	Q	13	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 22773 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 RagA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	903	Total	C	N	O	S	0	0	0
			7068	4476	1183	1377	32			
1	B	902	Total	C	N	O	S	0	0	0
			7064	4474	1182	1376	32			

- Molecule 2 is a protein called Lipoprotein RagB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	481	Total	C	N	O	S	0	0	0
			3834	2434	655	736	9			
2	D	482	Total	C	N	O	S	0	0	0
			3842	2440	656	737	9			

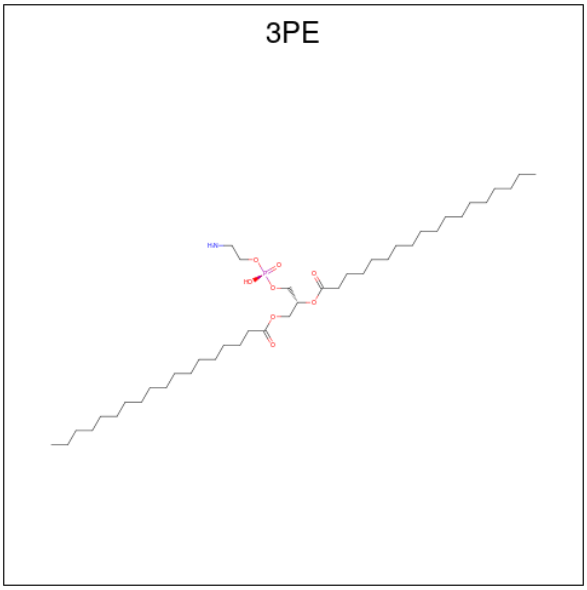
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	502	HIS	-	expression tag	UNP F5H948
C	503	HIS	-	expression tag	UNP F5H948
C	504	HIS	-	expression tag	UNP F5H948
C	505	HIS	-	expression tag	UNP F5H948
C	506	HIS	-	expression tag	UNP F5H948
C	507	HIS	-	expression tag	UNP F5H948
D	502	HIS	-	expression tag	UNP F5H948
D	503	HIS	-	expression tag	UNP F5H948
D	504	HIS	-	expression tag	UNP F5H948
D	505	HIS	-	expression tag	UNP F5H948
D	506	HIS	-	expression tag	UNP F5H948
D	507	HIS	-	expression tag	UNP F5H948

- Molecule 3 is a protein called GLN-THR-ALA-GLY-ALA-ASN-SER-GLN-ARG-GLY-SER-ALA-GLY.

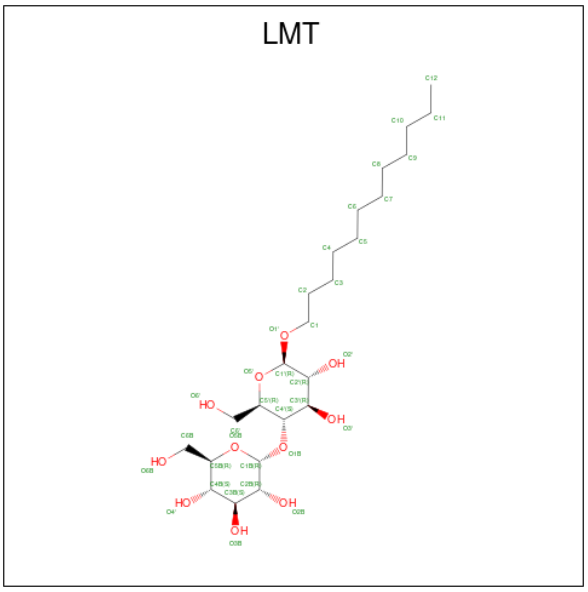
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	0	0	0
			83	45	19	19			
3	Q	13	Total	C	N	O	0	0	0
			83	45	19	19			

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



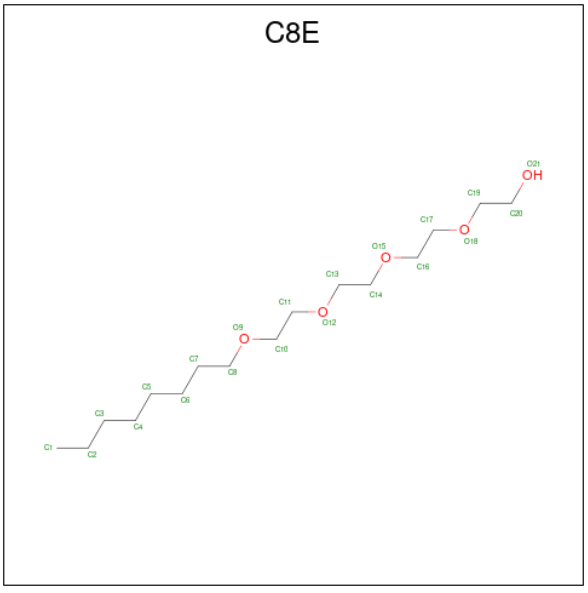
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			31	27	4		
4	B	1	Total	C	O	0	0
			32	28	4		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



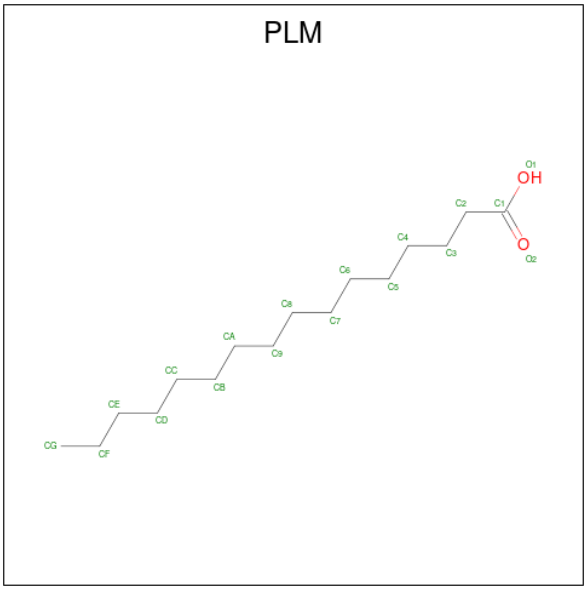
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 35 24 11	0	0
5	B	1	Total C O 35 24 11	0	0
5	C	1	Total C O 33 22 11	0	0
5	D	1	Total C O 33 22 11	0	0

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 21 16 5	0	0
6	A	1	Total C O 21 16 5	0	0
6	B	1	Total C O 7 5 2	0	0

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 14 13 1	0	0
7	D	1	Total C O 15 14 1	0	0

- Molecule 8 is water.

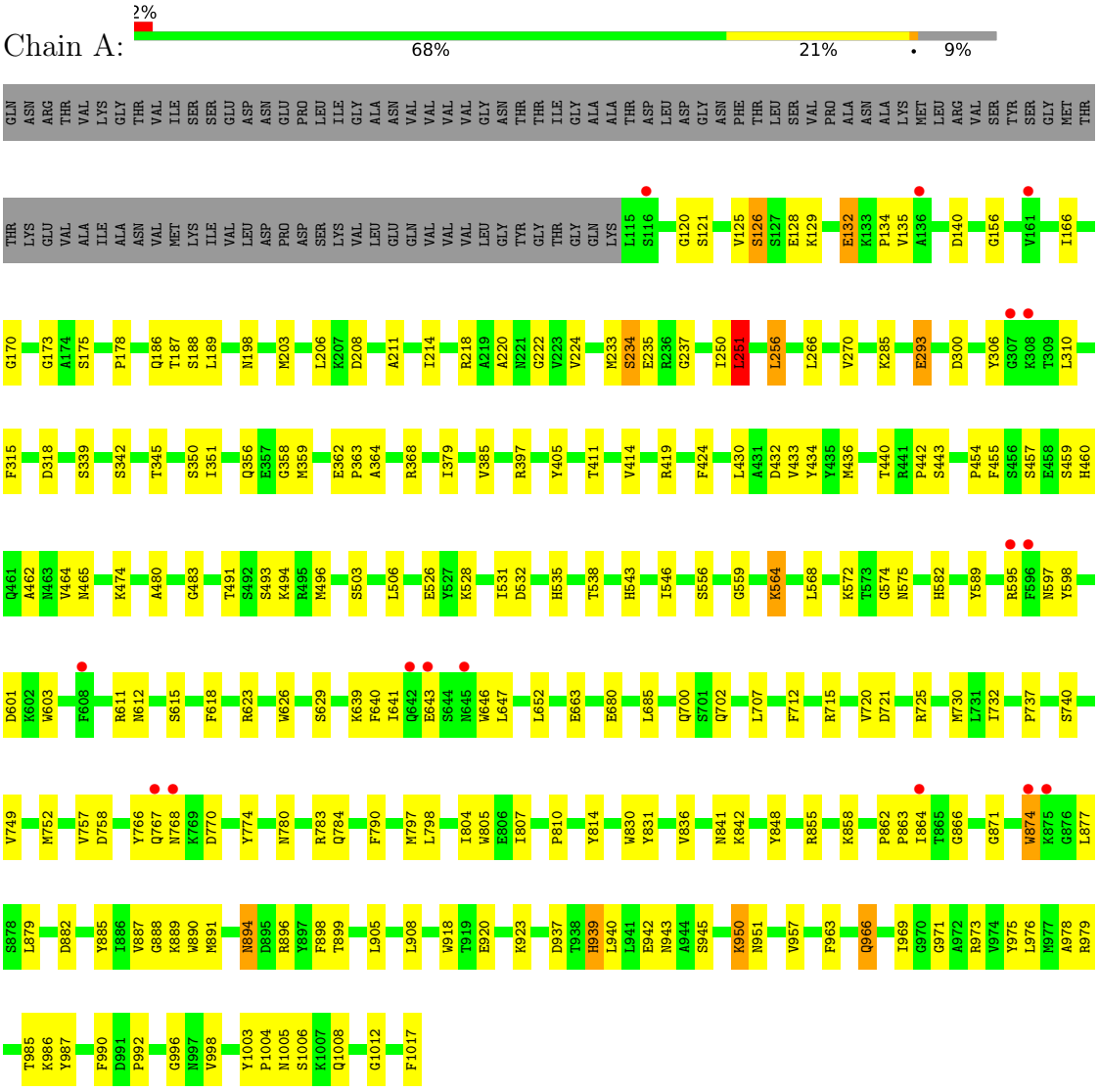
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	146	Total O 146 146	0	0
8	B	165	Total O 165 165	0	0
8	C	103	Total O 103 103	0	0
8	D	108	Total O 108 108	0	0

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.

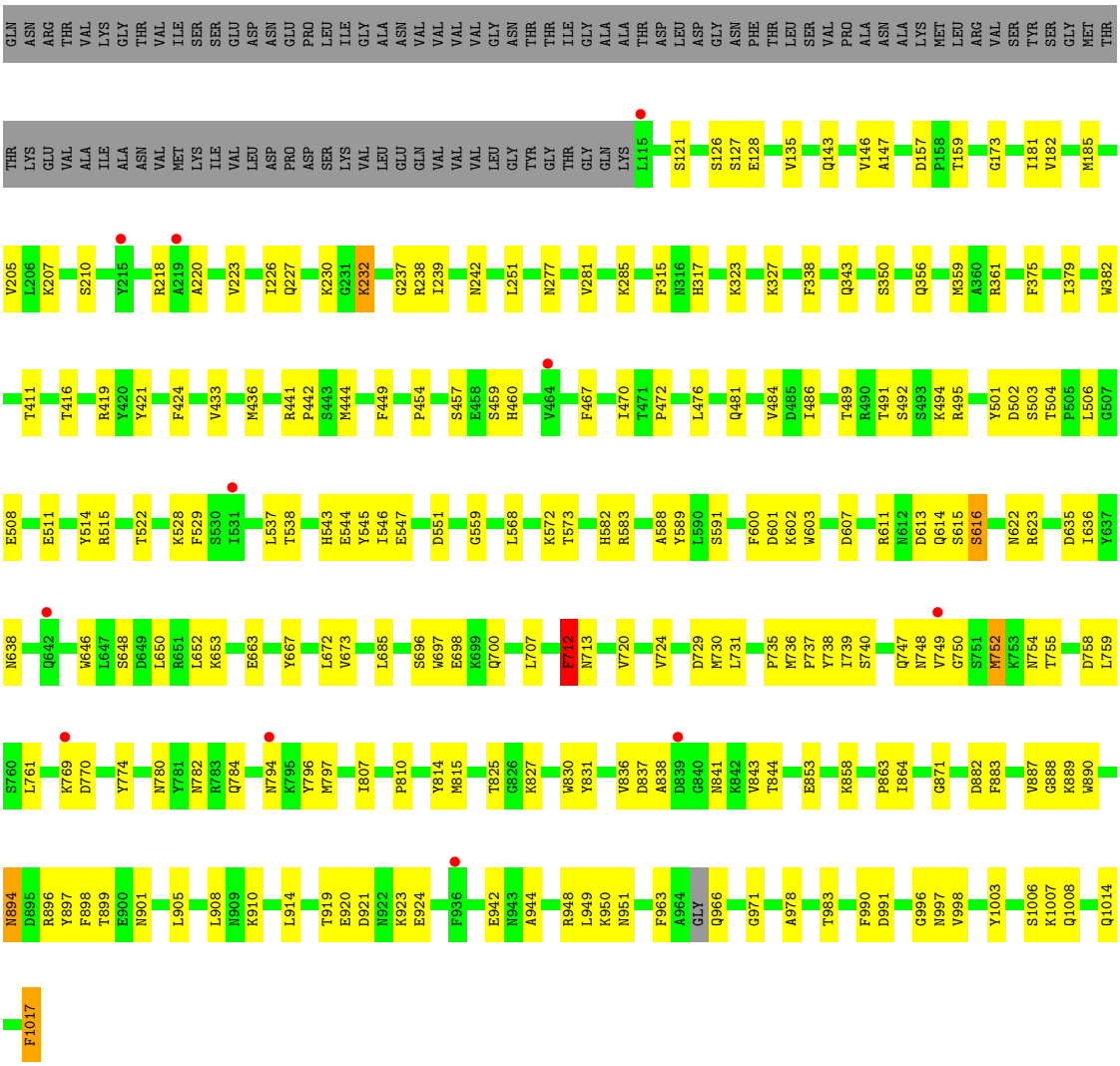
• Molecule 1: RagA protein

Chain A:



• Molecule 1: RagA protein

Chain B:

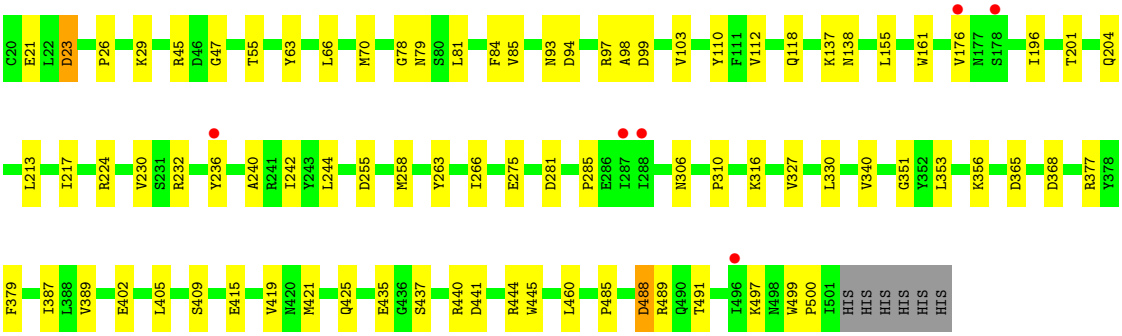


• Molecule 2: Lipoprotein RagB

Chain C:

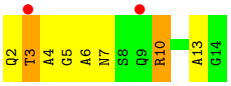
• Molecule 2: Lipoprotein RagB

Chain D:



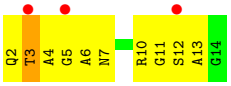
• Molecule 3: GLN-THR-ALA-GLY-ALA-ASN-SER-GLN-ARG-GLY-SER-ALA-GLY

Chain P:



• Molecule 3: GLN-THR-ALA-GLY-ALA-ASN-SER-GLN-ARG-GLY-SER-ALA-GLY

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	129.78Å 142.73Å 250.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.96 – 2.61 125.02 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (123.96-2.61) 99.8 (125.02-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.207 , 0.264 0.207 , 0.264	Depositor DCC
R_{free} test set	6897 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.876	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.3	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	0.89	EDS
Total number of atoms	22773	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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: 3PE, C8E, PLM, LMT

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	0.44	0/7232	0.63	2/9783 (0.0%)
1	B	0.44	0/7227	0.63	0/9775
2	C	0.42	0/3920	0.56	0/5320
2	D	0.44	0/3928	0.58	0/5331
3	P	0.54	0/82	0.94	0/108
3	Q	0.58	0/82	0.83	0/108
All	All	0.44	0/22471	0.61	2/30425 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	251	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	807	ILE	C-N-CA	-5.32	111.12	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	432	ASP	Peptide
1	B	712	PHE	Peptide
2	C	359	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7068	0	6806	159	0
1	B	7064	0	6802	143	0
2	C	3834	0	3728	72	0
2	D	3842	0	3739	50	0
3	P	83	0	75	7	0
3	Q	83	0	75	9	0
4	A	31	0	43	2	0
4	B	32	0	45	4	0
5	A	35	0	46	2	0
5	B	35	0	46	2	0
5	C	33	0	38	4	0
5	D	33	0	37	0	0
6	A	42	0	68	4	0
6	B	7	0	6	0	0
7	C	14	0	22	1	0
7	D	15	0	24	0	0
8	A	146	0	0	5	0
8	B	165	0	0	8	0
8	C	103	0	0	6	0
8	D	108	0	0	2	0
All	All	22773	0	21600	412	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (412) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ARG:HD2	1:A:767:GLN:NE2	1.63	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:ARG:HD2	1:A:767:GLN:HE22	0.99	1.07
1:A:715:ARG:CD	1:A:767:GLN:HE22	1.70	1.03
1:A:318:ASP:HB2	1:A:419:ARG:HB3	1.47	0.97
1:B:919:THR:HG22	1:B:921:ASP:H	1.30	0.95
1:A:950:LYS:NZ	8:A:1201:HOH:O	1.99	0.94
1:B:157:ASP:OD1	1:B:159:THR:HG22	1.73	0.88
1:B:227:GLN:NE2	8:B:1201:HOH:O	2.08	0.87
2:C:20:CYS:N	5:C:602:LMT:H6'	1.75	0.85
2:C:79:ASN:HB3	3:P:5:GLY:HA2	1.56	0.84
2:C:97:ARG:HH21	2:C:102:GLU:HB3	1.42	0.84
1:A:623:ARG:NH2	2:D:23:ASP:OD1	2.11	0.83
1:A:250:ILE:HB	1:A:359:MET:HE3	1.61	0.82
1:A:218:ARG:HD3	1:A:663:GLU:HG2	1.60	0.81
1:B:794:ASN:HA	1:B:807:ILE:HD12	1.62	0.80
2:C:124:VAL:HG11	2:C:212:ARG:HH22	1.48	0.78
1:B:433:VAL:CG2	1:B:442:PRO:HB2	2.14	0.77
1:B:503:SER:HB2	2:C:310:PRO:HG2	1.66	0.77
1:B:737:PRO:HB2	1:B:739:ILE:HG12	1.65	0.77
2:C:124:VAL:HG11	2:C:212:ARG:NH2	2.00	0.77
1:A:969:ILE:HA	1:A:1017:PHE:HB3	1.66	0.76
1:A:506:LEU:HB3	1:A:559:GLY:HA2	1.67	0.76
1:A:342:SER:OG	1:B:343:GLN:NE2	2.16	0.75
1:A:250:ILE:HB	1:A:359:MET:CE	2.16	0.75
2:D:402:GLU:HA	2:D:419:VAL:HG21	1.69	0.75
1:B:948:ARG:NH2	1:B:991:ASP:OD1	2.20	0.75
1:B:147:ALA:HB1	1:B:758:ASP:HB2	1.67	0.74
1:A:140:ASP:OD2	1:A:979:ARG:NH1	2.20	0.74
1:A:218:ARG:HD3	1:A:663:GLU:CG	2.18	0.74
1:A:618:PHE:O	1:A:623:ARG:NH1	2.21	0.74
1:A:457:SER:HB2	1:A:491:THR:HG22	1.69	0.73
1:B:135:VAL:HG12	1:B:356:GLN:HE22	1.53	0.73
2:D:79:ASN:HD22	3:Q:5:GLY:HA3	1.52	0.73
1:B:416:THR:HB	1:B:908:LEU:HD22	1.69	0.73
1:A:460:HIS:HB3	6:A:1103:C8E:H131	1.71	0.73
1:A:749:VAL:HG11	1:A:790:PHE:HB3	1.73	0.71
1:A:937:ASP:OD1	1:A:939:HIS:ND1	2.25	0.69
1:B:433:VAL:HG22	1:B:442:PRO:HB2	1.74	0.69
1:A:379:ILE:HD11	1:A:385:VAL:HG22	1.75	0.68
2:C:331:TYR:HB2	2:C:338:LYS:HD3	1.74	0.68
1:A:121:SER:N	1:A:208:ASP:OD1	2.26	0.67
1:B:948:ARG:NH1	1:B:983:THR:OG1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:HIS:NE2	8:B:1207:HOH:O	2.27	0.67
1:B:724:VAL:HG22	1:B:755:THR:HG23	1.77	0.67
1:B:239:ILE:HG23	1:B:1017:PHE:HB2	1.78	0.66
1:B:1006:SER:OG	1:B:1008:GLN:NE2	2.29	0.65
1:A:920:GLU:N	8:A:1202:HOH:O	2.14	0.65
1:B:504:THR:HG22	1:B:506:LEU:H	1.62	0.65
3:Q:10:ARG:HB2	3:Q:13:ALA:HB3	1.77	0.65
1:B:495:ARG:HB2	1:B:508:GLU:HB3	1.80	0.64
1:B:698:GLU:HG3	1:B:730:MET:HA	1.79	0.64
2:D:85:VAL:O	8:D:701:HOH:O	2.15	0.64
1:B:858:LYS:HG2	1:B:890:TRP:CE2	2.32	0.64
1:A:234:SER:HB3	1:A:235:GLU:OE2	1.98	0.64
1:A:715:ARG:NH1	1:A:767:GLN:OE1	2.30	0.64
1:B:323:LYS:HD3	1:B:424:PHE:CE2	2.33	0.63
1:A:300:ASP:OD2	8:A:1203:HOH:O	2.15	0.63
2:D:356:LYS:NZ	2:D:435:GLU:OE1	2.29	0.63
1:B:433:VAL:HG21	1:B:442:PRO:HB2	1.80	0.63
1:A:918:TRP:NE1	1:A:923:LYS:HG2	2.13	0.62
1:B:758:ASP:HB3	1:B:780:ASN:HD22	1.65	0.62
2:C:227:VAL:HG22	2:C:290:ARG:HG2	1.81	0.62
1:A:766:TYR:HE2	1:A:768:ASN:HD22	1.48	0.62
1:A:503:SER:HB2	2:D:310:PRO:HG2	1.81	0.61
1:B:457:SER:HB2	1:B:491:THR:HG22	1.81	0.60
1:B:472:PRO:HG2	1:B:476:LEU:HD23	1.83	0.60
1:A:433:VAL:CG2	1:A:442:PRO:HB2	2.31	0.60
1:B:529:PHE:CE1	1:B:537:LEU:HD12	2.37	0.60
1:B:522:THR:HG22	1:B:544:GLU:HG3	1.85	0.59
1:A:318:ASP:CB	1:A:419:ARG:HB3	2.29	0.59
1:B:622:ASN:HB3	1:B:696:SER:HB2	1.85	0.58
1:A:685:LEU:O	2:D:47:GLY:HA3	2.03	0.58
1:B:495:ARG:NH2	8:B:1211:HOH:O	2.34	0.58
2:D:97:ARG:NH1	2:D:99:ASP:OD2	2.37	0.58
1:A:943:ASN:HB3	1:A:986:LYS:HE2	1.86	0.58
1:A:957:VAL:HG22	1:A:973:ARG:HG2	1.85	0.58
2:C:402:GLU:HA	2:C:419:VAL:HG11	1.86	0.58
1:B:515:ARG:HB3	1:B:551:ASP:HB3	1.85	0.58
2:C:287:ILE:HG21	2:C:290:ARG:HD3	1.85	0.57
2:D:440:ARG:O	2:D:444:ARG:HG3	2.04	0.57
1:A:715:ARG:NE	1:A:767:GLN:HE22	2.03	0.57
1:B:467:PHE:HB3	1:B:481:GLN:HG3	1.87	0.57
3:Q:2:GLN:O	3:Q:4:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1103:C8E:H161	1:B:460:HIS:HB3	1.87	0.56
1:B:327:LYS:HD2	1:B:361:ARG:NH1	2.20	0.56
1:A:351:ILE:HB	6:A:1103:C8E:H31	1.86	0.56
5:A:1102:LMT:H6'2	2:D:21:GLU:HB3	1.88	0.56
2:C:128:GLU:HG3	2:C:149:LEU:HD11	1.87	0.56
1:A:882:ASP:HB2	1:A:951:ASN:HB3	1.86	0.56
1:B:506:LEU:HB3	1:B:559:GLY:HA2	1.88	0.56
2:D:45:ARG:HD3	8:D:702:HOH:O	2.05	0.56
3:P:2:GLN:O	3:P:4:ALA:N	2.38	0.56
1:B:864:ILE:HB	1:B:887:VAL:HB	1.88	0.55
1:A:639:LYS:HG3	1:A:640:PHE:CE1	2.41	0.55
1:A:730:MET:HG2	1:A:732:ILE:HG13	1.88	0.55
1:A:783:ARG:HH11	1:A:783:ARG:HG3	1.72	0.55
1:B:589:TYR:CE1	1:B:615:SER:HB2	2.41	0.55
1:A:454:PRO:HG2	1:A:494:LYS:HB2	1.88	0.55
1:A:730:MET:HE1	1:A:752:MET:SD	2.47	0.55
2:C:20:CYS:N	5:C:602:LMT:O6'	2.39	0.55
1:B:232:LYS:HB2	1:B:238:ARG:HH21	1.71	0.55
1:B:559:GLY:HA3	1:B:572:LYS:HG3	1.89	0.55
1:B:754:ASN:OD1	1:B:782:ASN:ND2	2.36	0.55
1:B:898:PHE:HE1	3:P:5:GLY:H	1.54	0.55
1:A:894:ASN:HB2	1:A:998:VAL:CG2	2.37	0.54
2:C:360:ASP:HB3	2:C:363:TYR:CD2	2.42	0.54
2:C:410:LYS:HB2	2:C:415:GLU:HB2	1.89	0.54
1:A:963:PHE:CE2	1:A:971:GLY:HA2	2.42	0.54
2:D:489:ARG:HE	2:D:497:LYS:HD3	1.73	0.54
2:C:338:LYS:HD2	2:C:342:ILE:HD11	1.90	0.54
1:A:784:GLN:HB3	1:A:810:PRO:HB3	1.90	0.53
1:A:214:ILE:HD13	1:A:595:ARG:HH21	1.73	0.53
2:D:176:VAL:HA	2:D:500:PRO:HG3	1.89	0.53
1:B:730:MET:SD	1:B:752:MET:HE2	2.47	0.53
1:B:797:MET:HG3	1:B:814:TYR:CD1	2.44	0.53
3:Q:3:THR:O	3:Q:3:THR:OG1	2.23	0.53
1:B:863:PRO:HD2	1:B:888:GLY:HA3	1.91	0.52
1:A:702:GLN:HG3	1:A:725:ARG:HB2	1.92	0.52
1:B:614:GLN:HA	1:B:623:ARG:O	2.09	0.52
2:C:166:ARG:NH2	2:C:480:TYR:O	2.36	0.52
1:A:589:TYR:CE1	1:A:615:SER:HB2	2.45	0.52
2:C:223:ASN:O	8:C:701:HOH:O	2.19	0.52
1:B:882:ASP:HB2	1:B:951:ASN:HB3	1.91	0.52
2:D:78:GLY:HA3	3:Q:3:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG12	1:A:356:GLN:NE2	2.25	0.52
1:A:532:ASP:HB2	1:A:535:HIS:HB2	1.92	0.52
1:B:382:TRP:HD1	1:B:470:ILE:HG23	1.75	0.52
1:B:454:PRO:HG2	1:B:494:LYS:HB2	1.92	0.52
1:B:996:GLY:O	1:B:997:ASN:HB3	2.10	0.52
1:B:698:GLU:HB2	1:B:731:LEU:HD12	1.91	0.52
2:C:368:ASP:HB3	2:C:369:LYS:HE3	1.91	0.52
2:D:70:MET:HB3	2:D:327:VAL:HG21	1.92	0.52
1:B:667:TYR:CD2	2:C:26:PRO:HB3	2.45	0.51
2:C:113:TYR:CE1	2:C:162:ARG:HG3	2.46	0.51
2:C:390:GLU:HB2	2:C:424:LEU:HD11	1.92	0.51
1:B:896:ARG:NH1	1:B:942:GLU:OE2	2.36	0.51
2:C:351:GLY:HA3	2:C:460:LEU:HD21	1.92	0.51
1:A:233:MET:HE1	1:A:345:THR:H	1.76	0.51
1:B:492:SER:OG	1:B:511:GLU:OE2	2.22	0.51
1:B:685:LEU:O	2:C:47:GLY:HA3	2.11	0.51
1:A:715:ARG:CZ	1:A:767:GLN:OE1	2.59	0.51
1:B:182:VAL:HG22	1:B:226:ILE:HB	1.92	0.51
1:A:582:HIS:HB2	1:B:568:LEU:HB2	1.92	0.51
1:B:218:ARG:NH1	1:B:663:GLU:OE1	2.43	0.51
2:C:331:TYR:CB	2:C:338:LYS:HD3	2.41	0.51
1:B:601:ASP:HB3	1:B:603:TRP:HD1	1.75	0.51
1:B:251:LEU:HA	1:B:1007:LYS:HE3	1.93	0.50
2:C:160:ILE:HG22	2:C:209:ILE:HD11	1.92	0.50
1:A:433:VAL:HG22	1:A:442:PRO:HB2	1.92	0.50
1:B:648:SER:OG	1:B:713:ASN:HA	2.11	0.50
2:C:389:VAL:HG11	2:C:405:LEU:HD13	1.93	0.50
1:B:232:LYS:HB2	1:B:238:ARG:NH2	2.26	0.50
1:B:896:ARG:HA	1:B:899:THR:OG1	2.11	0.50
2:C:420:ASN:O	2:C:422:GLU:N	2.43	0.50
2:D:224:ARG:NH1	2:D:263:TYR:HE2	2.10	0.50
1:A:433:VAL:HG21	1:A:442:PRO:HB2	1.93	0.50
1:B:736:MET:O	2:C:487:ARG:HD2	2.12	0.50
1:B:502:ASP:OD1	1:B:503:SER:N	2.44	0.50
1:A:379:ILE:HG23	1:B:237:GLY:HA3	1.94	0.50
1:A:543:HIS:CE1	4:A:1101:3PE:H331	2.47	0.50
2:C:427:GLU:OE1	2:C:430:ARG:NH2	2.32	0.50
1:B:740:SER:O	2:C:118:GLN:HG3	2.12	0.49
1:B:836:VAL:HG23	1:B:841:ASN:HB2	1.93	0.49
1:A:526:GLU:OE1	1:A:528:LYS:NZ	2.38	0.49
1:A:996:GLY:HA3	3:Q:13:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:CD	1:B:128:GLU:H	2.15	0.49
2:C:213:LEU:HD13	2:C:239:ARG:HG3	1.94	0.49
1:B:242:ASN:OD1	1:B:1014:GLN:HG3	2.12	0.49
1:A:233:MET:HE1	1:A:345:THR:N	2.27	0.49
1:B:544:GLU:OE1	1:B:546:ILE:HD11	2.12	0.49
1:B:774:TYR:CE2	1:B:871:GLY:HA3	2.47	0.49
1:A:405:TYR:HB2	3:Q:4:ALA:HB2	1.93	0.49
1:A:797:MET:HG3	1:A:814:TYR:CD1	2.48	0.49
2:C:34:PRO:HB3	8:C:798:HOH:O	2.13	0.49
1:B:239:ILE:HD12	1:B:338:PHE:HE2	1.77	0.49
2:C:97:ARG:HH21	2:C:102:GLU:CB	2.19	0.49
1:A:170:GLY:HA3	1:A:725:ARG:NH2	2.28	0.49
1:B:411:THR:HB	1:B:990:PHE:CE2	2.48	0.49
1:B:825:THR:HB	1:B:827:LYS:HG3	1.94	0.49
2:C:156:GLN:OE1	2:C:212:ARG:NH2	2.40	0.49
1:B:646:TRP:O	1:B:712:PHE:N	2.40	0.48
1:A:1006:SER:OG	1:A:1008:GLN:NE2	2.46	0.48
1:A:220:ALA:HB1	1:A:700:GLN:CD	2.34	0.48
1:A:440:THR:HB	2:D:316:LYS:HB3	1.95	0.48
1:A:680:GLU:O	1:B:572:LYS:HD3	2.13	0.48
2:C:79:ASN:HB3	3:P:5:GLY:CA	2.37	0.48
2:D:93:ASN:HB2	2:D:499:TRP:CZ3	2.48	0.48
1:A:250:ILE:CB	1:A:359:MET:HE1	2.44	0.48
1:B:489:THR:HB	1:B:514:TYR:HB2	1.95	0.48
2:C:123:PHE:HZ	2:C:148:PHE:HB3	1.79	0.48
1:A:250:ILE:CB	1:A:359:MET:CE	2.89	0.48
7:C:601:PLM:H51	5:C:602:LMT:H32	1.95	0.48
1:A:531:ILE:HG23	1:A:532:ASP:OD2	2.13	0.48
1:A:646:TRP:O	1:A:712:PHE:N	2.43	0.48
1:A:405:TYR:OH	1:A:894:ASN:HB3	2.13	0.48
1:A:858:LYS:HB3	1:A:890:TRP:CD1	2.48	0.48
1:B:573:THR:HG23	8:B:1326:HOH:O	2.12	0.48
2:D:351:GLY:HA3	2:D:460:LEU:HD21	1.95	0.48
2:D:441:ASP:HB3	2:D:445:TRP:CZ3	2.48	0.48
1:B:650:LEU:HD11	1:B:707:LEU:HD21	1.95	0.48
1:B:836:VAL:HG22	1:B:837:ASP:H	1.79	0.48
3:P:10:ARG:H	3:P:10:ARG:HD3	1.78	0.48
2:C:67:GLN:HA	2:C:84:PHE:O	2.14	0.47
2:D:55:THR:HG23	2:D:112:VAL:HG23	1.96	0.47
1:B:285:LYS:HB3	1:B:315:PHE:CE2	2.48	0.47
1:B:920:GLU:HA	1:B:923:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:425:GLN:O	2:C:429:THR:OG1	2.25	0.47
1:B:359:MET:HG2	8:B:1269:HOH:O	2.14	0.47
1:B:815:MET:HA	1:B:853:GLU:HG2	1.95	0.47
1:A:266:LEU:O	1:A:270:VAL:HG23	2.15	0.47
1:B:281:VAL:O	1:B:285:LYS:HG2	2.13	0.47
1:A:424:PHE:CE2	1:A:430:LEU:HD13	2.50	0.47
1:B:146:VAL:HG21	1:B:205:VAL:HG21	1.97	0.47
1:B:508:GLU:OE2	8:B:1202:HOH:O	2.20	0.47
1:A:641:ILE:O	1:A:643:GLU:N	2.44	0.47
1:A:237:GLY:HA3	1:B:379:ILE:HG23	1.96	0.47
1:A:612:ASN:HB2	1:A:626:TRP:CE3	2.50	0.47
1:B:181:ILE:HD12	1:B:223:VAL:HG13	1.97	0.47
1:B:635:ASP:OD2	1:B:638:ASN:ND2	2.41	0.47
1:B:831:TYR:HA	1:B:843:VAL:O	2.14	0.47
2:D:236:TYR:CZ	2:D:258:MET:HG2	2.50	0.47
1:B:747:GLN:HB3	1:B:749:VAL:HG13	1.96	0.47
2:D:63:TYR:HB3	2:D:84:PHE:CE2	2.50	0.47
2:D:201:THR:OG1	2:D:204:GLN:HG3	2.15	0.47
1:A:652:LEU:HD23	1:A:707:LEU:HD13	1.97	0.47
1:A:546:ILE:HG12	1:A:589:TYR:HB2	1.96	0.47
1:B:636:ILE:HG21	1:B:650:LEU:HD23	1.96	0.47
2:C:301:THR:O	8:C:702:HOH:O	2.21	0.47
1:A:293:GLU:OE2	8:A:1204:HOH:O	2.21	0.46
1:A:866:GLY:HA3	1:A:885:TYR:CZ	2.49	0.46
1:A:894:ASN:OD1	3:Q:7:ASN:HA	2.15	0.46
2:C:66:LEU:HD13	2:C:81:LEU:HD22	1.98	0.46
1:B:126:SER:OG	1:B:127:SER:N	2.48	0.46
2:C:472:GLN:NE2	8:C:705:HOH:O	2.47	0.46
2:D:110:TYR:CD2	2:D:485:PRO:HG2	2.51	0.46
3:Q:11:GLY:O	3:Q:12:SER:HB3	2.15	0.46
1:A:564:LYS:HE2	2:C:30:ASP:OD2	2.16	0.46
1:B:963:PHE:CE2	1:B:971:GLY:HA2	2.50	0.46
1:A:411:THR:HB	1:A:990:PHE:CE1	2.51	0.46
1:A:918:TRP:HE1	1:A:923:LYS:HG2	1.80	0.46
2:C:106:ILE:HG23	2:C:482:TRP:CE3	2.50	0.46
2:C:344:LYS:HD2	2:C:352:TYR:CE1	2.50	0.46
2:C:38:PHE:H	2:C:137:LYS:HZ1	1.64	0.46
1:A:464:VAL:O	1:A:483:GLY:HA2	2.16	0.46
1:A:730:MET:HG2	1:A:732:ILE:CG1	2.46	0.46
1:A:757:VAL:O	1:A:780:ASN:ND2	2.49	0.46
2:C:106:ILE:HD13	2:C:482:TRP:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:GLU:HG2	1:A:198:ASN:OD1	2.16	0.46
1:A:134:PRO:HG2	1:A:1008:GLN:OE1	2.15	0.46
1:A:804:ILE:HG21	1:A:855:ARG:HG3	1.97	0.46
1:B:327:LYS:HD2	1:B:361:ARG:HH12	1.81	0.46
1:B:484:VAL:HG22	1:B:486:ILE:HG13	1.98	0.46
1:A:740:SER:O	2:D:118:GLN:HG3	2.16	0.45
5:A:1102:LMT:H12	5:A:1102:LMT:O2'	2.14	0.45
1:B:910:LYS:HB3	1:B:914:LEU:HD12	1.98	0.45
2:D:244:LEU:HD22	2:D:387:ILE:HG12	1.98	0.45
1:A:187:THR:HG22	1:A:188:SER:O	2.16	0.45
1:A:218:ARG:HD3	1:A:663:GLU:HG3	1.97	0.45
1:B:588:ALA:H	1:B:616:SER:HB3	1.80	0.45
1:B:652:LEU:HD12	1:B:652:LEU:HA	1.81	0.45
1:B:444:MET:CE	1:B:449:PHE:HA	2.47	0.45
1:B:735:PRO:HG2	1:B:796:TYR:CE2	2.52	0.45
1:B:905:LEU:HB3	1:B:908:LEU:HD12	1.97	0.45
1:B:281:VAL:HG12	1:B:285:LYS:HE2	1.98	0.45
2:D:155:LEU:HD13	2:D:230:VAL:HG21	1.98	0.45
3:P:3:THR:O	3:P:3:THR:OG1	2.24	0.45
1:A:251:LEU:HG	1:A:1005:ASN:O	2.17	0.45
1:A:120:GLY:HA3	1:A:211:ALA:HB2	1.99	0.45
1:A:538:THR:HB	1:A:597:ASN:HB2	1.98	0.45
1:A:574:GLY:HA2	2:C:296:THR:HG21	1.97	0.45
1:A:206:LEU:HD13	1:A:211:ALA:O	2.17	0.45
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.87	0.45
1:B:635:ASP:CG	1:B:638:ASN:HD22	2.20	0.45
2:C:206:TYR:CE1	2:C:246:LEU:HD21	2.51	0.45
1:A:214:ILE:HD13	1:A:595:ARG:NH2	2.32	0.45
1:A:978:ALA:HA	1:A:1008:GLN:O	2.18	0.44
2:C:58:PRO:HD3	8:C:729:HOH:O	2.17	0.44
2:C:403:LYS:HG2	2:C:404:TYR:CD1	2.52	0.44
1:A:783:ARG:NH1	1:A:810:PRO:HD3	2.32	0.44
1:A:896:ARG:HD3	1:A:942:GLU:OE2	2.18	0.44
1:B:883:PHE:CZ	1:B:949:LEU:HD13	2.52	0.44
1:B:601:ASP:HB3	1:B:602:LYS:H	1.64	0.44
1:B:738:TYR:CZ	2:C:98:ALA:HB3	2.52	0.44
2:D:161:TRP:CD1	2:D:242:ILE:HG12	2.52	0.44
2:D:217:ILE:HG23	2:D:232:ARG:HD3	2.00	0.44
1:B:696:SER:OG	1:B:697:TRP:N	2.49	0.44
1:B:239:ILE:HD12	1:B:338:PHE:CE2	2.51	0.44
1:A:877:LEU:HD12	1:A:877:LEU:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:CG	1:B:159:THR:HG22	2.37	0.44
2:C:176:VAL:HG23	2:C:177:ASN:O	2.17	0.44
1:A:178:PRO:HB2	1:A:224:VAL:HG23	2.00	0.44
1:A:831:TYR:CG	1:A:842:LYS:HE3	2.53	0.43
2:C:268:ALA:HB1	2:C:273:GLU:HB3	2.00	0.43
2:D:240:ALA:HB2	2:D:255:ASP:HB2	1.99	0.43
1:A:125:VAL:HG13	1:A:129:LYS:HD3	2.00	0.43
1:A:575:ASN:HB3	2:D:365:ASP:HA	2.00	0.43
1:A:397:ARG:HG3	1:A:455:PHE:CD1	2.53	0.43
1:B:591:SER:OG	1:B:613:ASP:OD1	2.24	0.43
1:B:673:VAL:HG23	2:C:32:GLN:HG3	1.99	0.43
1:B:836:VAL:CG2	1:B:841:ASN:HB2	2.48	0.43
2:D:98:ALA:HA	2:D:103:VAL:HG22	1.99	0.43
1:B:784:GLN:HB3	1:B:810:PRO:HB3	2.00	0.43
2:C:137:LYS:HD3	2:C:137:LYS:N	2.34	0.43
1:A:186:GLN:NE2	1:A:546:ILE:HD13	2.34	0.43
1:A:203:MET:HB2	1:A:203:MET:HE2	1.80	0.43
1:A:774:TYR:CE2	1:A:871:GLY:HA3	2.54	0.43
1:B:601:ASP:HB3	1:B:603:TRP:CD1	2.52	0.43
1:A:721:ASP:HB2	1:A:758:ASP:HB2	2.01	0.43
2:C:212:ARG:HA	2:C:212:ARG:HD2	1.76	0.43
1:A:896:ARG:HA	1:A:899:THR:OG1	2.17	0.43
1:A:985:THR:HG21	1:A:992:PRO:HG3	2.01	0.43
1:B:444:MET:HB3	1:B:444:MET:HE2	1.90	0.43
2:C:206:TYR:CZ	2:C:246:LEU:HD21	2.53	0.43
1:A:898:PHE:CD1	1:A:905:LEU:HD13	2.54	0.43
1:A:966:GLN:NE2	1:A:969:ILE:O	2.51	0.43
2:D:137:LYS:HG3	2:D:138:ASN:HD22	1.83	0.43
2:C:22:LEU:HA	2:C:22:LEU:HD23	1.75	0.43
2:C:27:GLU:OE1	8:C:703:HOH:O	2.22	0.43
2:C:441:ASP:HB3	2:C:445:TRP:CZ3	2.53	0.43
1:A:175:SER:HB3	1:A:663:GLU:HB3	2.01	0.42
1:A:293:GLU:HB3	1:A:306:TYR:CE1	2.54	0.42
1:A:531:ILE:HD12	1:A:531:ILE:HA	1.87	0.42
1:A:976:LEU:HD12	1:A:976:LEU:HA	1.80	0.42
1:A:250:ILE:HG13	1:A:359:MET:HE1	1.99	0.42
1:B:121:SER:HB3	1:B:207:LYS:HB2	2.00	0.42
1:A:166:ILE:HD12	1:A:222:GLY:HA3	2.01	0.42
1:A:358:GLY:N	1:A:364:ALA:O	2.50	0.42
1:B:737:PRO:HG3	2:C:196:ILE:HG12	2.01	0.42
1:B:889:LYS:HG2	1:B:944:ALA:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:416:VAL:HG21	2:C:423:ALA:HB1	2.02	0.42
1:A:568:LEU:HB2	1:B:582:HIS:HB2	2.02	0.42
1:A:720:VAL:HA	1:A:758:ASP:O	2.20	0.42
1:B:185:MET:SD	8:B:1344:HOH:O	2.61	0.42
1:B:441:ARG:HD2	1:B:501:TYR:O	2.19	0.42
2:D:275:GLU:HB2	2:D:340:VAL:HG22	2.00	0.42
1:A:864:ILE:HB	1:A:887:VAL:HB	2.01	0.42
5:B:1102:LMT:H6'1	2:C:24:ARG:CZ	2.50	0.42
1:A:905:LEU:HD22	1:A:908:LEU:HD11	2.02	0.42
2:D:327:VAL:O	2:D:330:LEU:HB2	2.20	0.42
1:A:433:VAL:HA	1:A:443:SER:O	2.20	0.42
2:C:306:ASN:OD1	2:C:307:GLY:N	2.53	0.42
2:D:213:LEU:HD23	2:D:213:LEU:HA	1.93	0.42
1:A:639:LYS:HG3	1:A:640:PHE:CZ	2.54	0.42
2:C:421:MET:O	2:C:425:GLN:HG3	2.19	0.42
2:D:66:LEU:HD13	2:D:81:LEU:HD22	2.02	0.42
2:D:155:LEU:CD1	2:D:230:VAL:HG21	2.49	0.42
1:A:434:TYR:HE1	1:A:436:MET:CE	2.33	0.42
1:A:889:LYS:HE3	1:A:992:PRO:O	2.20	0.42
1:B:894:ASN:OD1	3:P:7:ASN:HA	2.19	0.41
2:C:182:ASP:HA	2:C:202:LYS:HD3	2.01	0.41
2:C:222:GLU:HA	2:C:232:ARG:HD2	2.02	0.41
2:D:421:MET:O	2:D:425:GLN:HG3	2.20	0.41
1:A:189:LEU:HD23	1:A:189:LEU:HA	1.79	0.41
1:A:362:GLU:HA	1:A:363:PRO:HD3	1.94	0.41
2:D:409:SER:OG	2:D:415:GLU:HA	2.20	0.41
1:A:256:LEU:HD21	1:A:414:VAL:CG1	2.50	0.41
1:A:863:PRO:HD2	1:A:888:GLY:HA3	2.02	0.41
1:A:891:MET:HE3	1:A:987:TYR:CZ	2.55	0.41
1:A:975:TYR:CZ	1:A:1012:GLY:HA3	2.55	0.41
4:B:1101:3PE:H222	4:B:1101:3PE:H31	2.02	0.41
1:A:496:MET:HB3	1:A:496:MET:HE3	1.95	0.41
1:A:737:PRO:HG3	2:D:196:ILE:HG12	2.02	0.41
1:B:545:TYR:OH	1:B:547:GLU:OE1	2.24	0.41
1:A:285:LYS:HG2	1:A:315:PHE:CD2	2.56	0.41
1:A:233:MET:O	1:A:234:SER:HB2	2.21	0.41
2:D:306:ASN:HB2	2:D:353:LEU:HD13	2.02	0.41
5:C:602:LMT:O3'	5:C:602:LMT:H1B	2.20	0.41
1:A:126:SER:OG	1:A:128:GLU:OE2	2.39	0.41
1:A:462:ALA:HB2	6:A:1103:C8E:H141	2.03	0.41
1:A:798:LEU:HD11	1:A:805:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:ASN:HB2	1:A:626:TRP:CZ3	2.56	0.41
1:A:646:TRP:CH2	1:A:647:LEU:HD12	2.56	0.41
1:A:836:VAL:HG13	1:A:841:ASN:O	2.21	0.41
1:B:143:GLN:OE1	1:B:950:LYS:NZ	2.25	0.41
1:B:830:TRP:O	1:B:844:THR:HA	2.20	0.41
1:B:894:ASN:HB2	1:B:998:VAL:CG2	2.51	0.41
2:C:161:TRP:CD1	2:C:242:ILE:HG12	2.56	0.41
2:C:405:LEU:HD12	2:C:405:LEU:HA	1.91	0.41
1:A:595:ARG:NH1	8:A:1215:HOH:O	2.38	0.41
1:B:729:ASP:HB3	1:B:748:ASN:HB3	2.01	0.41
2:C:171:GLU:OE2	2:C:171:GLU:N	2.47	0.41
2:D:389:VAL:HG11	2:D:405:LEU:HB2	2.03	0.41
1:A:830:TRP:CZ3	1:A:848:TYR:HB2	2.56	0.40
4:B:1101:3PE:H271	5:B:1102:LMT:H101	2.02	0.40
1:A:156:GLY:HA3	1:A:1004:PRO:O	2.21	0.40
1:A:939:HIS:O	1:A:940:LEU:HB2	2.22	0.40
1:B:421:TYR:CE2	1:B:436:MET:HG2	2.56	0.40
1:B:528:LYS:HG2	1:B:538:THR:HG22	2.02	0.40
1:B:672:LEU:HD23	1:B:672:LEU:HA	1.92	0.40
1:A:480:ALA:HB1	4:A:1101:3PE:H292	2.03	0.40
1:A:559:GLY:HA3	1:A:572:LYS:HG3	2.02	0.40
1:A:887:VAL:HA	1:A:945:SER:HB3	2.02	0.40
1:B:543:HIS:NE2	4:B:1101:3PE:H321	2.37	0.40
2:C:51:LEU:HD12	2:C:51:LEU:HA	1.96	0.40
2:C:65:GLU:OE2	2:C:434:GLY:N	2.41	0.40
2:D:45:ARG:HD3	2:D:45:ARG:HH11	1.75	0.40
2:D:266:ILE:HG12	2:D:285:PRO:HD2	2.04	0.40
2:D:488:ASP:HA	2:D:491:THR:HG22	2.04	0.40
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.89	0.40
1:A:737:PRO:HB3	2:D:491:THR:HG21	2.04	0.40
1:B:220:ALA:HB1	1:B:700:GLN:OE1	2.22	0.40
1:B:769:LYS:HA	1:B:769:LYS:HD2	1.92	0.40
1:B:897:TYR:O	1:B:901:ASN:HB2	2.22	0.40
2:D:26:PRO:HG2	2:D:29:LYS:HB2	2.02	0.40
2:D:281:ASP:OD1	2:D:377:ARG:NH2	2.52	0.40
1:A:535:HIS:CE1	1:A:598:TYR:HH	2.36	0.40
1:B:543:HIS:CE1	4:B:1101:3PE:H332	2.57	0.40
1:B:583:ARG:HD2	8:B:1351:HOH:O	2.20	0.40
1:B:653:LYS:HE2	1:B:653:LYS:HB2	1.61	0.40
1:B:720:VAL:HG23	1:B:759:LEU:HB3	2.04	0.40
1:B:730:MET:HE2	1:B:750:GLY:HA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:ALA:HA	1:B:1008:GLN:O	2.22	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	901/997 (90%)	836 (93%)	60 (7%)	5 (1%)	25	45
1	B	898/997 (90%)	844 (94%)	51 (6%)	3 (0%)	41	62
2	C	479/488 (98%)	453 (95%)	23 (5%)	3 (1%)	25	45
2	D	480/488 (98%)	460 (96%)	20 (4%)	0	100	100
3	P	11/13 (85%)	7 (64%)	1 (9%)	3 (27%)	0	0
3	Q	11/13 (85%)	7 (64%)	2 (18%)	2 (18%)	0	0
All	All	2780/2996 (93%)	2607 (94%)	157 (6%)	16 (1%)	25	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Q	3	THR
1	A	234	SER
3	P	3	THR
3	P	6	ALA
3	Q	6	ALA
1	A	132	GLU
1	A	173	GLY
1	A	770	ASP
1	B	838	ALA
3	P	13	ALA
1	B	712	PHE

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Mol	Chain	Res	Type
2	C	68	SER
2	C	174	THR
2	C	420	ASN
1	A	874	TRP
1	B	173	GLY

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	754/832 (91%)	730 (97%)	24 (3%)	39 63
1	B	754/832 (91%)	734 (97%)	20 (3%)	44 69
2	C	401/408 (98%)	397 (99%)	4 (1%)	76 89
2	D	402/408 (98%)	396 (98%)	6 (2%)	65 82
3	P	7/7 (100%)	6 (86%)	1 (14%)	3 5
3	Q	7/7 (100%)	7 (100%)	0	100 100
All	All	2325/2494 (93%)	2270 (98%)	55 (2%)	49 72

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	251	LEU
1	A	256	LEU
1	A	293	GLU
1	A	339	SER
1	A	350	SER
1	A	368	ARG
1	A	459	SER
1	A	465	ASN
1	A	474	LYS
1	A	493	SER
1	A	556	SER
1	A	564	LYS

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Mol	Chain	Res	Type
1	A	601	ASP
1	A	603	TRP
1	A	611	ARG
1	A	629	SER
1	A	874	TRP
1	A	879	LEU
1	A	894	ASN
1	A	939	HIS
1	A	950	LYS
1	A	966	GLN
1	A	1003	TYR
1	B	210	SER
1	B	230	LYS
1	B	232	LYS
1	B	277	ASN
1	B	350	SER
1	B	375	PHE
1	B	419	ARG
1	B	459	SER
1	B	600	PHE
1	B	607	ASP
1	B	611	ARG
1	B	616	SER
1	B	752	MET
1	B	761	LEU
1	B	770	ASP
1	B	894	ASN
1	B	924	GLU
1	B	966	GLN
1	B	1003	TYR
1	B	1017	PHE
2	C	99	ASP
2	C	368	ASP
2	C	379	PHE
2	C	488	ASP
2	D	23	ASP
2	D	94	ASP
2	D	368	ASP
2	D	379	PHE
2	D	437	SER
2	D	488	ASP
3	P	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	356	GLN
1	B	388	ASN
1	B	713	ASN
1	B	768	ASN
2	C	276	ASN
2	D	79	ASN
2	D	223	ASN

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)

11 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	$\#\|Z\| > 2$
5	LMT	D	602	-	34,34,36	1.17	5 (14%)	45,45,47	1.14	3 (6%)
5	LMT	A	1102	-	36,36,36	1.01	3 (8%)	47,47,47	1.70	7 (14%)
7	PLM	C	601	2	13,13,17	0.89	0	12,12,17	0.49	0
6	C8E	A	1104	-	20,20,20	0.50	0	19,19,19	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	3PE	A	1101	2	30,30,50	1.17	3 (10%)	32,32,55	1.45	3 (9%)
5	LMT	B	1102	-	36,36,36	1.06	2 (5%)	47,47,47	1.21	4 (8%)
4	3PE	B	1101	2	31,31,50	1.18	4 (12%)	33,33,55	1.46	3 (9%)
6	C8E	A	1103	-	20,20,20	0.53	0	19,19,19	0.51	0
5	LMT	C	602	-	34,34,36	1.18	4 (11%)	45,45,47	1.15	3 (6%)
7	PLM	D	601	2	14,14,17	0.54	0	13,13,17	0.59	0
6	C8E	B	1103	-	6,6,20	0.58	0	5,5,19	0.57	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
5	LMT	D	602	-	-	9/19/59/61	0/2/2/2
5	LMT	A	1102	-	-	10/21/61/61	0/2/2/2
7	PLM	C	601	2	-	5/10/11/15	-
6	C8E	A	1104	-	-	10/18/18/18	-
4	3PE	A	1101	2	-	12/31/31/54	-
5	LMT	B	1102	-	-	14/21/61/61	0/2/2/2
4	3PE	B	1101	2	-	12/32/32/54	-
6	C8E	A	1103	-	-	11/18/18/18	-
5	LMT	C	602	-	-	9/19/59/61	0/2/2/2
7	PLM	D	601	2	-	3/11/12/15	-
6	C8E	B	1103	-	-	4/4/4/18	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	3PE	O21-C2	-3.37	1.41	1.47
4	B	1101	3PE	O31-C31	3.27	1.42	1.33
5	C	602	LMT	O3'-C3'	-3.24	1.35	1.43
4	B	1101	3PE	O21-C2	-3.14	1.41	1.47
5	D	602	LMT	O3'-C3'	-2.92	1.36	1.43
4	A	1101	3PE	O31-C31	2.64	1.41	1.33
4	B	1101	3PE	O21-C21	2.59	1.41	1.34
4	A	1101	3PE	O21-C21	2.49	1.41	1.34
5	B	1102	LMT	O2B-C2B	-2.40	1.37	1.43
5	D	602	LMT	O3B-C3B	-2.39	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	LMT	O4'-C4B	-2.36	1.37	1.43
5	C	602	LMT	O2B-C2B	-2.29	1.37	1.43
5	A	1102	LMT	C1B-C2B	2.25	1.59	1.52
4	B	1101	3PE	O31-C3	-2.24	1.40	1.45
5	B	1102	LMT	O3'-C3'	-2.24	1.37	1.43
5	A	1102	LMT	O3B-C3B	-2.20	1.37	1.43
5	D	602	LMT	O2'-C2'	-2.17	1.37	1.43
5	D	602	LMT	O2B-C2B	-2.14	1.37	1.43
5	D	602	LMT	O1'-C1'	-2.08	1.36	1.40
5	C	602	LMT	O3B-C3B	-2.02	1.38	1.43
5	A	1102	LMT	C4'-C5'	2.02	1.58	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1102	LMT	O1'-C1'-C2'	5.24	116.48	108.30
5	A	1102	LMT	C1-O1'-C1'	5.13	122.34	113.84
4	A	1101	3PE	O21-C21-C22	4.61	121.45	111.50
4	B	1101	3PE	O21-C21-C22	4.50	121.19	111.50
4	B	1101	3PE	O31-C31-C32	4.46	125.92	111.91
5	A	1102	LMT	C3B-C4B-C5B	-4.37	102.44	110.24
5	A	1102	LMT	O5'-C5'-C4'	3.58	117.29	109.75
4	A	1101	3PE	O21-C2-C3	3.57	114.41	106.13
5	C	602	LMT	C1'-O5'-C5'	-3.56	106.71	113.69
5	C	602	LMT	C1-O1'-C1'	3.33	119.36	113.84
5	B	1102	LMT	C3'-C4'-C5'	-3.09	103.84	110.93
5	D	602	LMT	C3'-C4'-C5'	-3.03	103.98	110.93
5	B	1102	LMT	O1'-C1'-C2'	2.94	112.90	108.30
5	B	1102	LMT	O5B-C5B-C6B	2.79	113.37	106.44
4	A	1101	3PE	O31-C31-C32	2.73	120.49	111.91
5	A	1102	LMT	O5B-C5B-C6B	2.70	113.15	106.44
5	A	1102	LMT	C1'-C2'-C3'	-2.61	104.55	110.00
5	A	1102	LMT	O5B-C1B-C2B	2.53	115.70	110.35
5	D	602	LMT	O5B-C5B-C4B	2.36	113.98	109.69
4	B	1101	3PE	O31-C31-O32	-2.30	117.80	123.59
5	D	602	LMT	C1B-O5B-C5B	2.18	117.97	113.69
5	B	1102	LMT	O5B-C5B-C4B	2.02	113.37	109.69
5	C	602	LMT	O1'-C1-C2	-2.01	102.53	109.56

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	3PE	C22-C21-O21-C2
4	B	1101	3PE	C22-C21-O21-C2
5	A	1102	LMT	C2'-C1'-O1'-C1
5	B	1102	LMT	O5B-C1B-O1B-C4'
5	C	602	LMT	O5'-C1'-O1'-C1
5	B	1102	LMT	C4B-C5B-C6B-O6B
5	A	1102	LMT	C4'-C5'-C6'-O6'
4	B	1101	3PE	O32-C31-O31-C3
4	A	1101	3PE	O22-C21-O21-C2
4	B	1101	3PE	O22-C21-O21-C2
4	B	1101	3PE	C32-C31-O31-C3
5	C	602	LMT	O5B-C5B-C6B-O6B
5	A	1102	LMT	C4B-C5B-C6B-O6B
5	D	602	LMT	O5B-C5B-C6B-O6B
7	C	601	PLM	C7-C8-C9-CA
5	A	1102	LMT	O5B-C5B-C6B-O6B
5	A	1102	LMT	O5'-C5'-C6'-O6'
5	B	1102	LMT	O5B-C5B-C6B-O6B
6	A	1104	C8E	O12-C13-C14-O15
6	A	1103	C8E	C17-C16-O15-C14
5	C	602	LMT	C4B-C5B-C6B-O6B
5	B	1102	LMT	O5'-C5'-C6'-O6'
4	A	1101	3PE	C21-C22-C23-C24
4	B	1101	3PE	C31-C32-C33-C34
7	C	601	PLM	C5-C6-C7-C8
5	C	602	LMT	O1'-C1-C2-C3
5	D	602	LMT	O1'-C1-C2-C3
7	C	601	PLM	C9-CA-CB-CC
5	B	1102	LMT	C5'-C4'-O1B-C1B
6	A	1104	C8E	C6-C7-C8-O9
5	B	1102	LMT	O1'-C1-C2-C3
4	B	1101	3PE	C33-C34-C35-C36
4	B	1101	3PE	C32-C33-C34-C35
7	D	601	PLM	C4-C5-C6-C7
7	D	601	PLM	C6-C7-C8-C9
4	A	1101	3PE	C22-C23-C24-C25
5	A	1102	LMT	O5'-C1'-O1'-C1
4	A	1101	3PE	C32-C33-C34-C35
7	D	601	PLM	C3-C4-C5-C6
5	D	602	LMT	C1-C2-C3-C4
6	A	1104	C8E	O18-C19-C20-O21
5	D	602	LMT	C3-C4-C5-C6
4	B	1101	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	A	1102	LMT	C2-C3-C4-C5
5	A	1102	LMT	C3-C4-C5-C6
5	D	602	LMT	C7-C8-C9-C10
6	A	1104	C8E	O9-C10-C11-O12
4	A	1101	3PE	C28-C29-C2A-C2B
5	B	1102	LMT	C9-C10-C11-C12
5	B	1102	LMT	C3'-C4'-O1B-C1B
4	A	1101	3PE	C29-C2A-C2B-C2C
5	C	602	LMT	C5'-C4'-O1B-C1B
5	B	1102	LMT	C1-C2-C3-C4
6	A	1103	C8E	O12-C13-C14-O15
4	A	1101	3PE	C33-C34-C35-C36
5	D	602	LMT	C4B-C5B-C6B-O6B
6	A	1103	C8E	C3-C4-C5-C6
4	A	1101	3PE	C27-C28-C29-C2A
5	D	602	LMT	C2-C3-C4-C5
6	A	1103	C8E	C13-C14-O15-C16
6	A	1104	C8E	C11-C10-O9-C8
6	A	1104	C8E	C10-C11-O12-C13
6	A	1103	C8E	C5-C6-C7-C8
6	A	1104	C8E	C16-C17-O18-C19
7	C	601	PLM	C4-C5-C6-C7
5	D	602	LMT	C4-C5-C6-C7
5	C	602	LMT	C2-C3-C4-C5
6	B	1103	C8E	C17-C16-O15-C14
5	B	1102	LMT	C4'-C5'-C6'-O6'
5	C	602	LMT	C3'-C4'-O1B-C1B
6	A	1103	C8E	C1-C2-C3-C4
4	B	1101	3PE	C35-C36-C37-C38
5	A	1102	LMT	C1-C2-C3-C4
6	A	1103	C8E	C2-C3-C4-C5
6	A	1104	C8E	C20-C19-O18-C17
6	A	1103	C8E	C7-C8-O9-C10
6	A	1103	C8E	O15-C16-C17-O18
4	A	1101	3PE	C34-C35-C36-C37
7	C	601	PLM	C8-C9-CA-CB
5	C	602	LMT	C7-C8-C9-C10
5	B	1102	LMT	C7-C8-C9-C10
6	A	1103	C8E	C6-C7-C8-O9
6	A	1104	C8E	C17-C16-O15-C14
5	B	1102	LMT	C3-C4-C5-C6
5	B	1102	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	D	602	LMT	C5'-C4'-O1B-C1B
5	C	602	LMT	C3-C4-C5-C6
6	B	1103	C8E	C20-C19-O18-C17
4	B	1101	3PE	O31-C31-C32-C33
4	A	1101	3PE	O31-C31-C32-C33
6	B	1103	C8E	C16-C17-O18-C19
6	A	1104	C8E	O15-C16-C17-O18
4	A	1101	3PE	O32-C31-C32-C33
6	A	1103	C8E	O9-C10-C11-O12
4	B	1101	3PE	O32-C31-C32-C33
4	B	1101	3PE	C37-C38-C39-C3A
5	A	1102	LMT	C2-C1-O1'-C1'
5	B	1102	LMT	C2-C1-O1'-C1'
6	B	1103	C8E	O15-C16-C17-O18

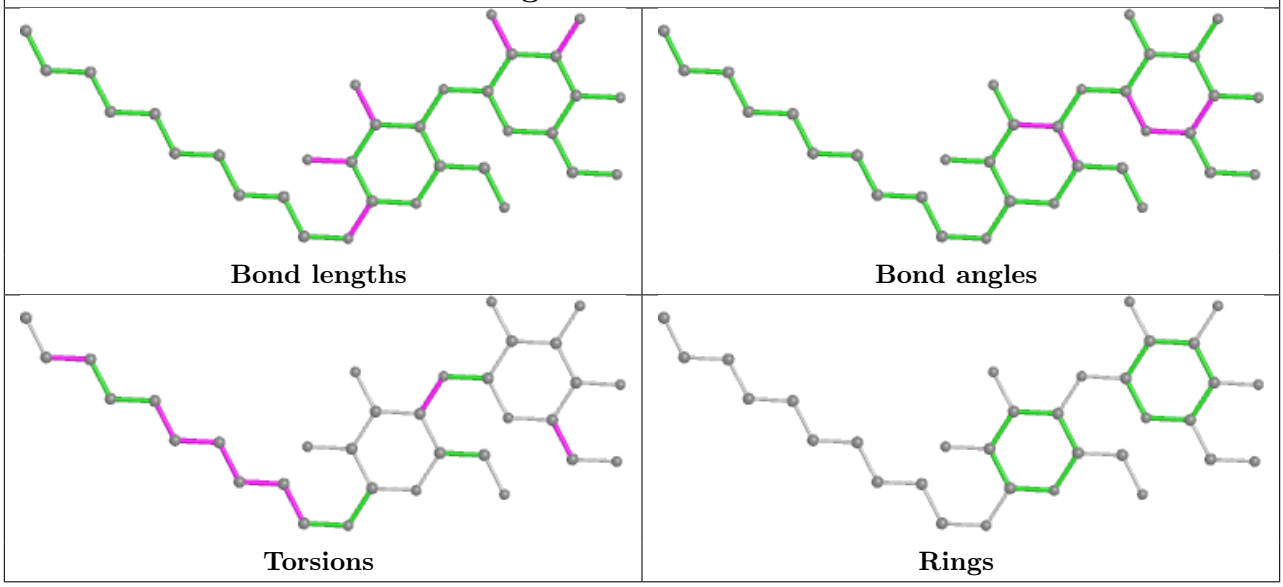
There are no ring outliers.

7 monomers are involved in 17 short contacts:

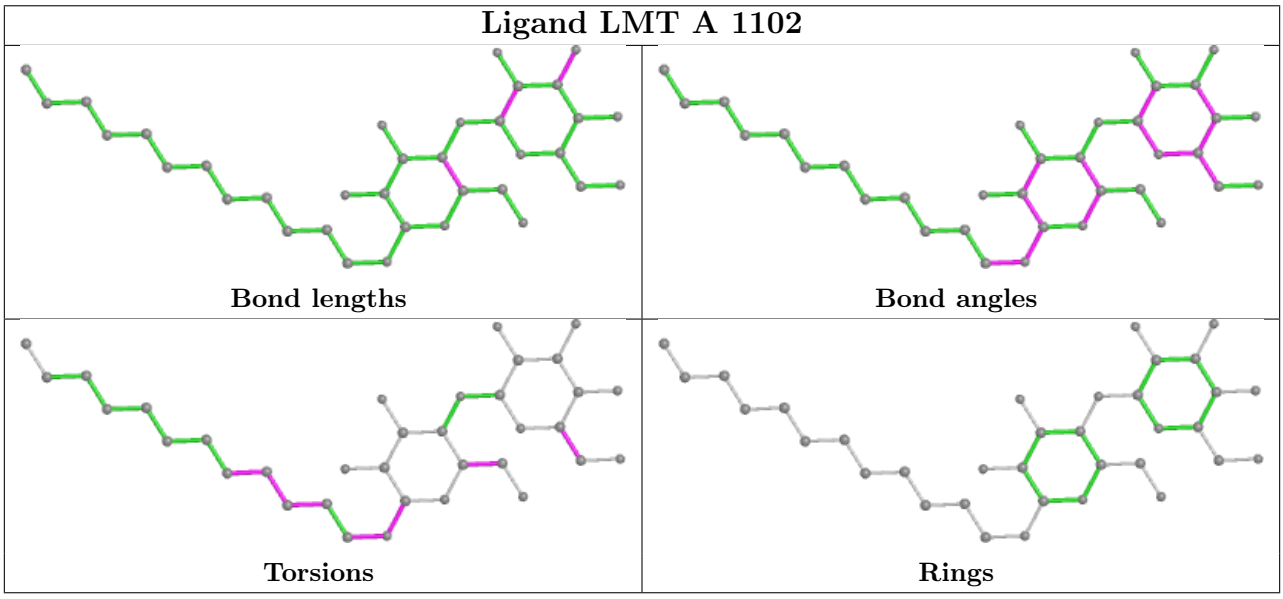
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1102	LMT	2	0
7	C	601	PLM	1	0
4	A	1101	3PE	2	0
5	B	1102	LMT	2	0
4	B	1101	3PE	4	0
6	A	1103	C8E	4	0
5	C	602	LMT	4	0

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.

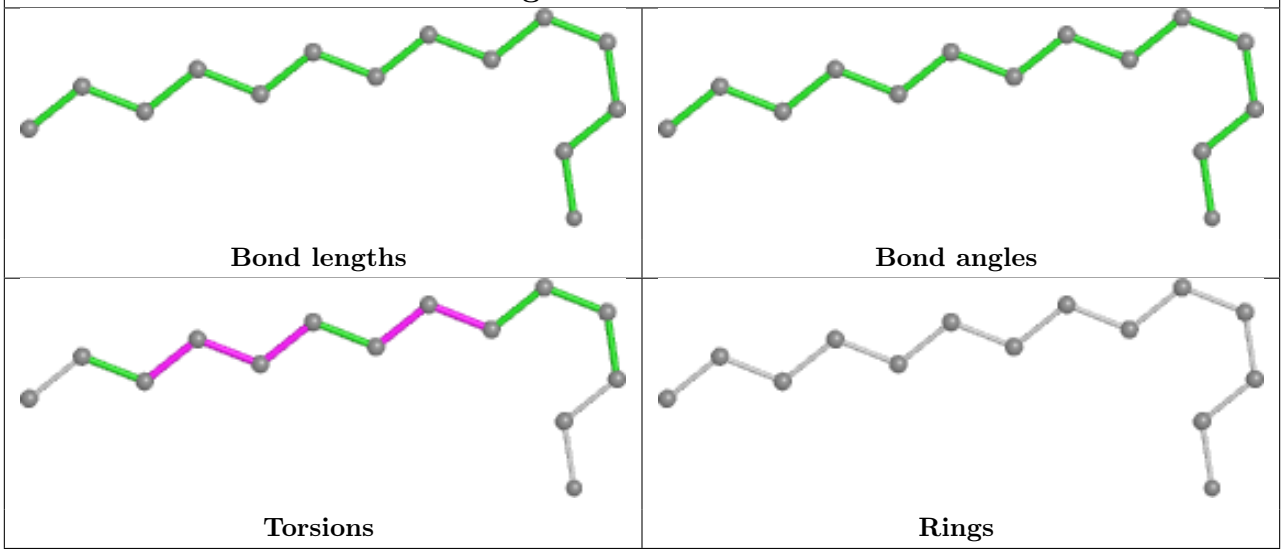
Ligand LMT D 602



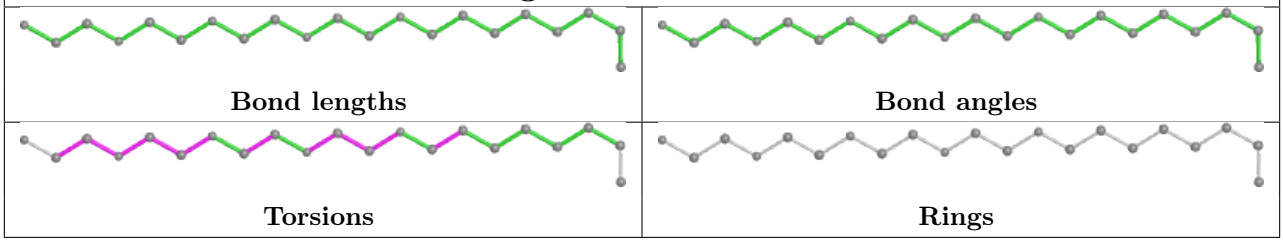
Ligand LMT A 1102



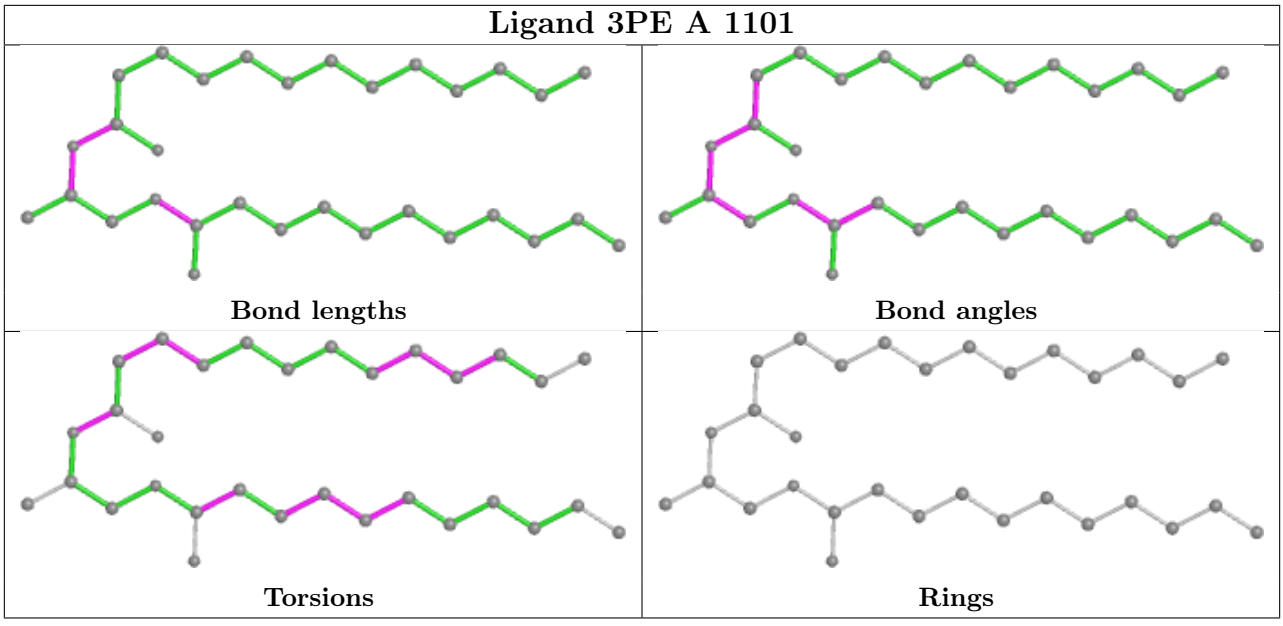
Ligand PLM C 601



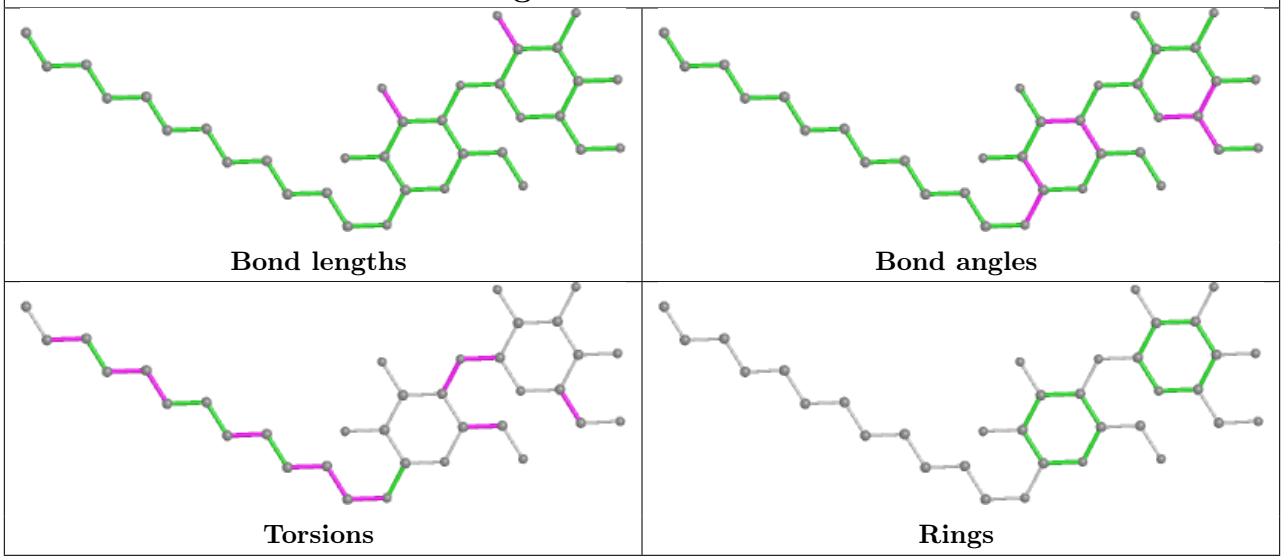
Ligand C8E A 1104



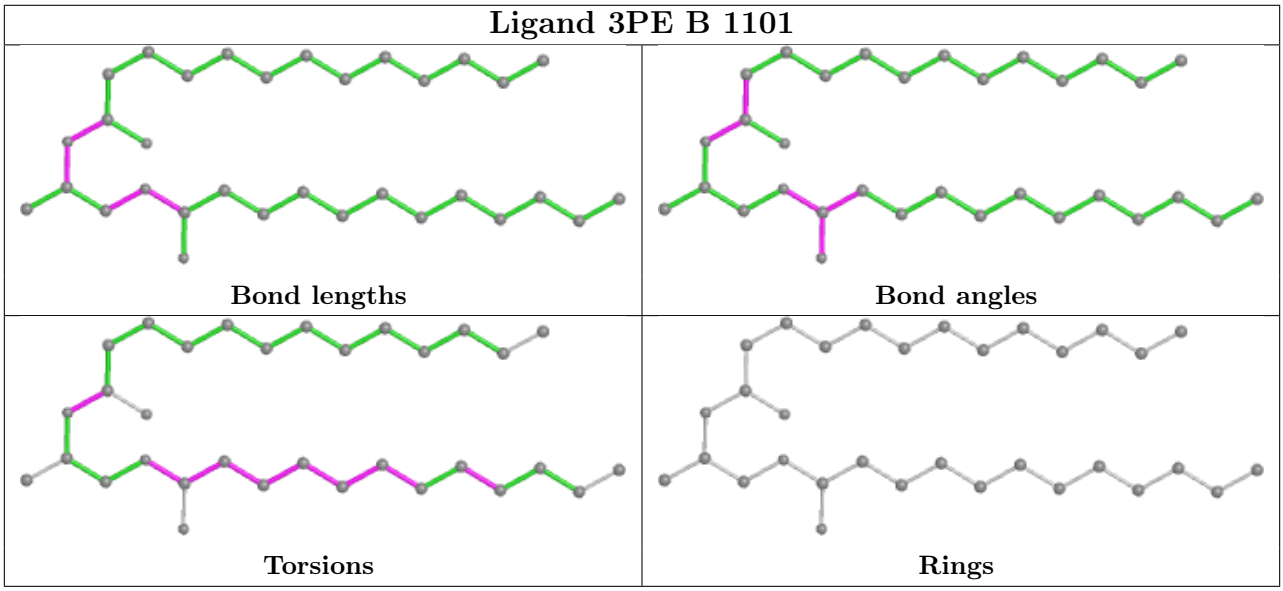
Ligand 3PE A 1101



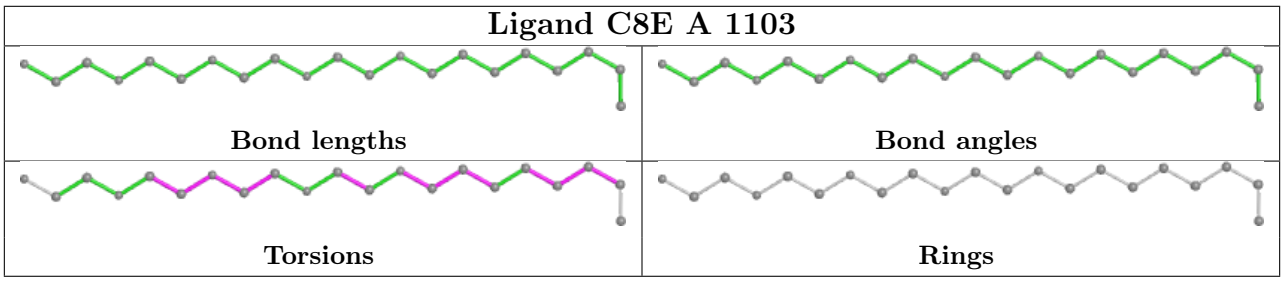
Ligand LMT B 1102

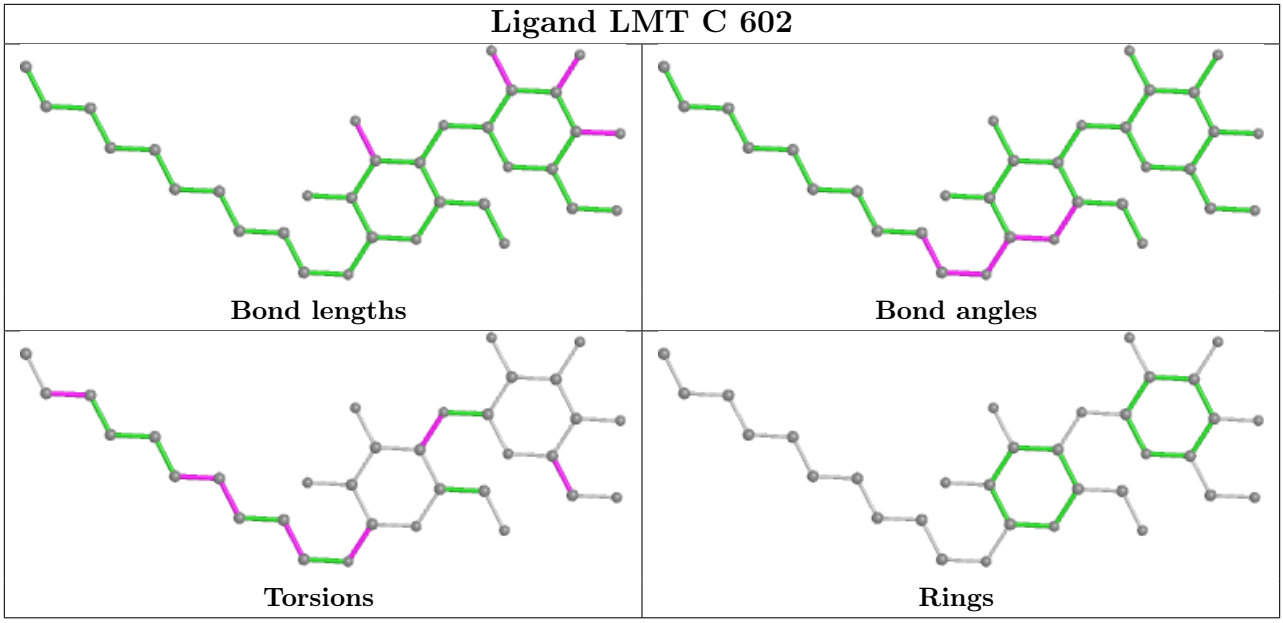


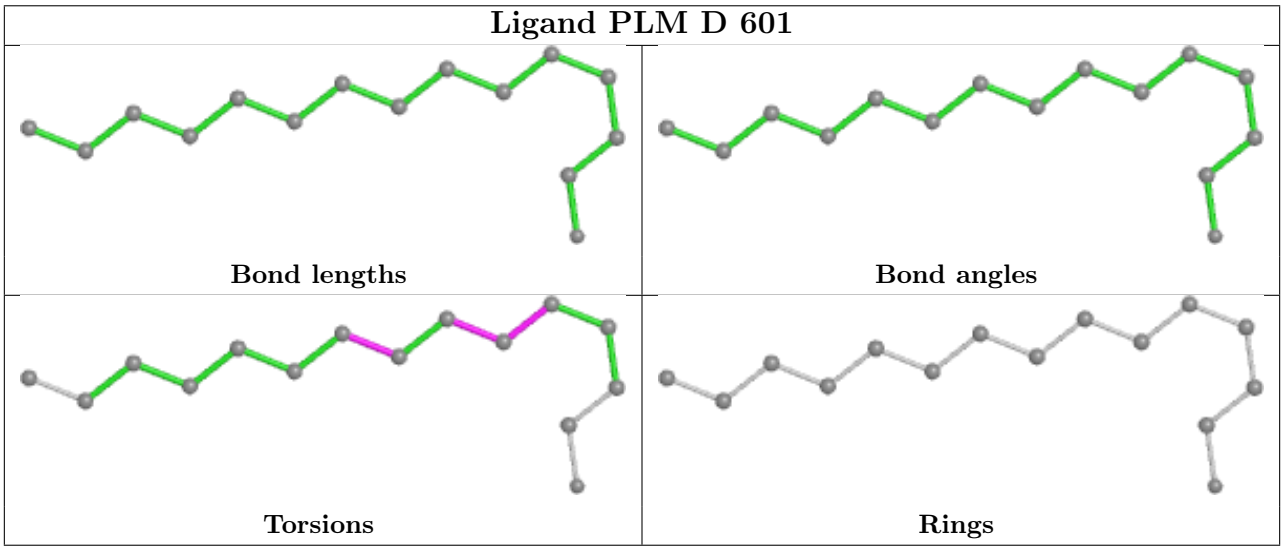
Ligand 3PE B 1101

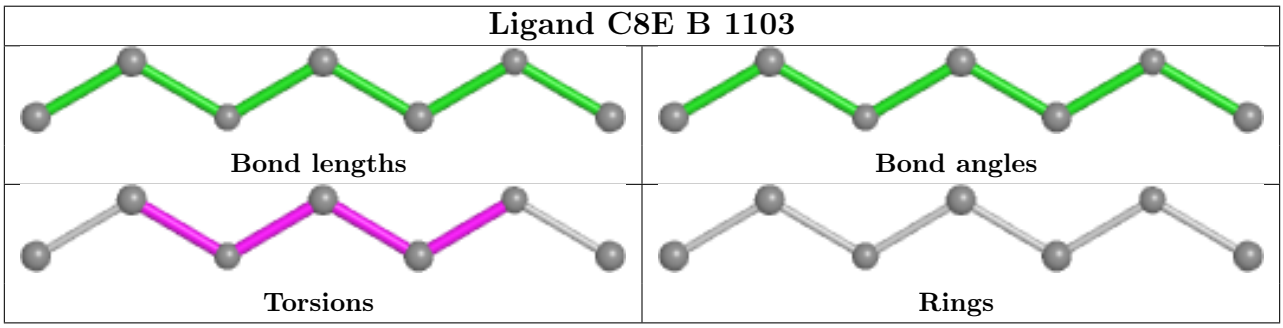


Ligand C8E A 1103









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	903/997 (90%)	0.12	16 (1%)	68	64	27, 52, 96, 161	0
1	B	902/997 (90%)	0.08	11 (1%)	79	76	29, 51, 94, 153	0
2	C	481/488 (98%)	0.08	1 (0%)	95	95	33, 48, 70, 95	0
2	D	482/488 (98%)	0.10	6 (1%)	79	76	32, 48, 69, 82	0
3	P	13/13 (100%)	1.39	2 (15%)	2	1	68, 73, 87, 96	0
3	Q	13/13 (100%)	1.37	3 (23%)	0	0	51, 77, 117, 120	0
All	All	2794/2996 (93%)	0.11	39 (1%)	75	71	27, 50, 87, 161	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	GLN	5.7
3	Q	5	GLY	3.8
1	A	643	GLU	3.7
1	B	115	LEU	3.6
1	B	839	ASP	3.3
1	A	645	ASN	3.2
3	Q	12	SER	3.2
1	B	642	GLN	3.2
1	A	161	VAL	3.1
3	P	3	THR	3.1
3	Q	3	THR	2.9
1	A	608	PHE	2.9
1	A	864	ILE	2.8
2	D	287	ILE	2.7
1	A	308	LYS	2.7
1	A	307	GLY	2.6
1	B	531	ILE	2.6
1	A	875	LYS	2.5
2	D	236	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	749	VAL	2.5
3	P	9	GLN	2.4
1	B	769	LYS	2.4
1	B	464	VAL	2.4
1	A	595	ARG	2.3
2	C	433	ILE	2.3
1	A	136	ALA	2.3
2	D	496	ILE	2.3
2	D	288	ILE	2.2
1	A	116	SER	2.2
1	A	642	GLN	2.2
2	D	176	VAL	2.2
1	A	768	ASN	2.2
1	A	874	TRP	2.2
1	B	794	ASN	2.2
1	B	936	PHE	2.2
2	D	178	SER	2.2
1	B	215	TYR	2.1
1	B	219	ALA	2.0
1	A	596	PHE	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
5	LMT	A	1102	35/35	0.79	0.26	53,90,105,107	0
6	C8E	B	1103	7/21	0.80	0.59	51,65,73,75	0
5	LMT	B	1102	35/35	0.84	0.18	51,90,117,120	0

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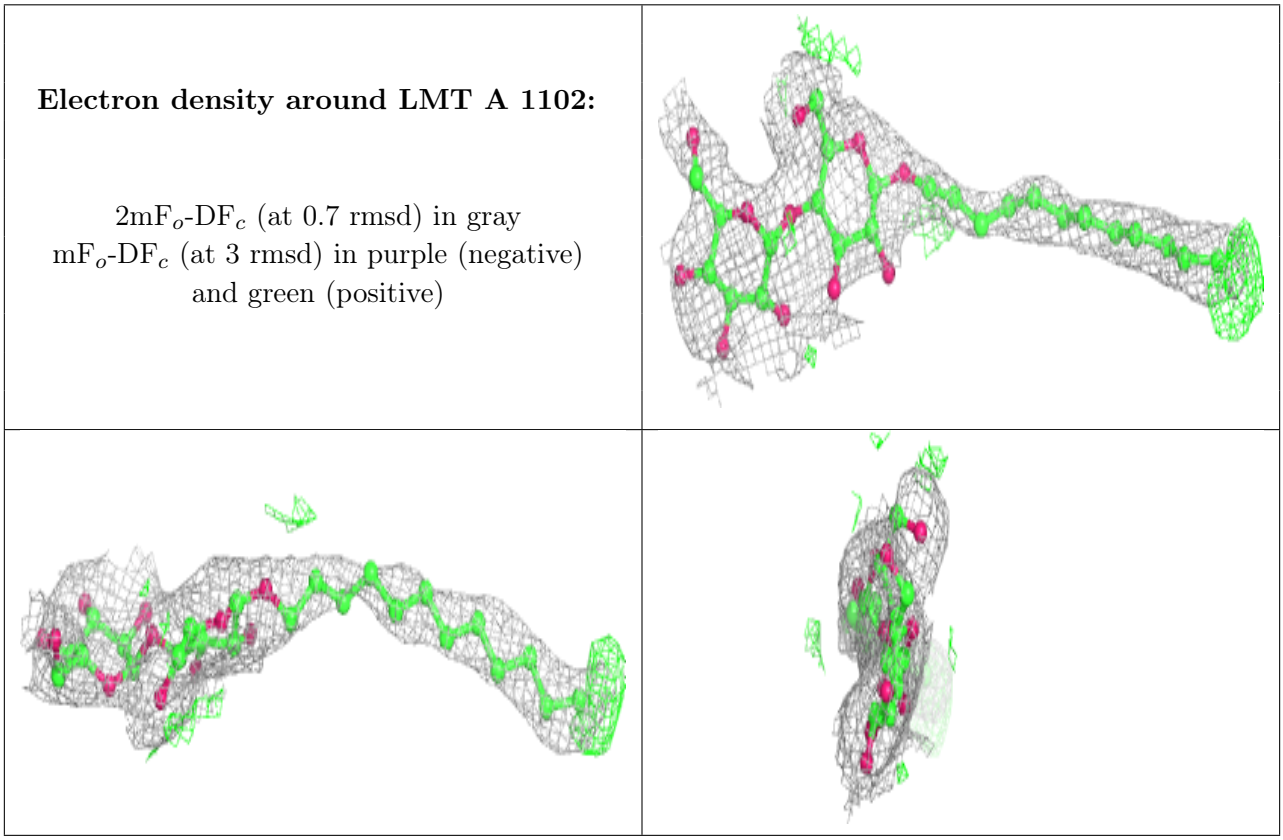
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PLM	C	601	14/18	0.88	0.37	42,49,59,62	0
5	LMT	C	602	33/35	0.89	0.22	54,64,80,83	0
6	C8E	A	1103	21/21	0.91	0.43	41,62,82,86	0
6	C8E	A	1104	21/21	0.91	0.30	35,60,65,66	0
4	3PE	A	1101	31/51	0.92	0.31	36,51,77,92	0
4	3PE	B	1101	32/51	0.93	0.26	34,49,60,73	0
5	LMT	D	602	33/35	0.93	0.27	61,71,88,90	0
7	PLM	D	601	15/18	0.93	0.38	34,50,59,61	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.

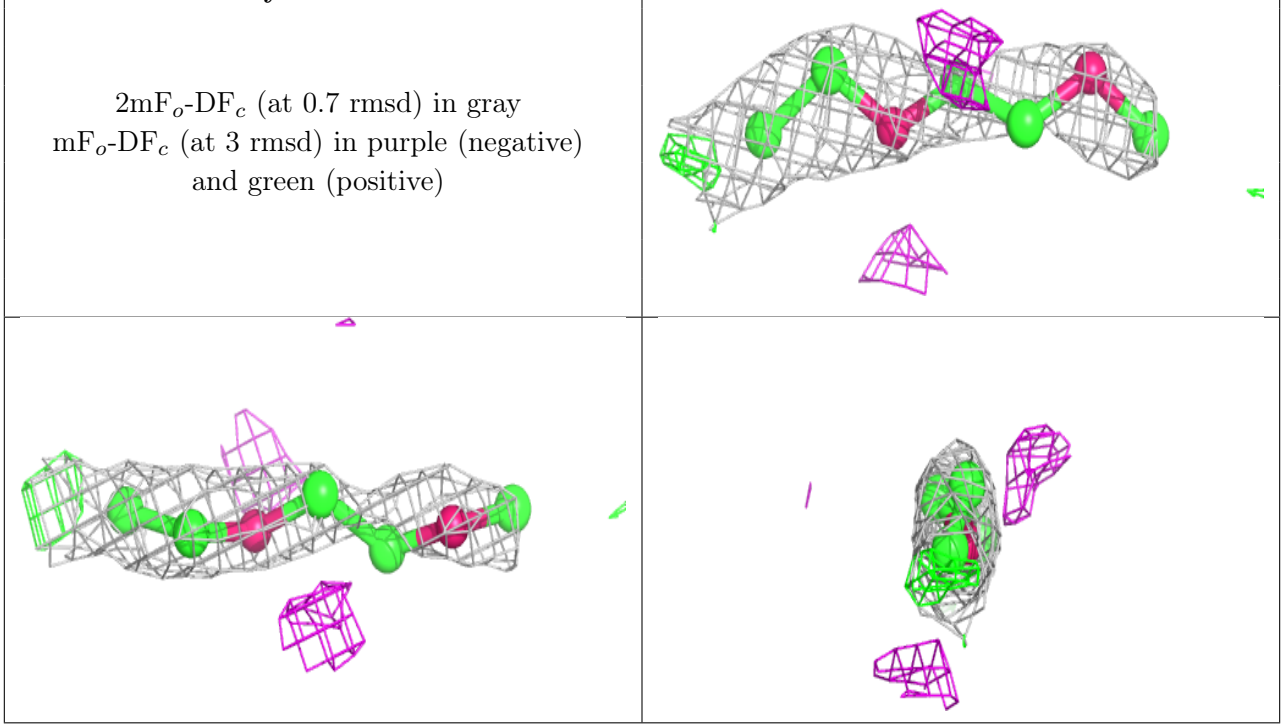
Electron density around LMT A 1102:

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



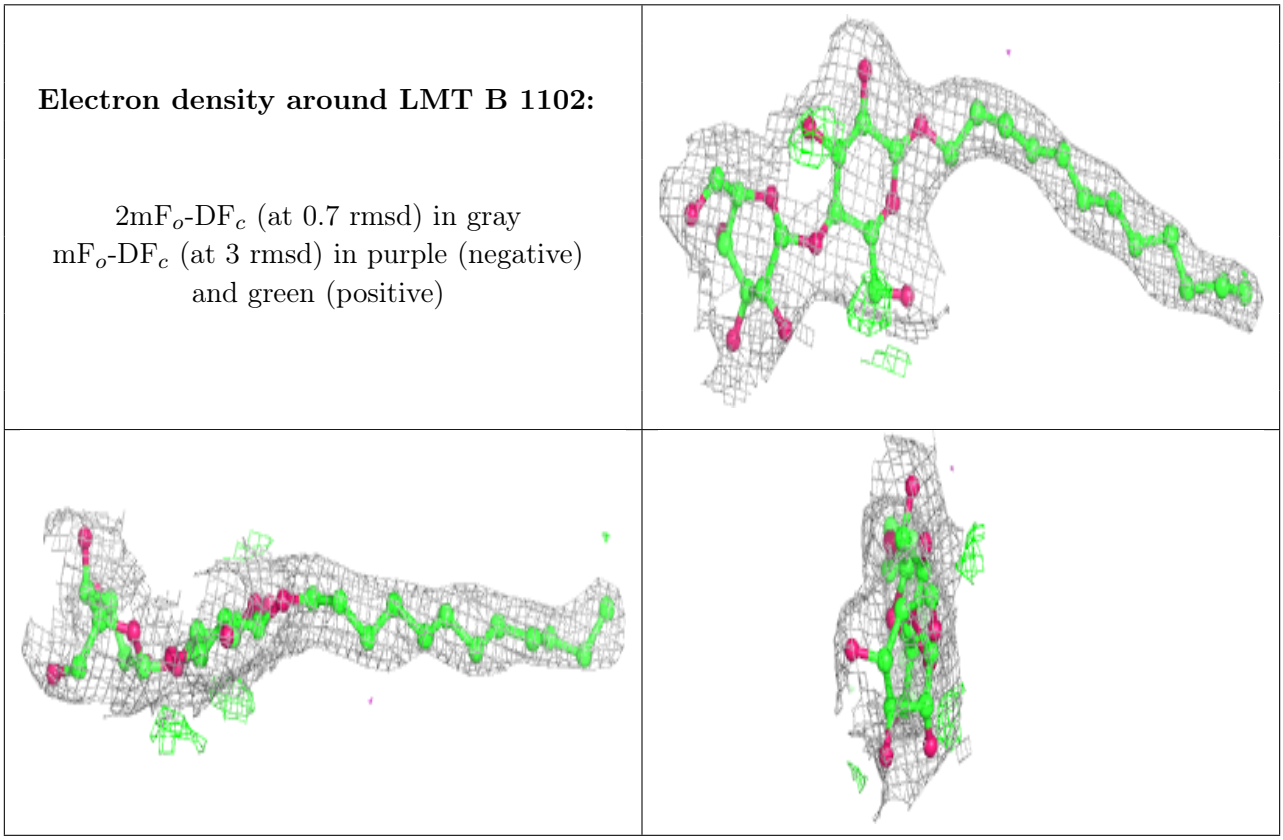
Electron density around C8E B 1103:

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



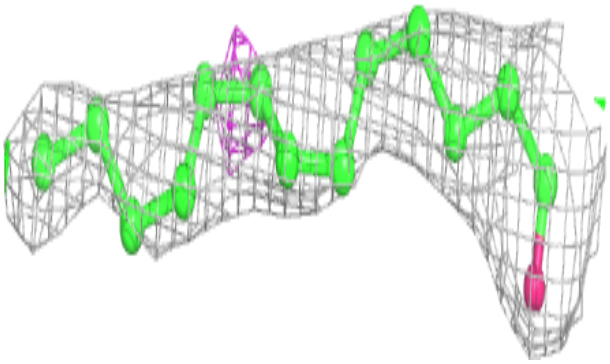
Electron density around LMT B 1102:

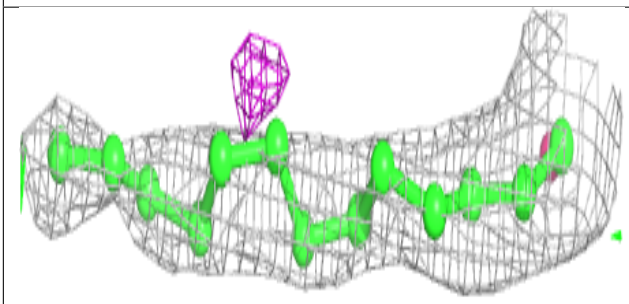
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

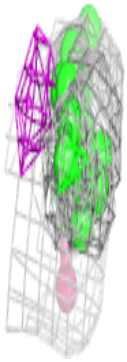


Electron density around PLM C 601:

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

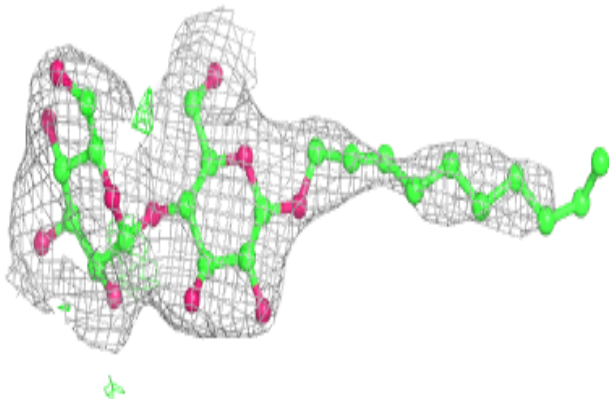


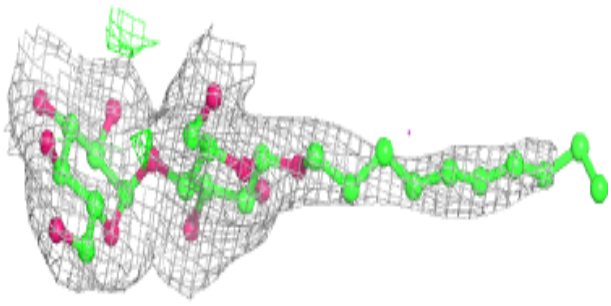


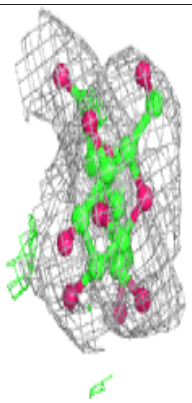


Electron density around LMT C 602:

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

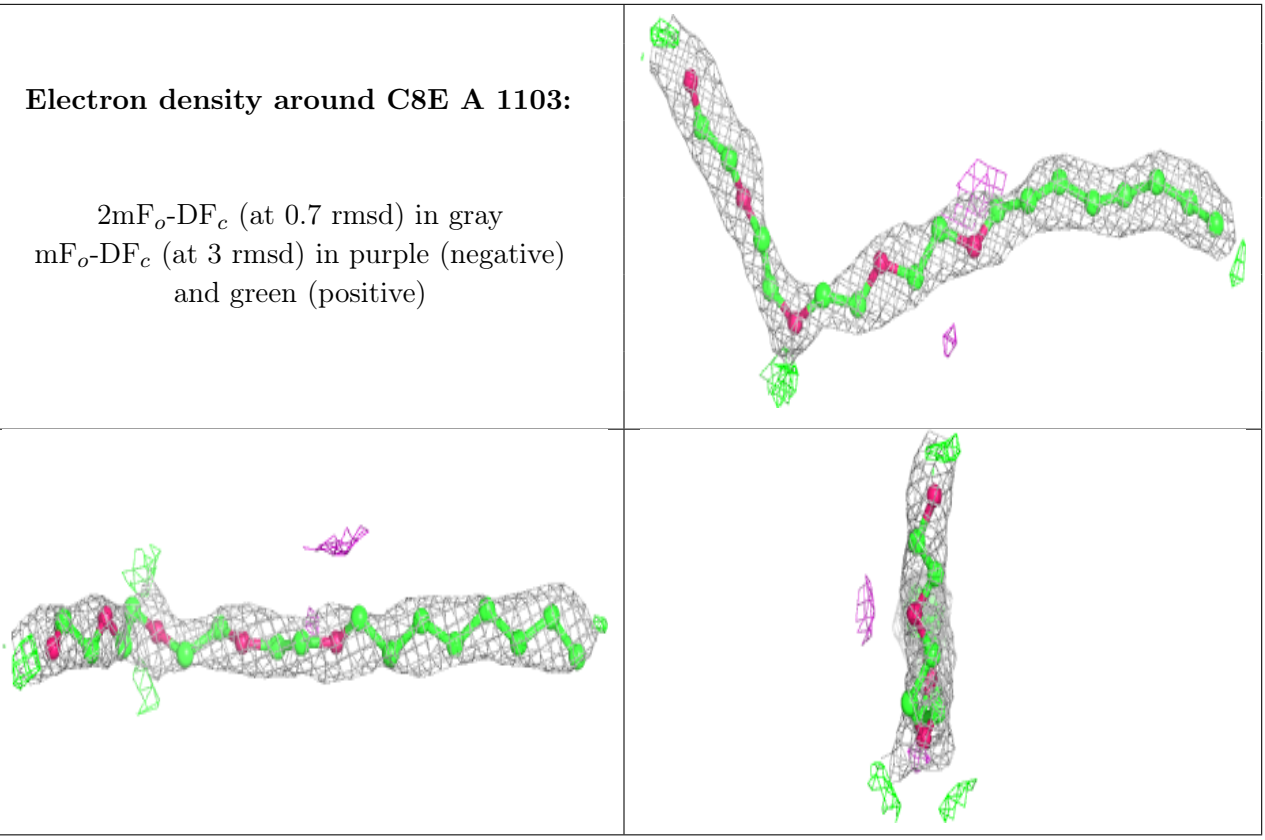






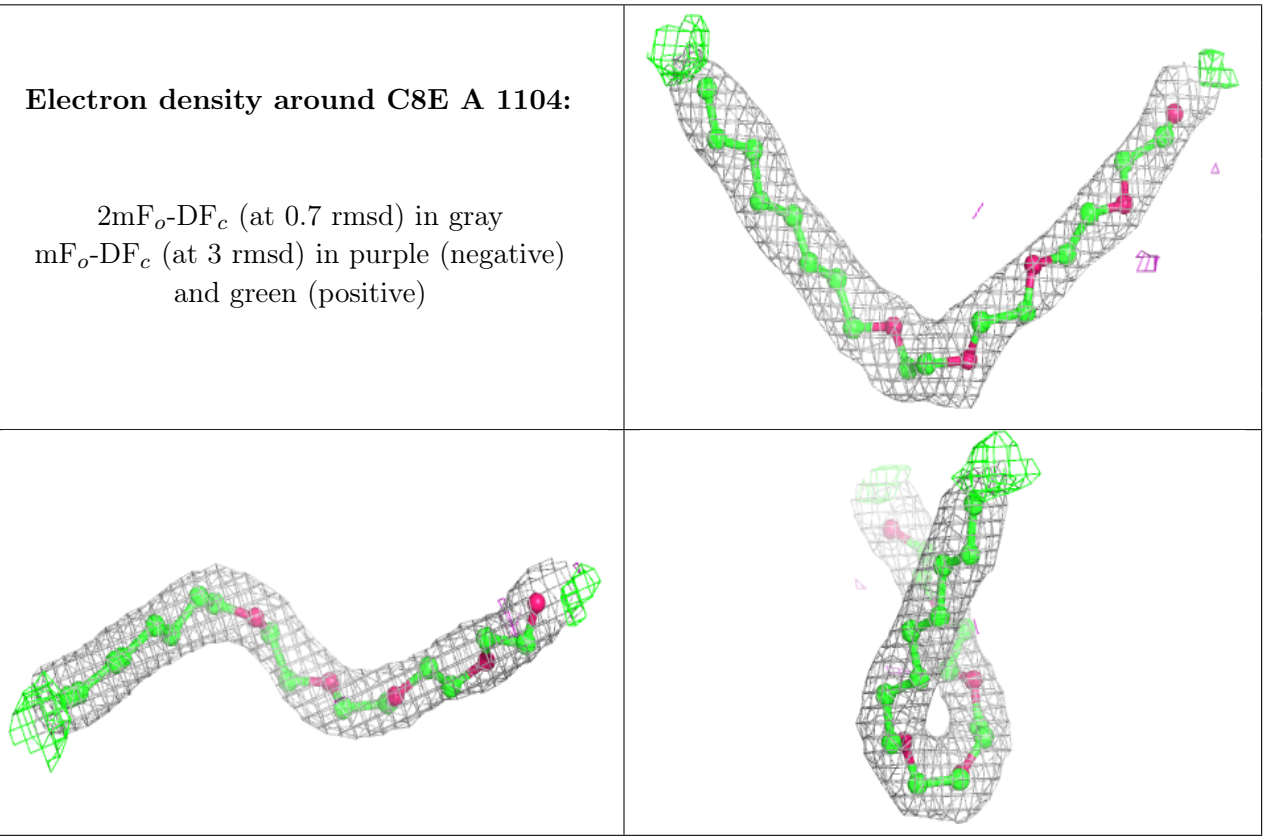
Electron density around C8E A 1103:

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



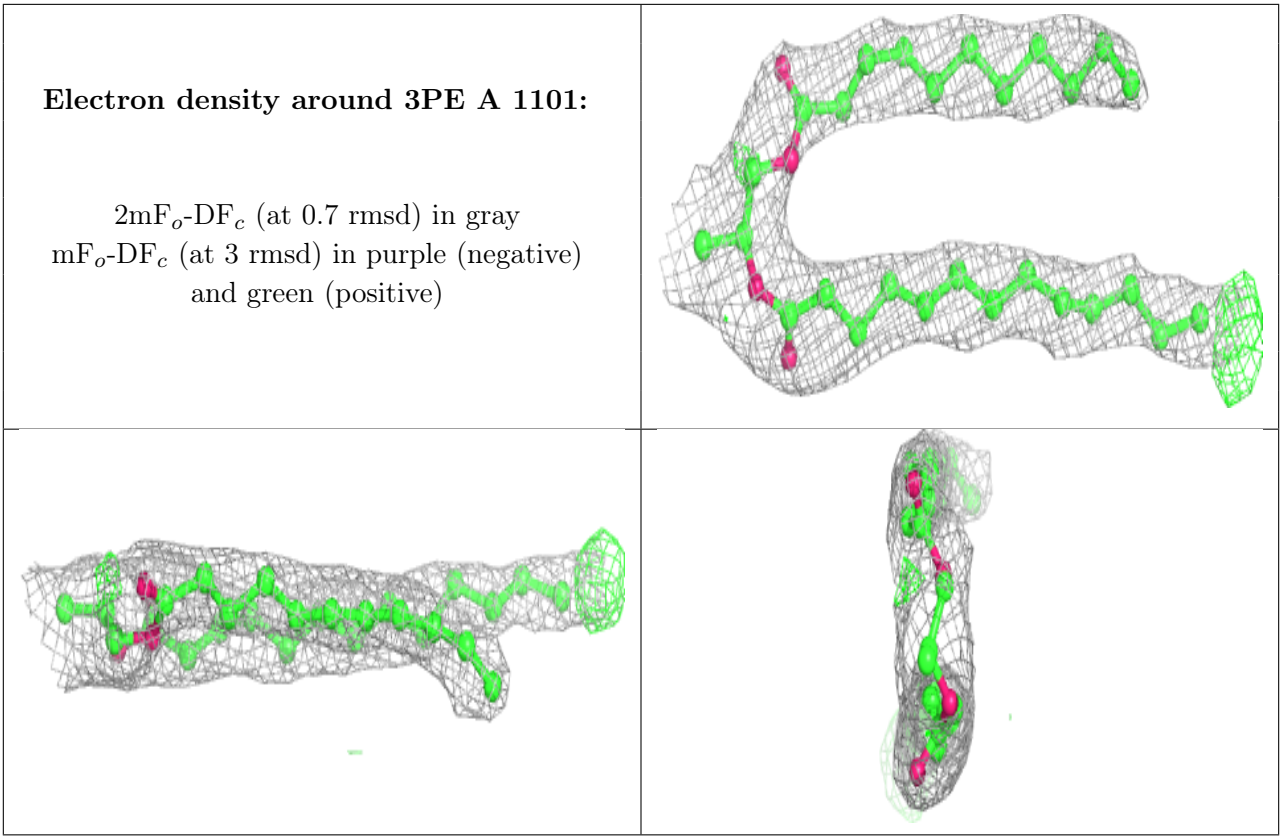
Electron density around C8E A 1104:

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



Electron density around 3PE A 1101:

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



Electron density around 3PE B 1101:

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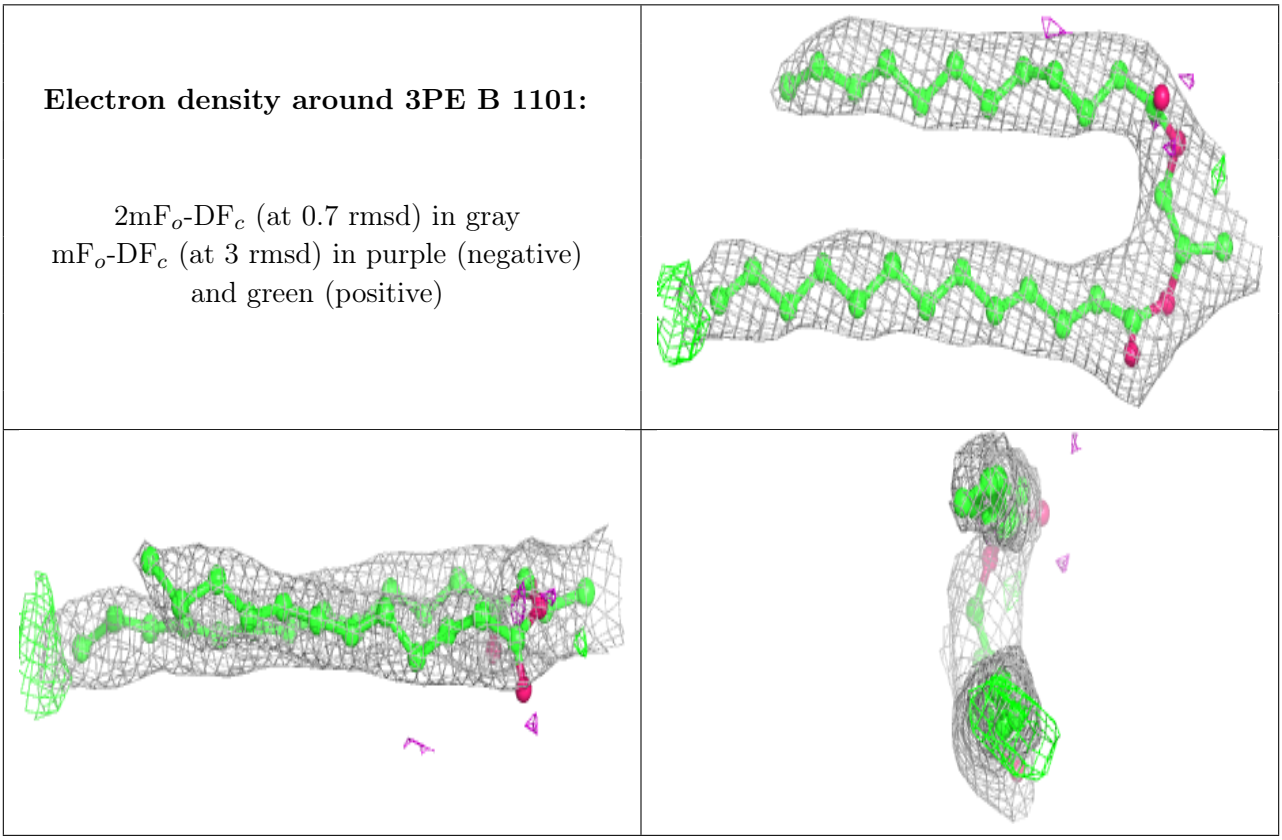
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT D 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
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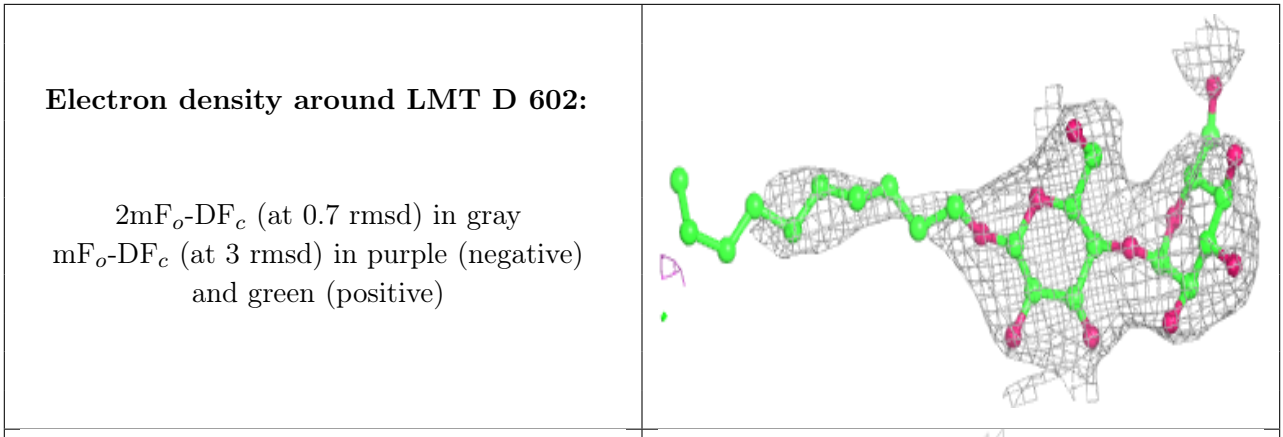
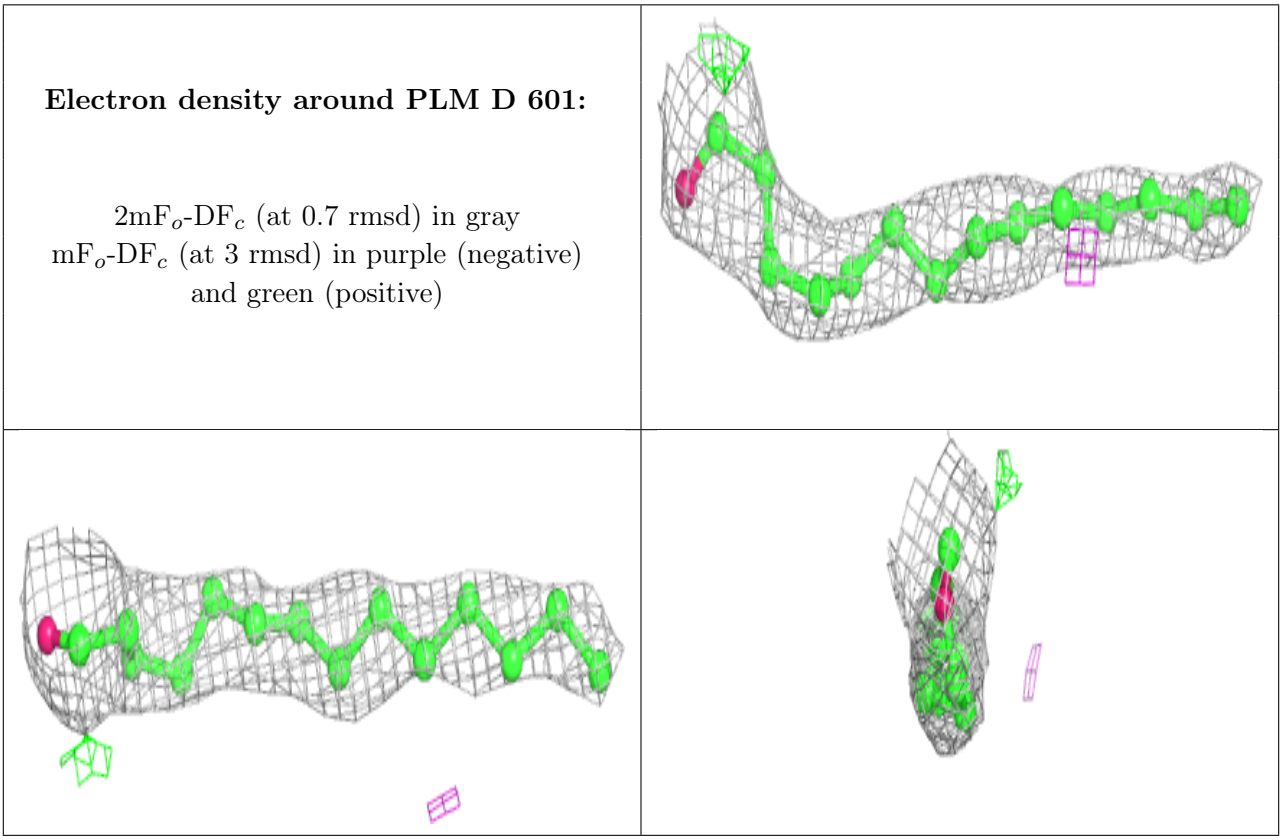


Electron density around PLM D 601:

$2mF_o$-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.