



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:15 AM UTC

PDB ID : 6SLN / pdb_00006sln
Title : Structure of the RagAB peptide transporter
Authors : Madej, M.; Ranson, N.A.; White, J.B.R.
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

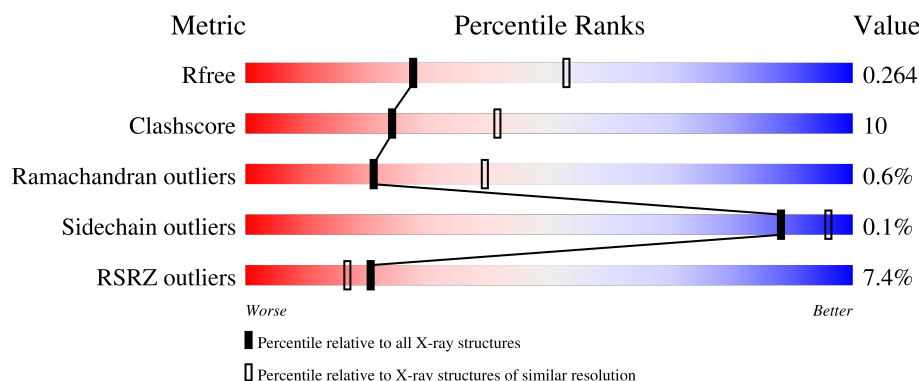
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 $\leq 5\%$. 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	997	
1	B	997	
2	C	488	
2	D	488	
3	P	13	

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Mol	Chain	Length	Quality of chain
3	Q	13	23%69%69%8%

2 Entry composition

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			

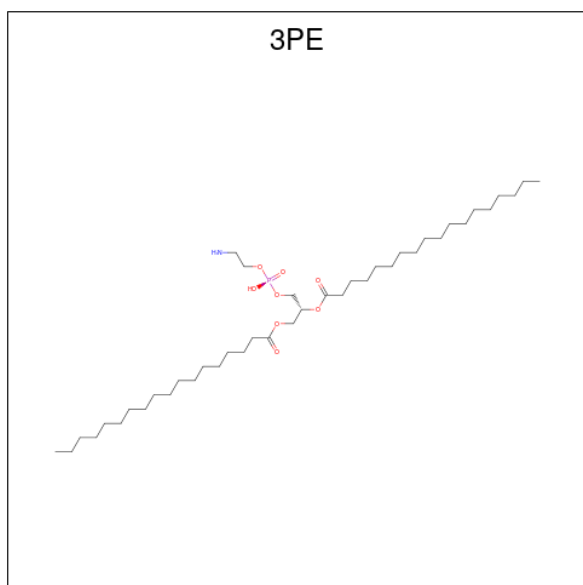
There are 12 discrepancies between the modelled and reference sequences:

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.

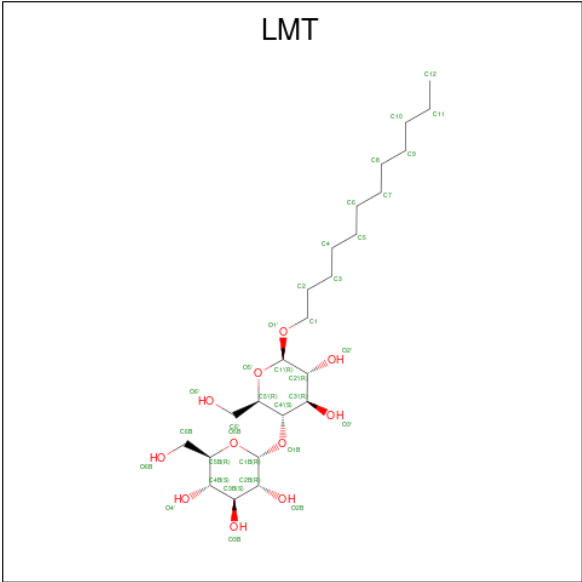
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	0	0	0
			83	45	19	19			
3	Q	13	Total	C	N	O	0	0	0
			83	45	19	19			

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



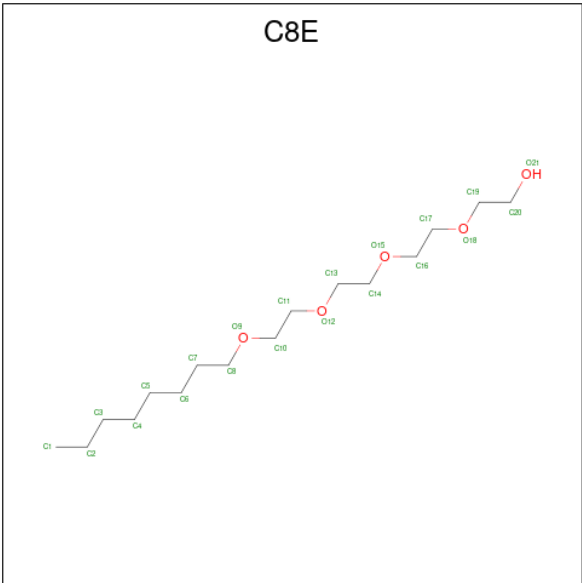
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			31	27	4		
4	B	1	Total	C	O	0	0
			32	28	4		

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



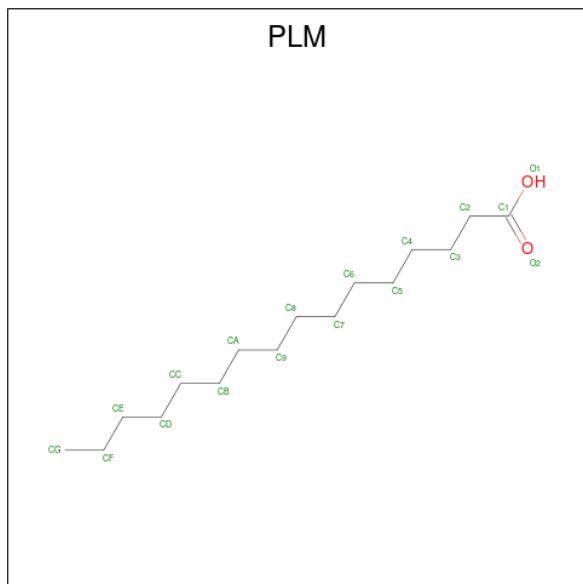
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			35	24	11		
5	B	1	Total	C	O	0	0
			35	24	11		
5	C	1	Total	C	O	0	0
			33	22	11		
5	D	1	Total	C	O	0	0
			33	22	11		

- Molecule 6 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



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

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

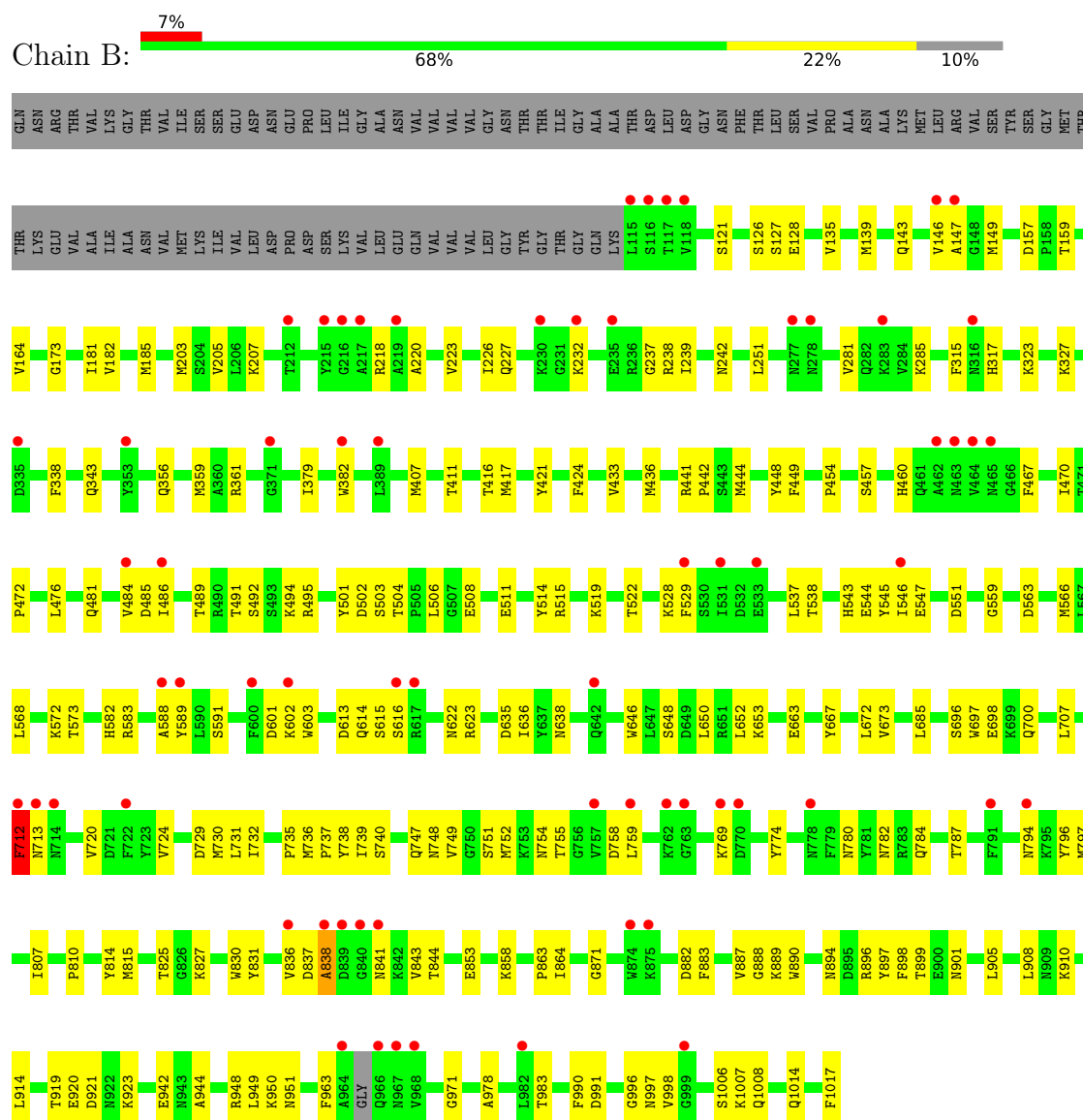


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			14	13	1		
7	D	1	Total	C	O	0	0
			15	14	1		

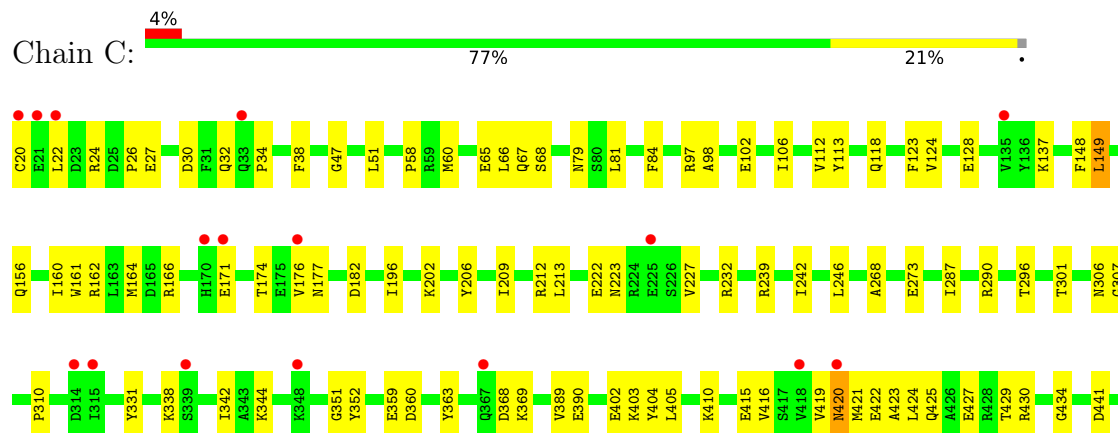
- Molecule 8 is water.

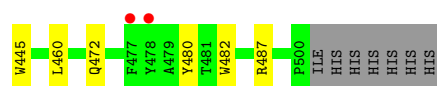
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	146	Total	O	0	0
			146	146		
8	B	165	Total	O	0	0
			165	165		
8	C	103	Total	O	0	0
			103	103		
8	D	108	Total	O	0	0
			108	108		

• Molecule 1: RagA protein

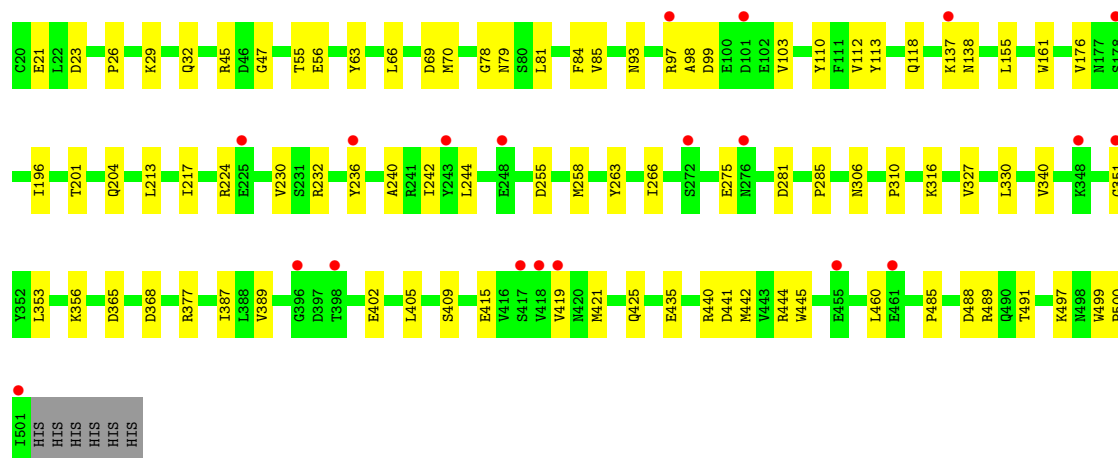
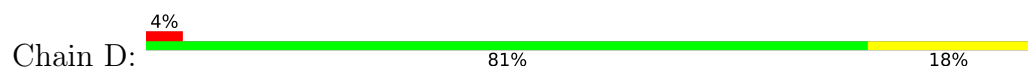


• Molecule 2: Lipoprotein RagB

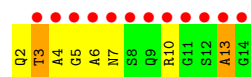
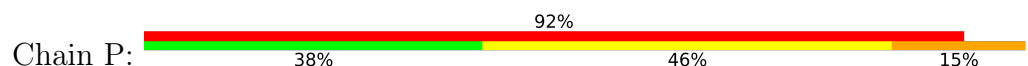




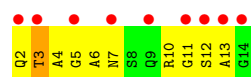
• Molecule 2: Lipoprotein RagB



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



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



4 Data and refinement statistics

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 – 2.61 123.96 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.7 (123.96-2.61) 99.8 (123.96-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 0.208 , 0.264	Depositor DCC
R_{free} test set	6906 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)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, LMT, C8E, PLM

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	0.37	0/7232	0.61	0/9783
1	B	0.37	0/7227	0.61	0/9775
2	C	0.34	0/3920	0.54	0/5320
2	D	0.37	0/3928	0.56	0/5331
3	P	0.62	0/82	1.14	1/108 (0.9%)
3	Q	0.53	0/82	1.01	0/108
All	All	0.37	0/22471	0.59	1/30425 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	13	ALA	N-CA-C	-5.16	99.80	110.80

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

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	170	0
1	B	7064	0	6802	156	0
2	C	3834	0	3728	75	0
2	D	3842	0	3739	53	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	10	0
8	C	103	0	0	6	0
8	D	108	0	0	2	0
All	All	22773	0	21600	440	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 10.

All (440) 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:250:ILE:HB	1:A:359:MET:HE1	1.41	1.01
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:250:ILE:CB	1:A:359:MET:HE1	1.97	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: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:434:TYR:HE1	1:A:436:MET:HE2	1.46	0.81
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:20:CYS:N	5:C:602:LMT:H6'	1.77	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
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:A:250:ILE:HB	1:A:359:MET:CE	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:N	1:A:208:ASP:OD1	2.26	0.67
1:A:203:MET:HE2	1:A:226:ILE:HG12	1.74	0.67
1:B:948:ARG:NH1	1:B:983:THR:OG1	2.26	0.67
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:A:171:SER:HA	1:A:730:MET:HE2	1.81	0.63
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
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:B:519:LYS:NZ	8:B:1210:HOH:O	2.32	0.61
1:A:503:SER:HB2	2:D:310:PRO:HG2	1.81	0.61
1:A:250:ILE:CA	1:A:359:MET:HE1	2.31	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:434:TYR:CE1	1:A:436:MET:HE2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:HB3	1:B:551:ASP:HB3	1.85	0.58
1:B:407:MET:HE3	8:B:1242:HOH:O	2.03	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
1:B:492:SER:OG	1:B:511:GLU:OE2	2.22	0.57
1:B:139:MET:HE1	1:B:203:MET:SD	2.45	0.57
3:Q:2:GLN:O	3:Q:4:ALA:N	2.38	0.56
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
2:C:38:PHE:H	2:C:137:LYS:HZ1	1.54	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
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
1:B:128:GLU:CD	1:B:128:GLU:H	2.15	0.54
1:B:730:MET:SD	1:B:752:MET:HE2	2.46	0.54
1:B:149:MET:HE2	1:B:164:VAL:HG11	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:VAL:HA	2:D:500:PRO:HG3	1.89	0.53
1:B:797:MET:HG3	1:B:814:TYR:CD1	2.44	0.53
1:A:220:ALA:HB1	1:A:700:GLN:CD	2.34	0.53
3:Q:3:THR:O	3:Q:3:THR:OG1	2.23	0.53
2:D:356:LYS:NZ	2:D:435:GLU:OE1	2.29	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
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:444:MET:HE3	1:B:448:TYR:CD2	2.45	0.52
2:D:69:ASP:HB3	2:D:442:MET:HE1	1.93	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: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:B:545:TYR:OH	1:B:547:GLU:OE1	2.24	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:A:134:PRO:HD3	1:A:977:MET:HE1	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:635:ASP:CG	1:B:638:ASN:HD22	2.20	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: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:157:ASP:CG	1:B:159:THR:HG22	2.37	0.48
1:B:646:TRP:O	1:B:712:PHE:N	2.40	0.48
1:A:149:MET:HE2	1:A:164:VAL:HG11	1.95	0.48
1:A:1006:SER:OG	1:A:1008:GLN:NE2	2.46	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:733:ASP:OD1	1:A:744:SER:OG	2.31	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
2:C:60:MET:HE3	2:C:112:VAL:HG21	1.96	0.47
2:C:425:GLN:O	2:C:429:THR:OG1	2.25	0.47
1:B:185:MET:HE3	1:B:485:ASP:OD1	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:ILE:CG1	1:A:359:MET:HE1	2.45	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
1:A:233:MET:HE1	1:A:345:THR:H	1.80	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
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:A:977:MET:HE2	1:A:977:MET:HB3	1.83	0.46
1:B:327:LYS:HD2	1:B:361:ARG:HH12	1.81	0.46
1:B:730:MET:HE3	1:B:732:ILE:HD11	1.98	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:813:PHE:HB3	1:A:815:MET:HE3	1.99	0.45
1:A:120:GLY:HA3	1:A:211:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:815:MET:HE2	1:B:815:MET:HB3	1.85	0.44
1:A:648:SER:OG	1:A:713:ASN:O	2.33	0.44
1:A:877:LEU:HD12	1:A:877:LEU:HA	1.74	0.44
1:B:407:MET:HG2	1:B:436:MET:HE1	1.99	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:250:ILE:HA	1:A:359:MET:HE1	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:496:MET:HE3	1:A:497:PRO:HD2	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:A:730:MET:HE1	1:A:752:MET:SD	2.59	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:736:MET:HE3	1:A:736:MET:HB3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
1:B:740:SER:C	2:C:118:GLN:HG3	2.45	0.42
2:C:164:MET:HE1	2:C:202:LYS:HG2	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
1:A:891:MET:HE3	1:A:987:TYR:CZ	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:LEU:CD1	2:D:230:VAL:HG21	2.49	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:56:GLU:OE1	2:D:113:TYR:OH	2.36	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: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:737:PRO:HG3	2:D:196:ILE:HG12	2.02	0.41
1:A:285:LYS:HG2	1:A:315:PHE:CD2	2.56	0.41
1:B:837:ASP:CG	1:B:838:ALA:H	2.20	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
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:407:MET:HE2	1:B:417:MET:SD	2.60	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:233:MET:HE1	1:A:345:THR:N	2.36	0.40
1:A:830:TRP:CZ3	1:A:848:TYR:HB2	2.56	0.40
1:B:220:ALA:HB1	1:B:700:GLN:CD	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ALA:C	2:D:32:GLN:HG3	2.46	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
1:B:751:SER:OG	1:B:787:THR:OG1	2.32	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:563:ASP:O	1:B:566:MET:HE2	2.21	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:978:ALA:HA	1:B:1008:GLN:O	2.22	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	901/997 (90%)	836 (93%)	60 (7%)	5 (1%)	21	39
1	B	898/997 (90%)	844 (94%)	51 (6%)	3 (0%)	36	56
2	C	479/488 (98%)	453 (95%)	23 (5%)	3 (1%)	21	39
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%)	21	39

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
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 ⓘ

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%)	754 (100%)	0	100	100
1	B	754/832 (91%)	754 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	401/408 (98%)	400 (100%)	1 (0%)	87	95
2	D	402/408 (98%)	401 (100%)	1 (0%)	87	95
3	P	7/7 (100%)	7 (100%)	0	100	100
3	Q	7/7 (100%)	7 (100%)	0	100	100
All	All	2325/2494 (93%)	2323 (100%)	2 (0%)	88	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	149	LEU
2	D	368	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	269	GLN
1	A	481	GLN
1	A	523	ASN
1	A	543	HIS
1	A	692	ASN
1	A	702	GLN
1	A	714	ASN
1	B	198	ASN
1	B	249	GLN
1	B	333	GLN
1	B	356	GLN
1	B	388	ASN
1	B	614	GLN
1	B	692	ASN
1	B	713	ASN
1	B	768	ASN
1	B	922	ASN
1	B	960	ASN
2	C	32	GLN
2	C	276	ASN
2	C	472	GLN
2	C	486	GLN
2	D	79	ASN
2	D	86	ASN

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Mol	Chain	Res	Type
2	D	117	ASN
2	D	192	ASN
2	D	223	ASN
3	P	9	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	1102	-	36,36,36	1.03	2 (5%)	47,47,47	1.23	4 (8%)
6	C8E	B	1103	-	6,6,20	0.58	0	5,5,19	0.57	0
5	LMT	D	602	-	34,34,36	1.14	5 (14%)	45,45,47	1.16	3 (6%)
6	C8E	A	1104	-	20,20,20	0.51	0	19,19,19	0.40	0
5	LMT	A	1102	-	36,36,36	0.98	2 (5%)	47,47,47	1.71	7 (14%)
5	LMT	C	602	-	34,34,36	1.15	3 (8%)	45,45,47	1.16	3 (6%)
7	PLM	D	601	2	13,14,17	0.51	0	12,13,17	0.48	0
4	3PE	A	1101	-	30,30,50	1.18	4 (13%)	32,32,55	1.45	3 (9%)
7	PLM	C	601	2	12,13,17	0.89	0	11,12,17	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	3PE	B	1101	-	31,31,50	1.19	4 (12%)	33,33,55	1.48	3 (9%)
6	C8E	A	1103	-	20,20,20	0.54	0	19,19,19	0.51	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	B	1102	-	-	13/21/61/61	0/2/2/2
6	C8E	B	1103	-	-	3/4/4/18	-
5	LMT	D	602	-	-	9/19/59/61	0/2/2/2
6	C8E	A	1104	-	-	10/18/18/18	-
5	LMT	A	1102	-	-	9/21/61/61	0/2/2/2
5	LMT	C	602	-	-	9/19/59/61	0/2/2/2
7	PLM	D	601	2	-	4/12/12/15	-
4	3PE	A	1101	-	-	12/31/31/54	-
7	PLM	C	601	2	-	5/11/11/15	-
4	3PE	B	1101	-	-	13/32/32/54	-
6	C8E	A	1103	-	-	11/18/18/18	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	3PE	O21-C2	-3.38	1.41	1.47
4	B	1101	3PE	O31-C31	3.27	1.42	1.33
4	B	1101	3PE	O21-C2	-3.16	1.41	1.47
5	C	602	LMT	O3'-C3'	-3.07	1.35	1.43
5	D	602	LMT	O3'-C3'	-2.77	1.36	1.43
4	A	1101	3PE	O31-C31	2.64	1.41	1.33
4	B	1101	3PE	O21-C21	2.60	1.41	1.34
4	A	1101	3PE	O21-C21	2.50	1.41	1.34
4	B	1101	3PE	O31-C3	-2.29	1.40	1.45
5	B	1102	LMT	O2B-C2B	-2.27	1.37	1.43
5	D	602	LMT	O3B-C3B	-2.26	1.37	1.43
5	C	602	LMT	O4'-C4B	-2.23	1.37	1.43
5	A	1102	LMT	C1B-C2B	2.21	1.59	1.52
5	C	602	LMT	O2B-C2B	-2.17	1.37	1.43
5	D	602	LMT	O1'-C1'	-2.16	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1102	LMT	O3'-C3'	-2.12	1.37	1.43
5	A	1102	LMT	O3B-C3B	-2.08	1.37	1.43
5	D	602	LMT	O2'-C2'	-2.05	1.37	1.43
5	D	602	LMT	O2B-C2B	-2.03	1.37	1.43
4	A	1101	3PE	O31-C3	-2.03	1.40	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1102	LMT	O1'-C1'-C2'	5.40	116.48	108.27
5	A	1102	LMT	C1-O1'-C1'	5.07	122.34	113.68
4	B	1101	3PE	O31-C31-C32	4.62	125.92	111.83
4	A	1101	3PE	O21-C21-C22	4.61	121.45	111.48
4	B	1101	3PE	O21-C21-C22	4.49	121.19	111.48
5	A	1102	LMT	C3B-C4B-C5B	-4.30	102.44	110.23
5	A	1102	LMT	O5'-C5'-C4'	3.66	117.29	109.72
5	C	602	LMT	C1'-O5'-C5'	-3.59	106.71	113.72
4	A	1101	3PE	O21-C2-C3	3.56	114.41	106.21
5	C	602	LMT	C1-O1'-C1'	3.33	119.36	113.68
5	B	1102	LMT	C3'-C4'-C5'	-3.20	103.84	110.93
5	D	602	LMT	C3'-C4'-C5'	-3.14	103.97	110.93
5	B	1102	LMT	O1'-C1'-C2'	3.05	112.90	108.27
4	A	1101	3PE	O31-C31-C32	2.84	120.49	111.83
5	B	1102	LMT	O5B-C5B-C6B	2.80	113.37	106.44
5	A	1102	LMT	O5B-C5B-C6B	2.71	113.15	106.44
5	A	1102	LMT	C1'-C2'-C3'	-2.59	104.55	110.01
5	A	1102	LMT	O5B-C1B-C2B	2.59	115.70	110.37
5	D	602	LMT	O5B-C5B-C4B	2.38	113.98	109.70
4	B	1101	3PE	O31-C31-O32	-2.33	117.80	123.63
5	D	602	LMT	C1B-O5B-C5B	2.18	117.97	113.72
5	B	1102	LMT	O5B-C5B-C4B	2.04	113.37	109.70
5	C	602	LMT	O1'-C1-C2	-2.01	102.53	109.37

There are no chirality outliers.

All (98) 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

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Mol	Chain	Res	Type	Atoms
5	B	1102	LMT	C4B-C5B-C6B-O6B
4	B	1101	3PE	O32-C31-O31-C3
5	A	1102	LMT	C4'-C5'-C6'-O6'
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
6	A	1104	C8E	O12-C13-C14-O15
5	A	1102	LMT	O5B-C5B-C6B-O6B
5	A	1102	LMT	O5'-C5'-C6'-O6'
5	B	1102	LMT	O5B-C5B-C6B-O6B
7	C	601	PLM	C7-C8-C9-CA
6	A	1103	C8E	C17-C16-O15-C14
5	B	1102	LMT	O5'-C5'-C6'-O6'
5	C	602	LMT	C4B-C5B-C6B-O6B
4	B	1101	3PE	C31-C32-C33-C34
5	C	602	LMT	O1'-C1-C2-C3
4	A	1101	3PE	C21-C22-C23-C24
5	D	602	LMT	O1'-C1-C2-C3
5	B	1102	LMT	C5'-C4'-O1B-C1B
7	C	601	PLM	C5-C6-C7-C8
5	B	1102	LMT	O1'-C1-C2-C3
6	A	1104	C8E	C6-C7-C8-O9
7	C	601	PLM	C9-CA-CB-CC
5	A	1102	LMT	O5'-C1'-O1'-C1
4	B	1101	3PE	C33-C34-C35-C36
4	B	1101	3PE	C32-C33-C34-C35
7	D	601	PLM	C4-C5-C6-C7
5	D	602	LMT	C1-C2-C3-C4
6	A	1104	C8E	O18-C19-C20-O21
4	A	1101	3PE	C32-C33-C34-C35
7	D	601	PLM	C6-C7-C8-C9
4	A	1101	3PE	C22-C23-C24-C25
7	D	601	PLM	C3-C4-C5-C6
5	D	602	LMT	C7-C8-C9-C10
5	B	1102	LMT	C3'-C4'-O1B-C1B
6	A	1104	C8E	O9-C10-C11-O12
5	D	602	LMT	C3-C4-C5-C6
4	B	1101	3PE	C34-C35-C36-C37
5	C	602	LMT	C5'-C4'-O1B-C1B

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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	B	1102	LMT	C9-C10-C11-C12
4	A	1101	3PE	C28-C29-C2A-C2B
5	D	602	LMT	C4B-C5B-C6B-O6B
5	B	1102	LMT	C1-C2-C3-C4
4	A	1101	3PE	C29-C2A-C2B-C2C
6	A	1103	C8E	O12-C13-C14-O15
4	A	1101	3PE	C33-C34-C35-C36
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	1104	C8E	C11-C10-O9-C8
6	A	1104	C8E	C10-C11-O12-C13
5	C	602	LMT	C3'-C4'-O1B-C1B
6	A	1103	C8E	C13-C14-O15-C16
6	A	1104	C8E	C16-C17-O18-C19
6	A	1103	C8E	C5-C6-C7-C8
7	C	601	PLM	C4-C5-C6-C7
5	B	1102	LMT	C4'-C5'-C6'-O6'
5	D	602	LMT	C4-C5-C6-C7
5	C	602	LMT	C2-C3-C4-C5
6	B	1103	C8E	C17-C16-O15-C14
6	A	1103	C8E	C7-C8-O9-C10
4	B	1101	3PE	C35-C36-C37-C38
4	B	1101	3PE	C3-C2-O21-C21
5	A	1102	LMT	C1-C2-C3-C4
6	A	1103	C8E	C1-C2-C3-C4
6	A	1104	C8E	C20-C19-O18-C17
6	A	1103	C8E	C2-C3-C4-C5
6	A	1103	C8E	O15-C16-C17-O18
5	C	602	LMT	C7-C8-C9-C10
4	A	1101	3PE	C34-C35-C36-C37
7	C	601	PLM	C8-C9-CA-CB
6	A	1103	C8E	C6-C7-C8-O9
6	A	1104	C8E	C17-C16-O15-C14
5	B	1102	LMT	C7-C8-C9-C10
5	D	602	LMT	C5'-C4'-O1B-C1B
5	B	1102	LMT	C3-C4-C5-C6
5	B	1102	LMT	C6-C7-C8-C9
6	B	1103	C8E	C20-C19-O18-C17
5	C	602	LMT	C3-C4-C5-C6

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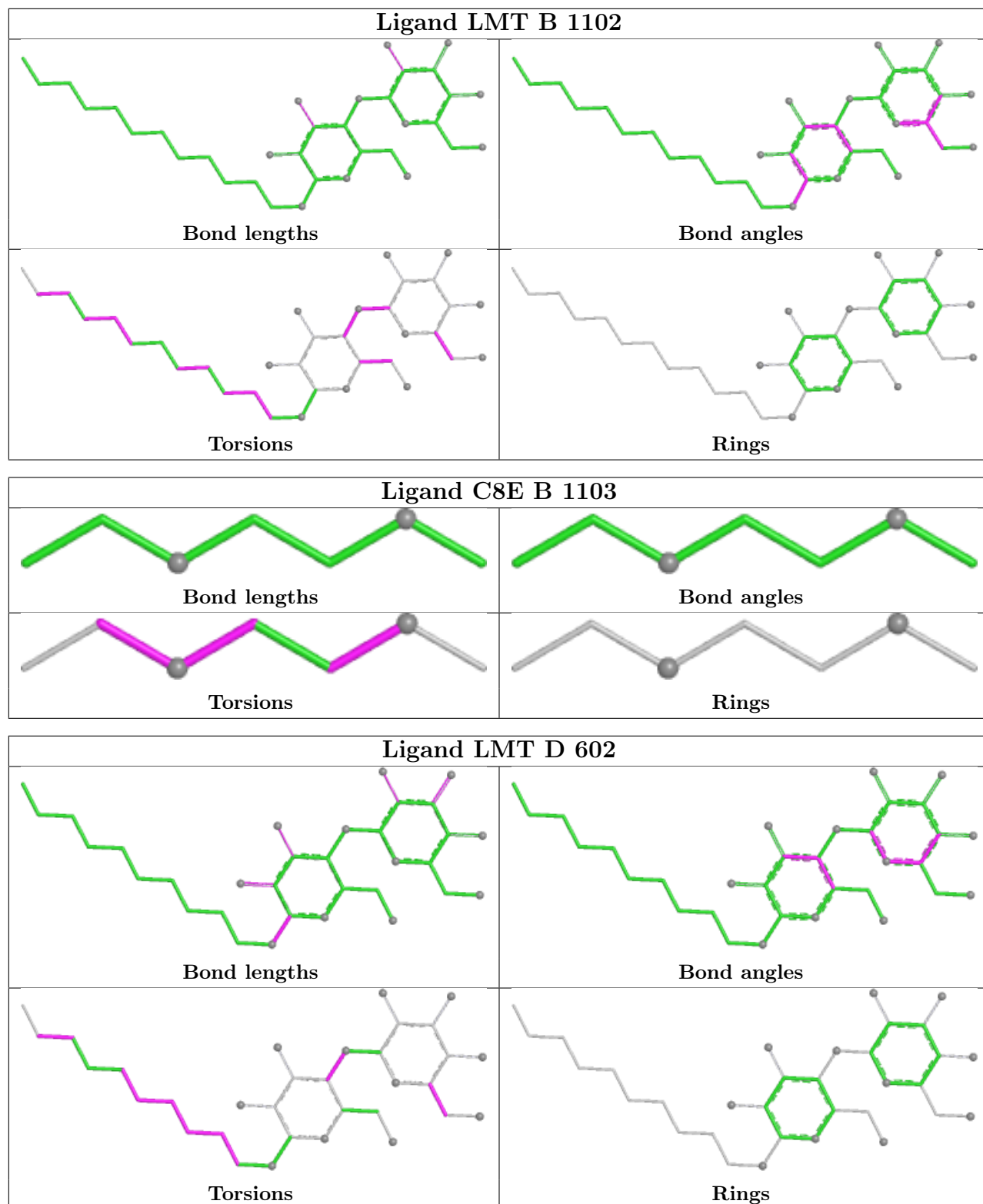
Mol	Chain	Res	Type	Atoms
4	B	1101	3PE	O31-C31-C32-C33
4	A	1101	3PE	O31-C31-C32-C33
6	B	1103	C8E	C16-C17-O18-C19
6	A	1104	C8E	O15-C16-C17-O18
4	A	1101	3PE	O32-C31-C32-C33
4	B	1101	3PE	C37-C38-C39-C3A
4	B	1101	3PE	O32-C31-C32-C33
7	D	601	PLM	C2-C3-C4-C5
6	A	1103	C8E	O9-C10-C11-O12

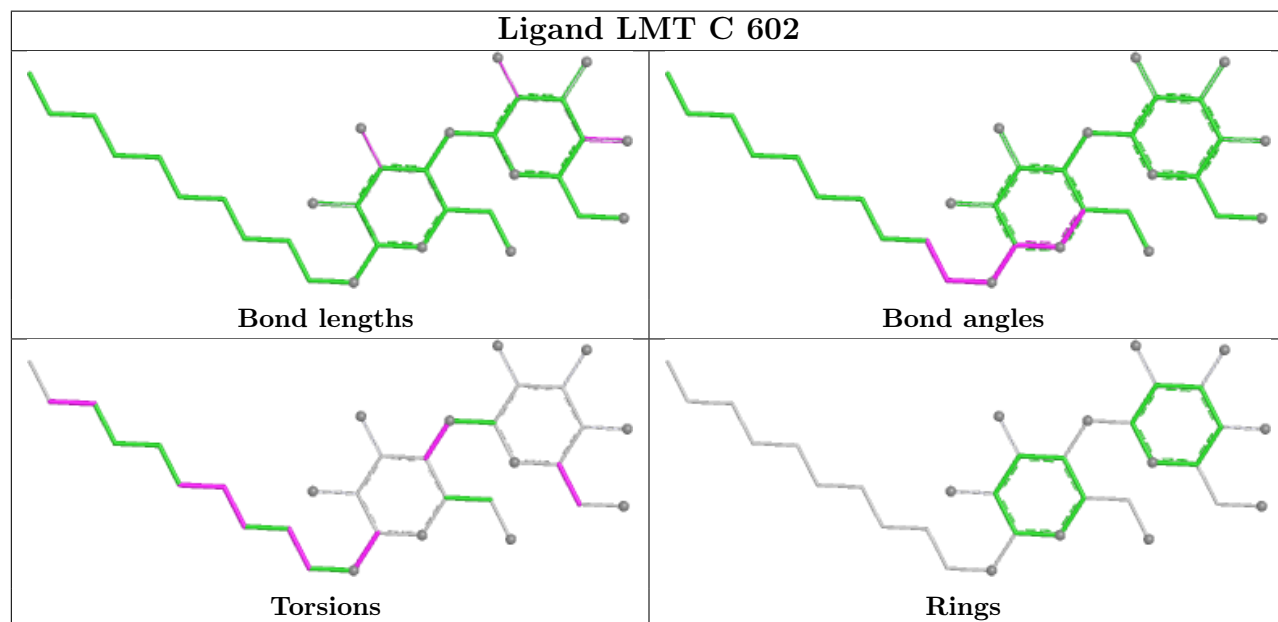
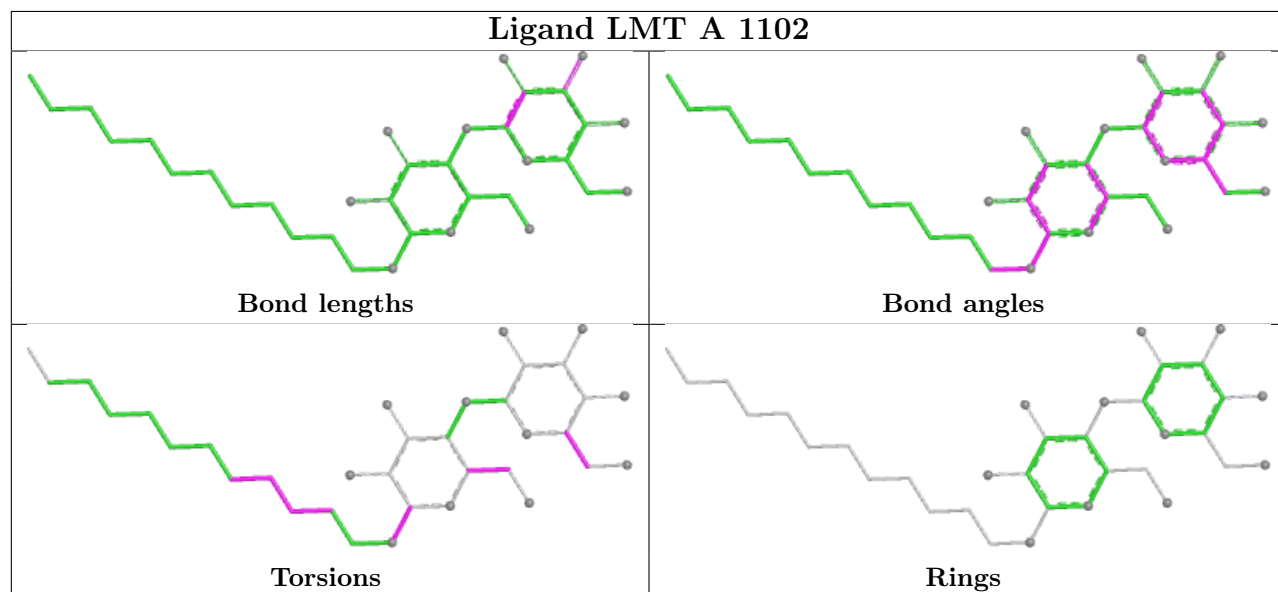
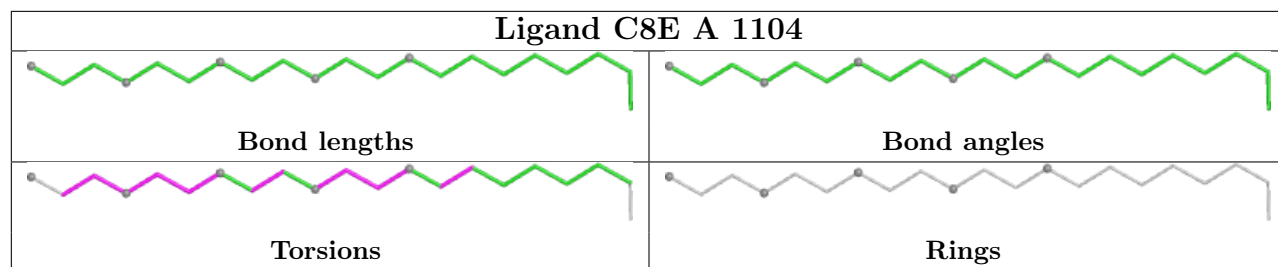
There are no ring outliers.

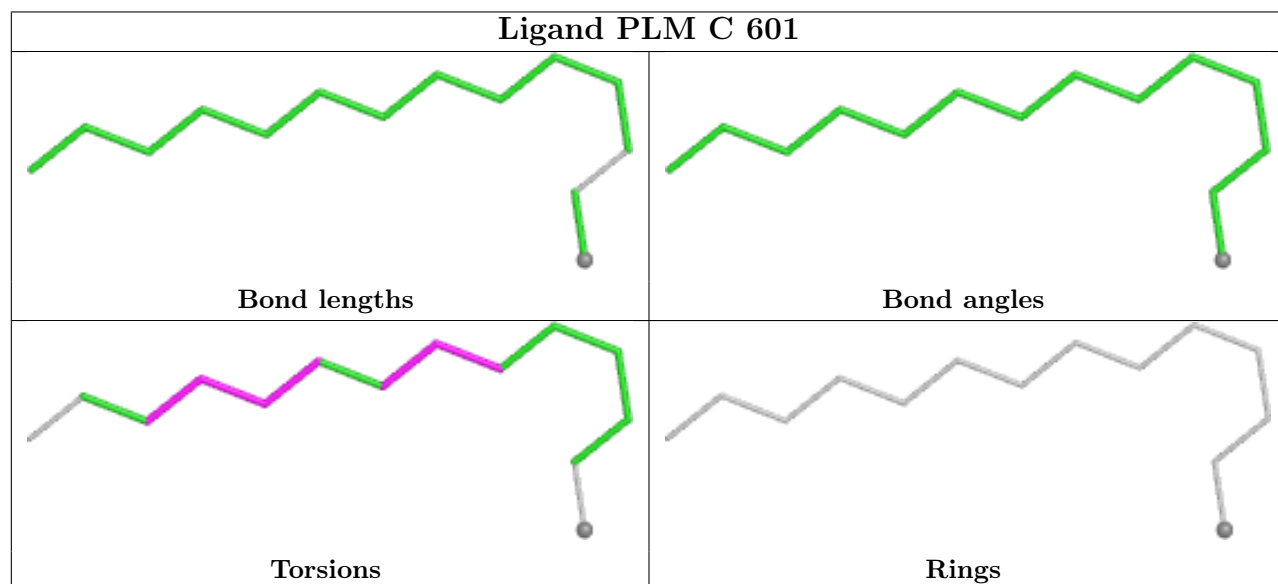
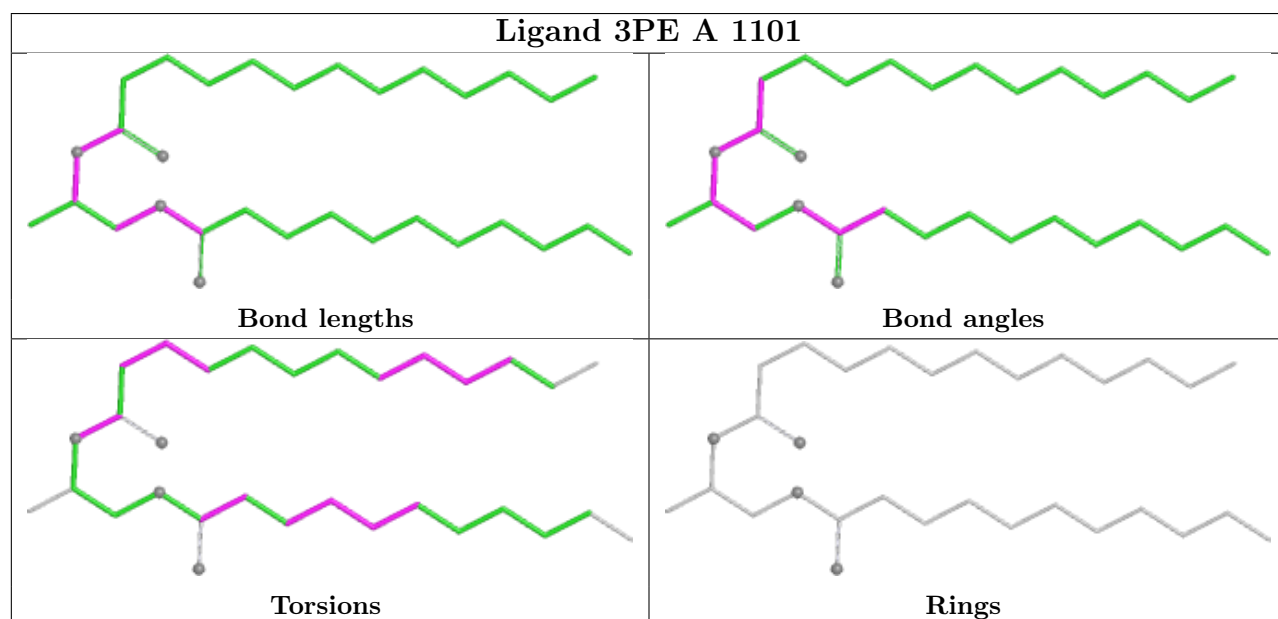
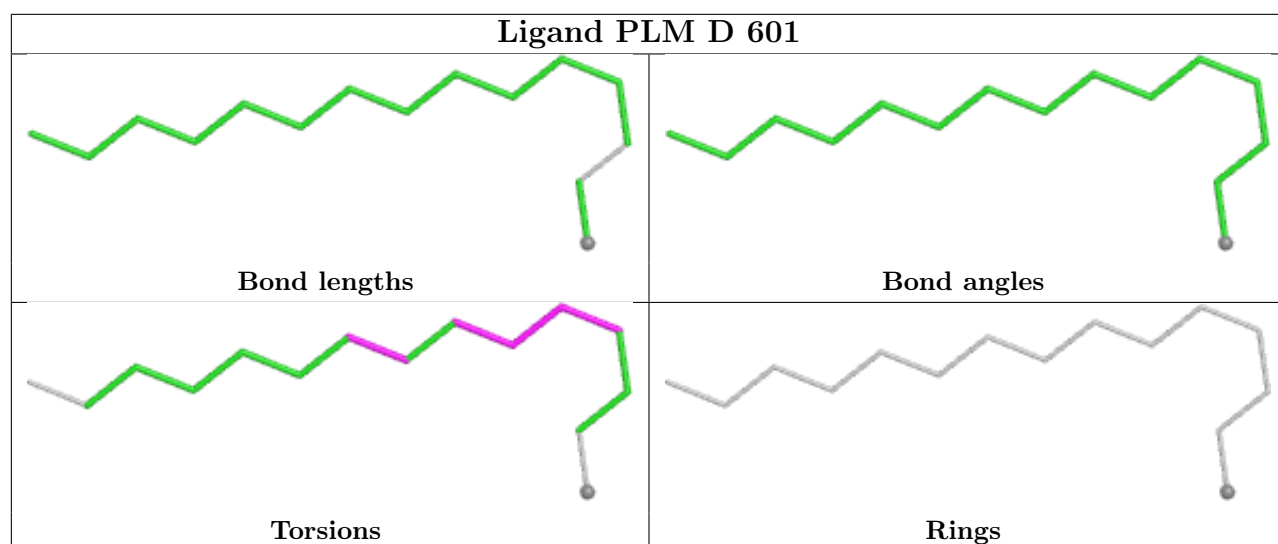
7 monomers are involved in 17 short contacts:

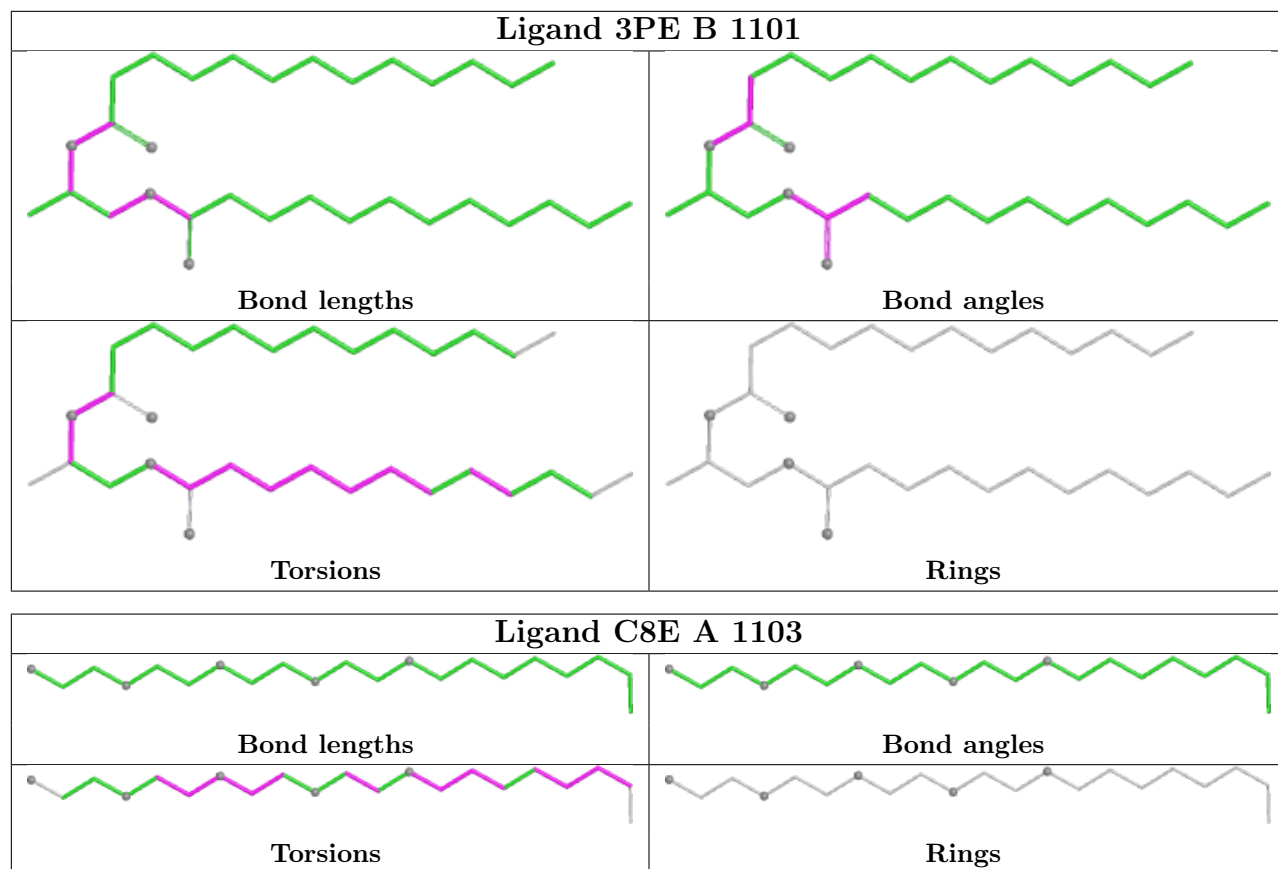
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	LMT	2	0
5	A	1102	LMT	2	0
5	C	602	LMT	4	0
4	A	1101	3PE	2	0
7	C	601	PLM	1	0
4	B	1101	3PE	4	0
6	A	1103	C8E	4	0

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 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	903/997 (90%)	0.46	82 (9%) 15 11	27, 52, 96, 161	0
1	B	902/997 (90%)	0.41	66 (7%) 21 17	29, 51, 94, 153	0
2	C	481/488 (98%)	0.18	18 (3%) 45 40	33, 48, 70, 95	0
2	D	482/488 (98%)	0.16	20 (4%) 41 36	32, 48, 69, 82	0
3	P	13/13 (100%)	3.17	12 (92%) 0 0	68, 73, 87, 96	0
3	Q	13/13 (100%)	3.15	9 (69%) 0 0	51, 77, 117, 120	0
All	All	2794/2996 (93%)	0.37	207 (7%) 20 17	27, 50, 87, 161	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	643	GLU	6.7
3	Q	12	SER	6.3
1	B	464	VAL	6.1
1	B	278	ASN	5.5
1	B	462	ALA	5.4
1	A	161	VAL	5.4
1	A	638	ASN	5.0
3	Q	3	THR	5.0
3	Q	5	GLY	4.8
1	A	459	SER	4.7
2	C	22	LEU	4.6
1	A	307	GLY	4.4
1	B	371	GLY	4.4
3	Q	9	GLN	4.4
3	P	9	GLN	4.4
2	D	501	ILE	4.4
1	A	115	LEU	4.3
1	B	762	LYS	4.3
3	P	12	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	192	VAL	4.2
3	P	10	ARG	4.2
3	Q	13	ALA	4.1
3	P	3	THR	3.9
1	B	533	GLU	3.8
1	A	426	VAL	3.8
1	B	115	LEU	3.8
1	A	642	GLN	3.7
1	A	465	ASN	3.6
3	Q	14	GLY	3.6
1	A	249	GLN	3.6
1	B	839	ASP	3.5
1	A	160	ALA	3.5
2	C	225	GLU	3.5
1	A	194	THR	3.5
1	A	193	ALA	3.5
1	B	316	ASN	3.5
1	A	136	ALA	3.5
2	C	418	VAL	3.5
1	A	116	SER	3.4
1	B	217	ALA	3.4
1	A	767	GLN	3.4
1	B	600	PHE	3.4
1	A	217	ALA	3.4
3	P	8	SER	3.4
1	A	541	MET	3.4
1	A	369	TYR	3.3
1	A	371	GLY	3.3
2	D	418	VAL	3.3
3	P	11	GLY	3.3
1	B	794	ASN	3.3
1	B	486	ILE	3.3
1	B	838	ALA	3.3
1	B	484	VAL	3.2
1	B	770	ASP	3.2
2	C	20	CYS	3.2
1	A	308	LYS	3.2
1	B	215	TYR	3.2
2	C	21	GLU	3.2
1	A	396	ARG	3.2
1	A	235	GLU	3.2
1	B	588	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	864	ILE	3.1
1	A	531	ILE	3.1
3	P	5	GLY	3.1
3	P	13	ALA	3.1
1	B	769	LYS	3.1
1	B	463	ASN	3.1
1	A	1017	PHE	3.0
1	B	616	SER	3.0
2	D	417	SER	3.0
1	A	768	ASN	3.0
1	A	190	ASP	3.0
1	B	277	ASN	3.0
1	B	230	LYS	3.0
1	B	757	VAL	3.0
1	A	986	LYS	2.9
1	A	464	VAL	2.9
1	A	189	LEU	2.9
1	A	648	SER	2.9
1	A	645	ASN	2.9
3	P	7	ASN	2.9
1	A	191	VAL	2.9
1	A	180	TYR	2.8
3	P	4	ALA	2.8
2	C	170	HIS	2.8
1	B	874	TRP	2.8
1	A	427	ASN	2.8
1	B	235	GLU	2.8
2	C	33	GLN	2.8
1	B	531	ILE	2.8
2	D	101	ASP	2.8
1	A	602	LYS	2.8
1	B	713	ASN	2.8
1	A	216	GLY	2.8
1	A	394	ALA	2.8
2	D	455	GLU	2.8
1	A	514	TYR	2.8
1	A	875	LYS	2.7
1	A	874	TRP	2.7
2	D	178	SER	2.7
1	A	819	ALA	2.7
2	C	314	ASP	2.7
2	D	272	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	311	PHE	2.7
2	C	315	ILE	2.7
1	B	722	PHE	2.7
1	A	608	PHE	2.7
3	Q	2	GLN	2.6
1	A	714	ASN	2.6
1	B	967	ASN	2.6
2	D	276	ASN	2.6
1	B	712	PHE	2.6
1	A	393	ILE	2.6
1	A	641	ILE	2.6
1	B	968	VAL	2.6
2	C	477	PHE	2.6
1	A	370	SER	2.6
1	A	859	SER	2.6
1	A	389	LEU	2.6
2	D	248	GLU	2.6
1	A	646	TRP	2.5
2	D	461	GLU	2.5
1	A	552	VAL	2.5
1	B	875	LYS	2.5
1	A	458	GLU	2.5
3	P	14	GLY	2.5
3	Q	11	GLY	2.5
1	B	116	SER	2.5
1	B	216	GLY	2.5
1	B	791	PHE	2.5
1	B	232	LYS	2.5
1	A	603	TRP	2.5
1	B	389	LEU	2.5
1	B	763	GLY	2.5
1	A	132	GLU	2.4
1	B	546	ILE	2.4
1	A	712	PHE	2.4
1	B	335	ASP	2.4
1	B	840	GLY	2.4
1	A	354	PHE	2.4
1	A	965	GLY	2.4
2	C	367	GLN	2.4
1	A	162	ALA	2.4
1	A	366	PHE	2.4
1	B	117	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	137	LYS	2.3
1	A	599	GLY	2.3
1	B	617	ARG	2.3
1	A	1009	TYR	2.3
2	C	420	ASN	2.3
1	A	230	LYS	2.3
1	B	999	GLY	2.3
1	B	589	TYR	2.3
2	D	236	TYR	2.3
1	B	465	ASN	2.3
2	D	225	GLU	2.3
1	A	118	VAL	2.3
1	B	836	VAL	2.3
1	B	529	PHE	2.3
1	A	367	LYS	2.3
1	B	382	TRP	2.3
3	P	6	ALA	2.2
1	B	283	LYS	2.2
1	B	841	ASN	2.2
1	B	219	ALA	2.2
1	A	601	ASP	2.2
1	A	982	LEU	2.2
1	A	159	THR	2.2
1	B	212	THR	2.2
1	B	759	LEU	2.2
2	C	171	GLU	2.2
1	A	762	LYS	2.2
2	D	351	GLY	2.2
1	A	400	ASP	2.2
2	C	135	VAL	2.2
2	C	176	VAL	2.2
2	C	339	SER	2.2
1	B	147	ALA	2.1
1	A	794	ASN	2.1
2	C	348	LYS	2.1
1	A	649	ASP	2.1
1	A	850	ALA	2.1
1	B	982	LEU	2.1
2	D	419	VAL	2.1
1	A	620	SER	2.1
1	A	634	PHE	2.1
1	A	489	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	602	LYS	2.1
1	B	966	GLN	2.1
1	B	778	ASN	2.1
2	C	478	TYR	2.1
1	A	887	VAL	2.1
1	A	600	PHE	2.1
1	A	722	PHE	2.1
1	B	642	GLN	2.1
2	D	396	GLY	2.1
1	B	353	TYR	2.1
2	D	243	TYR	2.1
1	B	964	ALA	2.0
2	D	348	LYS	2.0
1	A	309	THR	2.0
2	D	398	THR	2.0
1	B	118	VAL	2.0
1	B	146	VAL	2.0
2	D	97	ARG	2.0
1	B	714	ASN	2.0
3	Q	7	ASN	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	LMT	A	1102	35/35	0.77	0.18	53,90,105,107	0
6	C8E	B	1103	7/21	0.78	0.28	51,65,73,75	0
5	LMT	B	1102	35/35	0.82	0.18	51,90,117,120	0

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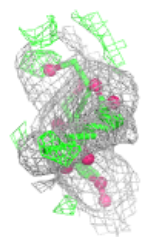
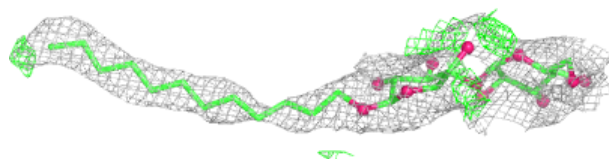
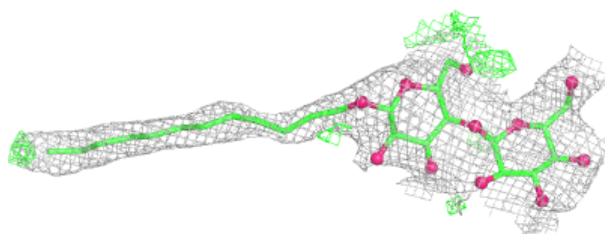
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	LMT	C	602	33/35	0.86	0.16	54,64,80,83	0
7	PLM	C	601	14/18	0.86	0.18	42,49,59,62	0
6	C8E	A	1103	21/21	0.88	0.18	41,62,82,86	0
6	C8E	A	1104	21/21	0.88	0.17	35,60,65,66	0
5	LMT	D	602	33/35	0.89	0.15	61,71,88,90	0
4	3PE	A	1101	31/51	0.90	0.16	36,51,77,92	0
4	3PE	B	1101	32/51	0.92	0.14	34,49,60,73	0
7	PLM	D	601	15/18	0.92	0.13	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.

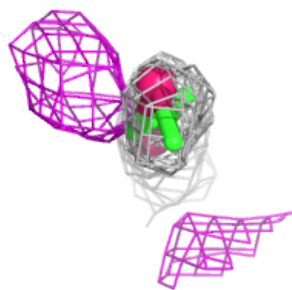
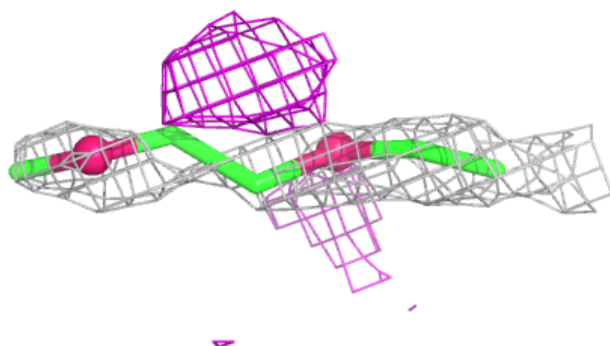
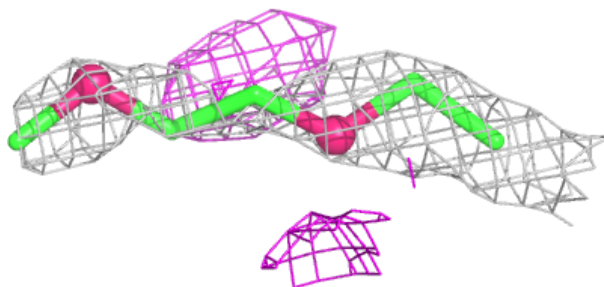
Electron density around LMT A 1102:

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

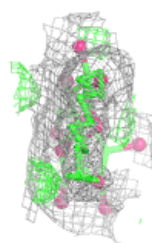
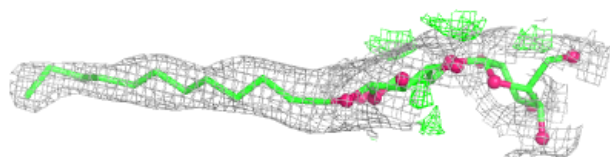
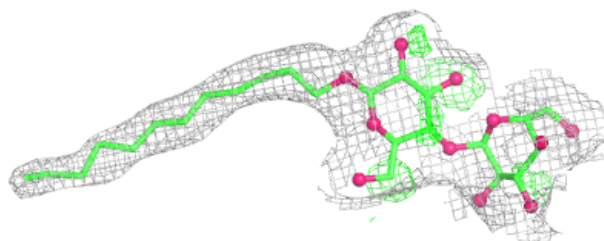


Electron density around C8E B 1103:

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

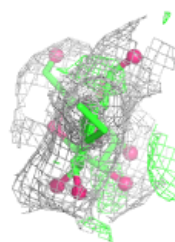
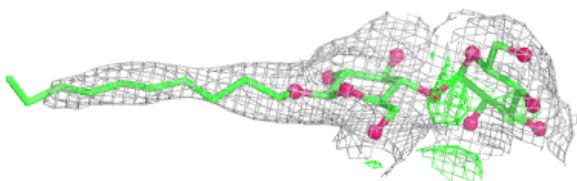
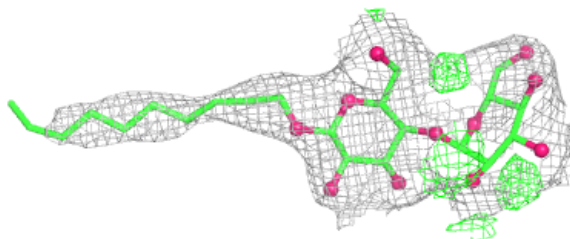
**Electron density around LMT B 1102:**

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

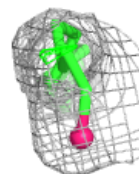
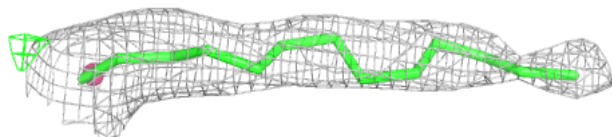
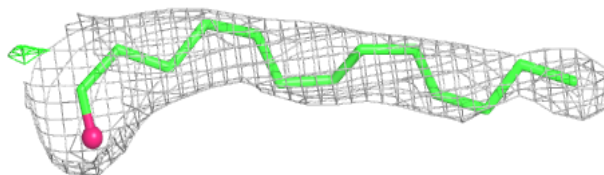


Electron density around LMT C 602:

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

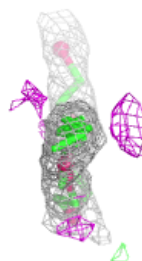
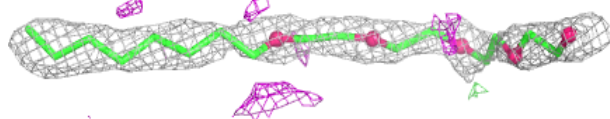
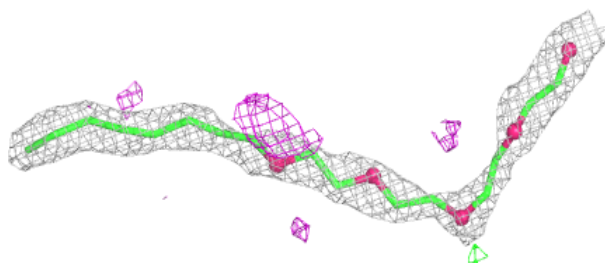
**Electron density around PLM C 601:**

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

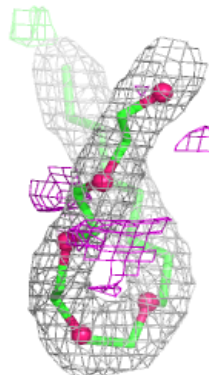
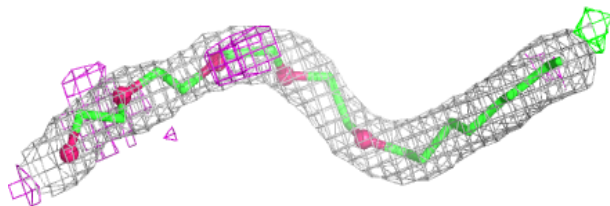
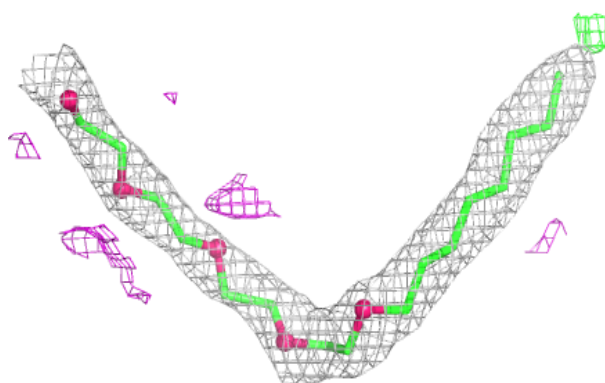


Electron density around C8E A 1103:

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

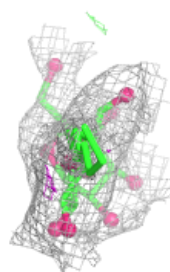
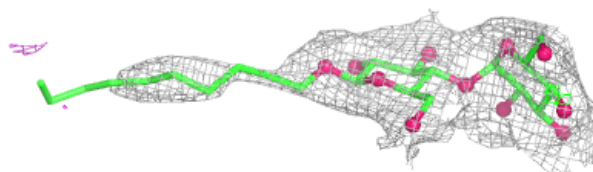
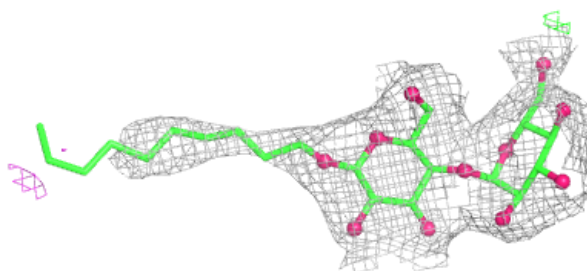
**Electron density around C8E A 1104:**

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

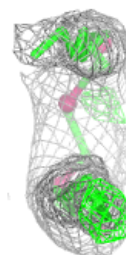
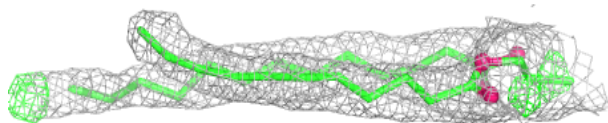
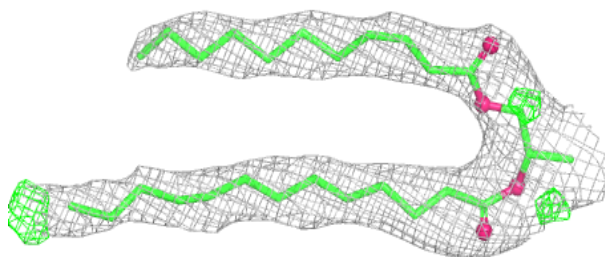


Electron density around LMT D 602:

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

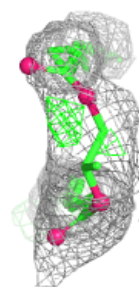
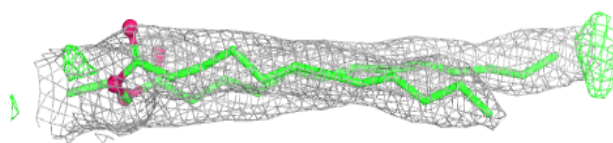
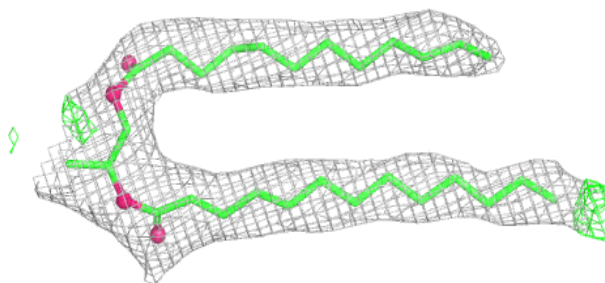
**Electron density around 3PE A 1101:**

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

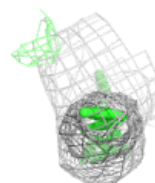
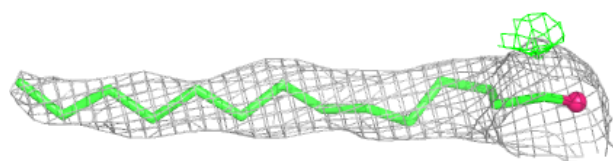
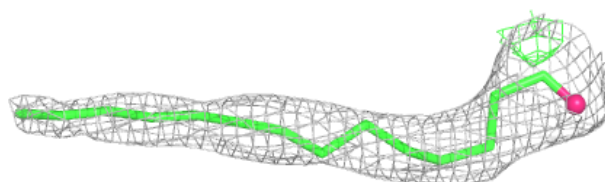


Electron density around 3PE B 1101:

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

**Electron density around PLM 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.