



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:53 PM UTC

PDB ID : 6V8Q / pdb_00006v8q
Title : Structure of an inner membrane protein required for PhoPQ regulated increases in outer membrane cardiolipin
Authors : Fan, J.; Miller, S.
Deposited on : 2019-12-11
Resolution : 2.70 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

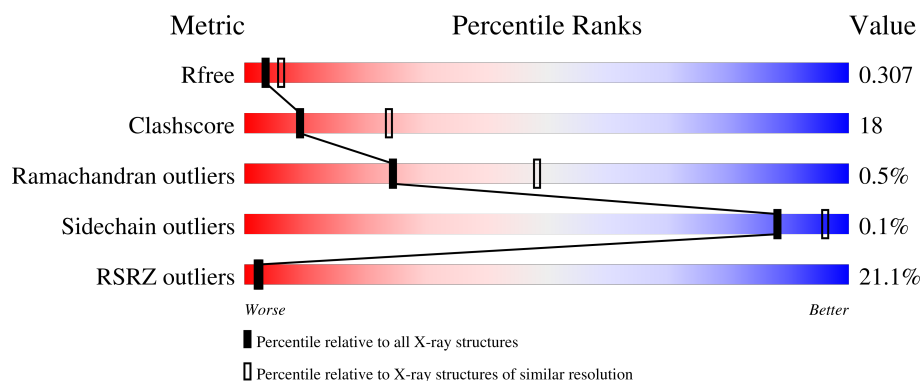
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	592	24% 61% 34% .
1	B	592	16% 61% 32% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9259 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 Inner membrane protein YejM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4473	2894	760	803	16			
1	B	565	Total	C	N	O	S	0	0	0
			4500	2917	765	802	16			

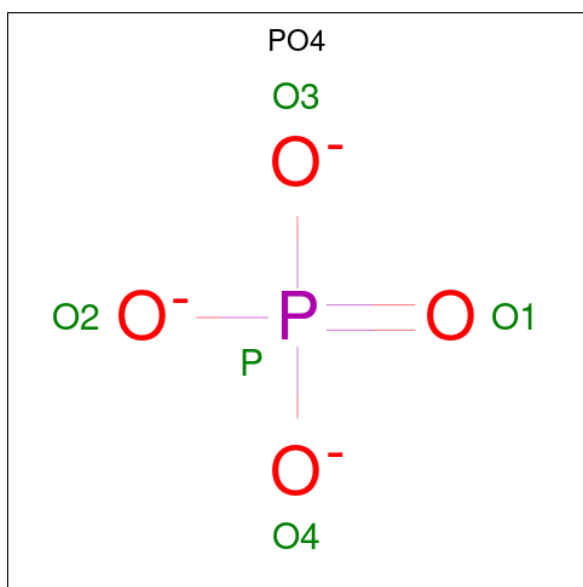
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	283	VAL	ALA	conflict	UNP P40709
A	587	HIS	-	expression tag	UNP P40709
A	588	HIS	-	expression tag	UNP P40709
A	589	HIS	-	expression tag	UNP P40709
A	590	HIS	-	expression tag	UNP P40709
A	591	HIS	-	expression tag	UNP P40709
A	592	HIS	-	expression tag	UNP P40709
B	283	VAL	ALA	conflict	UNP P40709
B	587	HIS	-	expression tag	UNP P40709
B	588	HIS	-	expression tag	UNP P40709
B	589	HIS	-	expression tag	UNP P40709
B	590	HIS	-	expression tag	UNP P40709
B	591	HIS	-	expression tag	UNP P40709
B	592	HIS	-	expression tag	UNP P40709

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

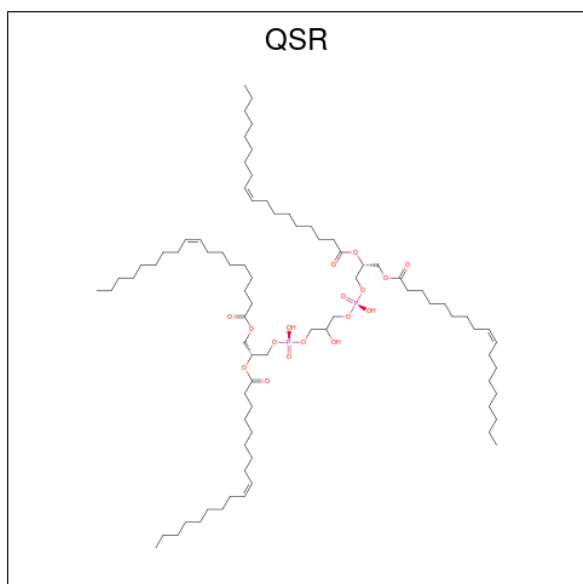
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



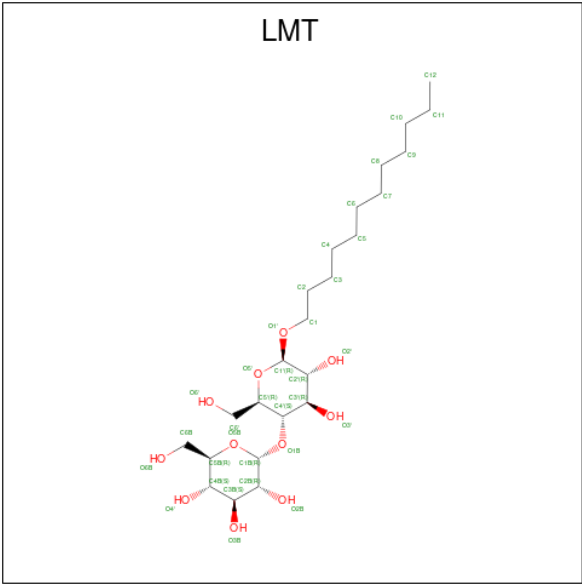
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is (9Z,21R,24R,30R,33R,44Z)-24,27,30-trihydroxy-18,24,30,36-tetraoxo-19,23,25,29,31,35-hexaoxa-24lambda 5 ,30lambda 5 -dip hosphatripentaconta-9,44-diene-21,33-diyl (9Z,9'Z)di-octadec-9-enoate (CCD ID: QSR) (formula: C₈₁H₁₅₀O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			52	33	17	2		
4	A	1	Total	C	O	P	0	0
			27	18	8	1		
4	B	1	Total	C	O	P	0	0
			67	48	17	2		
4	B	1	Total	C	O	P	0	0
			70	51	17	2		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	13	11		
5	B	1	Total	C	O	0	0
			35	24	11		

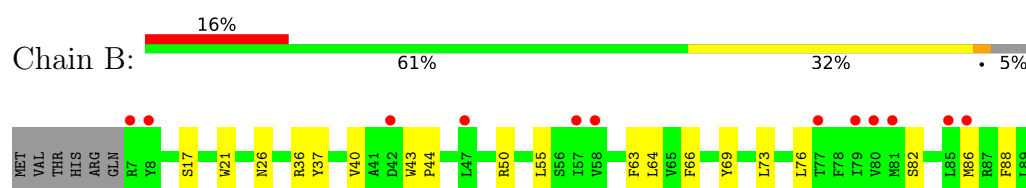
3 Residue-property plots [i](#)

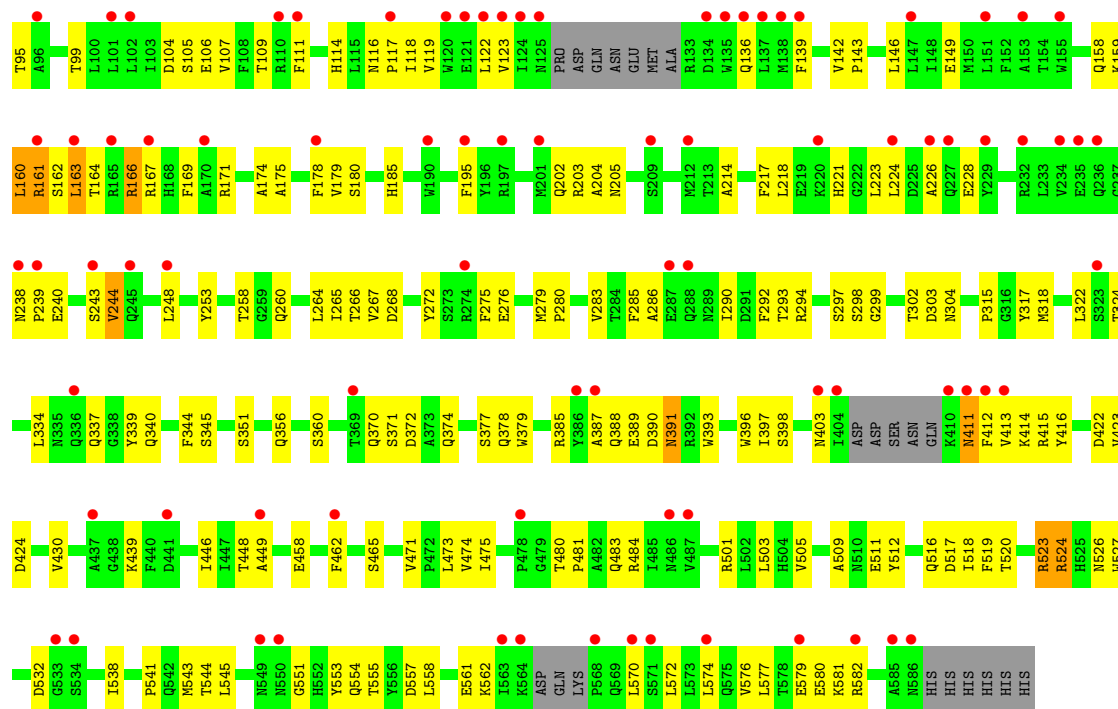
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Inner membrane protein YejM



• Molecule 1: Inner membrane protein YejM





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.83Å 64.85Å 146.36Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	48.34 – 2.70 48.34 – 2.70	Depositor EDS
% Data completeness (in resolution range)	76.7 (48.34-2.70) 76.7 (48.34-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.239 , 0.291 0.262 , 0.307	Depositor DCC
R_{free} test set	2716 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 21.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9259	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: CA, PO4, LMT, QSR

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	0.43	0/4589	0.77	7/6260 (0.1%)
1	B	0.43	0/4622	0.72	4/6303 (0.1%)
All	All	0.43	0/9211	0.75	11/12563 (0.1%)

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	B	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	81	MET	CB-CG-SD	-8.35	87.66	112.70
1	A	81	MET	CA-C-N	8.23	136.94	121.87
1	A	81	MET	C-N-CA	8.23	136.94	121.87
1	B	411	ASN	CB-CA-C	-7.97	95.37	109.71
1	B	523	ARG	CA-C-N	-6.67	105.92	121.52
1	B	523	ARG	C-N-CA	-6.67	105.92	121.52
1	A	126	PRO	N-CA-CB	6.07	109.67	103.00
1	A	172	PRO	N-CA-CB	5.57	109.40	103.39
1	A	227	GLN	CA-C-N	5.35	127.71	120.38
1	A	227	GLN	C-N-CA	5.35	127.71	120.38
1	B	524	ARG	N-CA-CB	5.22	119.61	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	161	ARG	Peptide
1	B	403	ASN	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	4473	0	4318	162	0
1	B	4500	0	4382	166	0
2	A	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
4	A	79	0	0	1	0
4	B	137	0	0	5	0
5	A	24	0	21	5	0
5	B	35	0	46	8	0
All	All	9259	0	8767	328	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 18.

All (328) 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:197:ARG:HH22	1:A:323:SER:CB	1.69	1.06
1:B:36:ARG:NE	1:B:105:SER:OG	1.92	1.01
1:A:197:ARG:NH2	1:A:323:SER:OG	1.94	1.01
1:A:197:ARG:HH22	1:A:323:SER:HB2	1.40	0.84
1:B:95:THR:HG22	1:B:149:GLU:HG3	1.60	0.83
1:B:317:TYR:OH	1:B:580:GLU:O	1.98	0.82
1:B:387:ALA:HB1	1:B:439:LYS:HZ3	1.46	0.81
1:A:95:THR:HG22	1:A:149:GLU:HG3	1.62	0.81
1:A:557:ASP:HB3	1:A:563:ILE:HD11	1.63	0.81
1:A:444:VAL:HG12	1:A:478:PRO:HD2	1.63	0.80
1:A:77:THR:O	1:A:81:MET:CE	2.31	0.77
1:A:121:GLU:N	1:A:121:GLU:OE1	2.17	0.76
1:A:135:TRP:HA	1:A:138:MET:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:MET:HG3	1:B:555:THR:HG23	1.69	0.74
1:A:142:VAL:HG13	1:A:143:PRO:HD3	1.69	0.74
1:A:36:ARG:HH12	1:A:106:GLU:HG2	1.51	0.74
1:B:258:THR:HG23	1:B:260:GLN:H	1.53	0.74
1:B:458:GLU:OE2	1:B:458:GLU:N	2.19	0.72
1:B:294:ARG:HG2	1:B:294:ARG:HH11	1.54	0.72
4:B:603:QSR:O9	4:B:603:QSR:O1	2.08	0.72
1:A:256:MET:HE1	1:B:374:GLN:HG3	1.71	0.71
1:A:91:ALA:O	1:A:95:THR:HG23	1.91	0.71
1:B:446:ILE:HG12	1:B:475:ILE:HG12	1.72	0.71
1:B:449:ALA:HB3	1:B:471:VAL:HB	1.72	0.71
1:B:387:ALA:HB1	1:B:439:LYS:NZ	2.07	0.70
4:B:603:QSR:O9	4:B:603:QSR:O5	2.10	0.69
1:A:77:THR:C	1:A:81:MET:HE3	2.17	0.69
1:A:493:ASP:HB3	1:A:518:ILE:HG23	1.74	0.69
1:B:95:THR:HG21	1:B:146:LEU:HA	1.75	0.69
1:B:292:PHE:HB2	1:B:473:LEU:HB3	1.72	0.69
5:B:604:LMT:O2B	5:B:604:LMT:O4'	2.10	0.68
1:A:38:LEU:HD13	1:A:57:ILE:HD11	1.75	0.68
1:A:487:VAL:HG11	1:A:523:ARG:HD3	1.76	0.68
1:A:76:LEU:HA	1:A:79:ILE:HG22	1.76	0.68
1:A:150:MET:O	1:A:154:THR:HG22	1.93	0.67
1:A:82:SER:HB3	1:A:85:LEU:HB3	1.76	0.67
1:B:36:ARG:NE	1:B:105:SER:HG	1.89	0.67
1:B:40:VAL:HG11	1:B:109:THR:HA	1.76	0.67
1:A:77:THR:O	1:A:81:MET:HE3	1.94	0.67
1:B:119:VAL:O	1:B:123:VAL:HG23	1.95	0.67
1:B:243:SER:O	1:B:244:VAL:HG22	1.95	0.67
1:B:114:HIS:NE2	1:B:204:ALA:O	2.29	0.66
1:B:411:ASN:CG	1:B:413:VAL:HG23	2.21	0.65
1:B:345:SER:HB2	1:B:398:SER:HB3	1.78	0.65
1:B:178:PHE:HA	5:B:604:LMT:H81	1.79	0.64
1:A:195:PHE:CE1	1:A:239:PRO:HG3	2.33	0.64
1:A:373:ALA:HA	1:A:426:GLN:OE1	1.98	0.64
1:B:91:ALA:O	1:B:95:THR:HG23	1.96	0.63
1:A:170:ALA:HB3	5:A:605:LMT:H6E	1.80	0.63
1:A:576:VAL:HG12	1:A:577:LEU:HD23	1.80	0.63
1:B:579:GLU:HB2	1:B:582:ARG:HH21	1.63	0.63
1:B:520:THR:O	1:B:523:ARG:NH1	2.32	0.63
1:B:543:MET:HG2	1:B:544:THR:N	2.14	0.62
1:B:36:ARG:HH22	1:B:106:GLU:CG	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HD12	1:B:118:ILE:H	1.64	0.62
1:B:122:LEU:HD22	1:B:574:LEU:HD13	1.81	0.62
1:B:279:MET:O	1:B:283:VAL:HG23	1.99	0.62
1:A:27:ILE:HG12	1:A:62:SER:HA	1.82	0.62
1:A:197:ARG:NH2	1:A:323:SER:CB	2.50	0.62
1:A:575:GLN:O	1:A:579:GLU:HG2	2.00	0.61
1:B:554:GLN:HE22	1:B:562:LYS:HD2	1.65	0.61
1:B:36:ARG:CZ	1:B:105:SER:OG	2.48	0.61
1:A:272:TYR:CB	1:A:470:GLN:HG2	2.31	0.60
1:A:347:ASP:O	1:A:350:ALA:HB2	2.01	0.60
1:A:12:VAL:HG22	1:A:81:MET:SD	2.41	0.60
1:A:276:GLU:HA	1:A:283:VAL:CG2	2.31	0.60
1:B:290:ILE:HG21	1:B:519:PHE:HE1	1.66	0.60
1:B:265:ILE:HD11	1:B:430:VAL:HG11	1.84	0.59
1:A:405:ASP:O	1:A:415:ARG:NH1	2.34	0.59
1:B:340:GLN:HG2	1:B:393:TRP:HB3	1.84	0.59
1:A:262:VAL:HG13	1:A:444:VAL:HG23	1.83	0.58
1:B:36:ARG:HH22	1:B:106:GLU:HG2	1.69	0.58
1:B:37:TYR:OH	1:B:104:ASP:OD2	2.13	0.58
1:A:262:VAL:HB	1:A:394:PHE:CD2	2.39	0.57
1:B:390:ASP:O	1:B:391:ASN:HB2	2.04	0.57
1:A:33:LEU:HD23	1:A:101:LEU:HD23	1.86	0.57
1:A:391:ASN:OD1	1:A:392:ARG:N	2.34	0.57
1:A:538:ILE:HG21	1:A:572:LEU:HD11	1.87	0.56
1:A:258:THR:OG1	1:A:260:GLN:HG3	2.05	0.56
1:B:379:TRP:CG	1:B:397:ILE:HD11	2.40	0.56
1:B:379:TRP:CD2	1:B:397:ILE:HD11	2.41	0.56
1:A:17:SER:OG	5:A:605:LMT:O6B	2.14	0.56
1:B:114:HIS:HE1	1:B:205:ASN:O	1.90	0.55
1:A:379:TRP:CG	1:A:397:ILE:HD11	2.41	0.55
1:A:119:VAL:O	1:A:123:VAL:HG23	2.07	0.55
1:A:318:MET:HE2	1:A:353:LEU:HD13	1.87	0.55
1:B:159:LYS:C	1:B:161:ARG:H	2.14	0.55
1:A:360:SER:O	1:B:415:ARG:HD2	2.06	0.55
1:B:118:ILE:HD11	1:B:551:GLY:O	2.07	0.55
1:B:238:ASN:ND2	1:B:240:GLU:HG3	2.22	0.54
1:A:189:ILE:HD11	1:A:212:MET:SD	2.48	0.54
1:B:337:GLN:NE2	1:B:503:LEU:O	2.38	0.54
1:B:370:GLN:NE2	1:B:378:GLN:OE1	2.34	0.54
1:B:76:LEU:HB3	1:B:86:MET:HE1	1.88	0.54
1:A:77:THR:O	1:A:81:MET:HE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:TYR:OH	1:A:580:GLU:O	2.22	0.54
1:B:243:SER:HB2	1:B:324:THR:HG21	1.89	0.54
1:B:36:ARG:NH2	1:B:106:GLU:HG2	2.23	0.54
1:A:43:TRP:NE1	1:A:50:ARG:HE	2.06	0.53
1:B:501:ARG:NH2	1:B:517:ASP:OD1	2.40	0.53
1:A:117:PRO:O	1:A:121:GLU:OE1	2.26	0.53
1:B:272:TYR:CE1	1:B:275:PHE:HE2	2.27	0.53
1:A:116:ASN:HB2	1:A:117:PRO:HD2	1.91	0.53
1:A:432:ASN:OD1	1:A:435:ARG:NH1	2.40	0.53
1:B:293:THR:HG21	1:B:484:ARG:NH1	2.24	0.53
1:A:111:PHE:O	1:A:113:LEU:HD12	2.07	0.53
1:A:276:GLU:HA	1:A:283:VAL:HG21	1.90	0.53
1:B:541:PRO:O	1:B:558:LEU:HD21	2.08	0.53
1:A:61:PHE:CE1	1:A:101:LEU:HD11	2.44	0.52
1:A:256:MET:HE2	1:B:377:SER:CB	2.39	0.52
1:A:142:VAL:CG1	1:A:143:PRO:HD3	2.39	0.52
1:B:36:ARG:HH22	1:B:106:GLU:HA	1.74	0.52
1:B:570:LEU:HB2	1:B:572:LEU:HB3	1.90	0.52
1:B:294:ARG:HG2	1:B:294:ARG:NH1	2.23	0.52
1:A:253:TYR:CD1	1:A:505:VAL:HG22	2.45	0.52
1:B:318:MET:HG3	1:B:322:LEU:HD13	1.92	0.52
1:B:114:HIS:CE1	1:B:205:ASN:O	2.62	0.52
1:A:118:ILE:HD11	1:A:573:LEU:HD13	1.91	0.51
1:A:175:ALA:O	1:A:179:VAL:HG23	2.10	0.51
1:B:167:ARG:O	1:B:171:ARG:HB2	2.10	0.51
1:A:262:VAL:HG13	1:A:444:VAL:CG2	2.40	0.51
1:B:579:GLU:HB2	1:B:582:ARG:NH2	2.24	0.51
1:A:581:LYS:HE2	1:A:584:ILE:HD11	1.91	0.51
1:B:226:ALA:HB3	1:B:228:GLU:HG3	1.91	0.51
1:A:253:TYR:CE1	1:A:505:VAL:HG22	2.45	0.51
1:B:36:ARG:NH2	1:B:105:SER:OG	2.44	0.51
1:A:18:TRP:CE2	1:A:87:ARG:HG2	2.45	0.51
1:B:160:LEU:HD23	1:B:160:LEU:O	2.10	0.51
1:B:572:LEU:O	1:B:576:VAL:HG13	2.10	0.51
1:B:411:ASN:OD1	1:B:411:ASN:O	2.29	0.51
1:B:458:GLU:H	1:B:458:GLU:CD	2.13	0.51
1:A:543:MET:CG	1:A:555:THR:HG23	2.42	0.50
1:B:171:ARG:HH22	5:B:604:LMT:H6'1	1.75	0.50
1:A:449:ALA:HB3	1:A:471:VAL:HB	1.93	0.50
1:A:516:GLN:HB3	1:A:524:ARG:NH2	2.26	0.50
1:B:334:LEU:HD23	1:B:503:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HB3	1:A:113:LEU:HD12	1.93	0.50
1:A:379:TRP:CH2	1:A:383:LEU:HD22	2.47	0.50
1:A:361:ASP:O	1:B:415:ARG:HG3	2.12	0.49
1:B:248:LEU:HB2	1:B:511:GLU:HG2	1.94	0.49
1:B:371:SER:HB2	1:B:374:GLN:H	1.76	0.49
1:B:526:ASN:OD1	1:B:541:PRO:HD2	2.12	0.49
1:B:545:LEU:HD11	1:B:553:TYR:CD2	2.46	0.49
1:A:18:TRP:CZ2	1:A:87:ARG:HG2	2.48	0.49
1:B:411:ASN:OD1	1:B:413:VAL:HG23	2.12	0.49
1:B:253:TYR:CE2	1:B:505:VAL:HG22	2.48	0.49
1:A:497:THR:OG1	1:A:518:ILE:HG12	2.13	0.49
1:A:197:ARG:NH2	1:A:323:SER:HB2	2.19	0.49
1:A:272:TYR:CE1	1:A:275:PHE:HE2	2.31	0.49
1:A:469:LEU:HD23	1:A:469:LEU:HA	1.57	0.49
1:B:481:PRO:HD2	1:B:483:GLN:NE2	2.27	0.49
1:A:197:ARG:N	1:A:198:PRO:CD	2.76	0.48
1:B:299:GLY:HA3	1:B:304:ASN:HB2	1.95	0.48
1:B:36:ARG:NH2	1:B:106:GLU:HA	2.28	0.48
1:A:118:ILE:HD12	1:A:121:GLU:HB2	1.95	0.48
1:B:166:ARG:HA	1:B:169:PHE:HB2	1.94	0.48
1:B:292:PHE:CE1	1:B:475:ILE:HD12	2.48	0.48
1:B:538:ILE:HD11	1:B:576:VAL:HG21	1.94	0.48
1:B:298:SER:O	1:B:315:PRO:HG2	2.13	0.48
1:B:174:ALA:HB1	5:B:604:LMT:H51	1.95	0.48
1:A:17:SER:O	1:A:21:TRP:HD1	1.97	0.48
1:A:370:GLN:NE2	1:A:378:GLN:OE1	2.44	0.48
1:B:136:GLN:HA	1:B:139:PHE:HB2	1.94	0.48
1:A:159:LYS:C	1:A:161:ARG:H	2.20	0.47
1:B:260:GLN:O	1:B:339:TYR:OH	2.17	0.47
1:B:276:GLU:HA	1:B:283:VAL:HG22	1.96	0.47
1:A:542:GLN:O	1:A:558:LEU:HD13	2.15	0.47
1:A:196:TYR:O	1:A:200:THR:HG23	2.14	0.47
1:B:509:ALA:HA	1:B:512:TYR:CZ	2.50	0.47
1:A:446:ILE:HG12	1:A:475:ILE:HG12	1.96	0.47
1:A:264:LEU:O	1:A:396:TRP:HA	2.15	0.47
1:A:355:ARG:CZ	1:A:364:MET:HE3	2.44	0.47
1:B:111:PHE:O	1:B:581:LYS:HD2	2.15	0.47
1:B:116:ASN:HB2	1:B:117:PRO:HD2	1.96	0.47
1:B:268:ASP:OD1	1:B:302:THR:HG21	2.14	0.47
1:A:272:TYR:O	1:A:275:PHE:HD2	1.98	0.47
1:A:17:SER:HG	5:A:605:LMT:H6B	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:603:QSR:O2	4:A:603:QSR:O9	2.32	0.47
1:B:36:ARG:NH2	1:B:106:GLU:CA	2.78	0.47
1:A:77:THR:C	1:A:81:MET:CE	2.82	0.47
1:A:290:ILE:HD13	1:A:519:PHE:CE1	2.49	0.47
1:A:342:GLY:O	1:A:395:SER:HA	2.14	0.47
1:B:73:LEU:HD13	1:B:90:SER:HB3	1.96	0.46
1:B:185:HIS:NE2	3:B:601:PO4:O4	2.48	0.46
1:A:26:ASN:OD1	1:A:94:ALA:HB1	2.15	0.46
1:A:43:TRP:HE1	1:A:50:ARG:HE	1.62	0.46
1:A:334:LEU:O	1:A:339:TYR:HB2	2.16	0.46
1:B:171:ARG:HH12	5:B:604:LMT:H6'1	1.80	0.46
1:A:531:ALA:HB2	1:A:536:LEU:HD12	1.97	0.46
1:B:111:PHE:HZ	1:B:574:LEU:HD11	1.81	0.46
1:B:267:VAL:O	1:B:449:ALA:HA	2.16	0.46
1:A:293:THR:HG21	1:A:484:ARG:NH1	2.31	0.45
1:B:17:SER:O	1:B:21:TRP:HD1	1.99	0.45
1:A:43:TRP:CE3	1:A:44:PRO:HD2	2.51	0.45
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.84	0.45
1:A:261:ASN:OD1	1:A:392:ARG:HA	2.16	0.45
1:A:297:SER:OG	1:A:298:SER:N	2.50	0.45
1:B:104:ASP:HA	1:B:107:VAL:HG22	1.98	0.45
1:A:256:MET:HE2	1:B:377:SER:HB3	1.98	0.45
1:A:545:LEU:HD11	1:A:553:TYR:HB2	1.97	0.45
1:B:248:LEU:HD23	1:B:248:LEU:HA	1.56	0.45
1:A:488:LEU:HB3	1:A:528:VAL:HG13	1.98	0.45
1:B:43:TRP:CE2	1:B:50:ARG:HG2	2.52	0.45
1:B:412:PHE:CD1	1:B:412:PHE:N	2.85	0.45
1:A:68:THR:O	1:A:72:ILE:HD12	2.16	0.45
1:A:117:PRO:HB2	1:A:551:GLY:O	2.17	0.45
1:B:290:ILE:HD11	1:B:480:THR:OG1	2.17	0.45
1:A:290:ILE:HD13	1:A:519:PHE:HE1	1.82	0.45
1:A:337:GLN:NE2	1:A:503:LEU:O	2.50	0.45
1:B:50:ARG:NH2	4:B:603:QSR:O11	2.50	0.45
1:B:297:SER:OG	1:B:298:SER:N	2.49	0.45
1:A:210:TYR:N	3:A:602:PO4:O4	2.35	0.45
1:B:63:PHE:HA	5:B:604:LMT:H101	1.99	0.44
1:B:88:PHE:O	1:B:92:ILE:HG12	2.17	0.44
1:B:142:VAL:HB	1:B:143:PRO:HD3	1.99	0.44
1:B:175:ALA:O	1:B:179:VAL:HG13	2.18	0.44
1:A:121:GLU:HB3	1:A:570:LEU:HD21	2.00	0.44
1:A:135:TRP:CA	1:A:138:MET:HB3	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HE2	1:A:90:SER:O	2.00	0.44
1:B:26:ASN:OD1	1:B:94:ALA:HB1	2.18	0.44
1:B:104:ASP:HA	1:B:107:VAL:CG2	2.48	0.44
1:B:509:ALA:HA	1:B:512:TYR:CE2	2.53	0.44
1:A:509:ALA:HA	1:A:512:TYR:CE2	2.53	0.44
1:B:379:TRP:CZ3	1:B:430:VAL:HG13	2.53	0.44
1:B:387:ALA:C	1:B:389:GLU:H	2.26	0.44
1:A:223:LEU:HA	1:A:224:LEU:HA	1.65	0.44
1:A:543:MET:HE3	1:A:543:MET:HB3	1.83	0.44
1:B:95:THR:O	1:B:99:THR:HG22	2.18	0.44
1:A:38:LEU:HD22	1:A:57:ILE:CD1	2.48	0.43
1:B:36:ARG:HH22	1:B:106:GLU:CA	2.31	0.43
1:A:218:LEU:HD23	1:A:218:LEU:HA	1.78	0.43
1:B:462:PHE:O	1:B:465:SER:HB3	2.19	0.43
1:B:524:ARG:NH1	1:B:524:ARG:HG2	2.32	0.43
1:A:293:THR:HG21	1:A:484:ARG:HH12	1.83	0.43
1:A:355:ARG:NH1	1:A:364:MET:HE3	2.33	0.43
1:B:292:PHE:CZ	1:B:518:ILE:HD12	2.53	0.43
1:A:125:ASN:CB	1:A:570:LEU:HD13	2.48	0.43
1:B:385:ARG:O	1:B:388:GLN:HG2	2.18	0.43
1:A:272:TYR:HB2	1:A:470:GLN:HG2	2.01	0.43
1:A:312:GLY:O	1:A:492:THR:HB	2.19	0.43
1:B:303:ASP:OD2	1:B:351:SER:OG	2.20	0.43
1:A:286:ALA:HB2	1:A:474:VAL:HG21	2.00	0.43
1:B:238:ASN:HD21	1:B:240:GLU:HG3	1.83	0.43
1:B:532:ASP:OD1	1:B:532:ASP:C	2.62	0.43
1:A:44:PRO:HG3	1:A:202:GLN:NE2	2.33	0.43
1:A:294:ARG:HB3	1:A:488:LEU:HD23	2.01	0.43
1:B:276:GLU:HA	1:B:283:VAL:CG2	2.49	0.43
1:B:481:PRO:O	1:B:483:GLN:HG2	2.19	0.43
1:A:562:LYS:HB2	1:A:562:LYS:HE3	1.78	0.42
1:B:66:PHE:O	1:B:69:TYR:HB3	2.18	0.42
1:B:159:LYS:C	1:B:161:ARG:N	2.77	0.42
1:B:285:PHE:HD2	1:B:474:VAL:HG11	1.83	0.42
1:A:37:TYR:OH	1:A:104:ASP:OD1	2.32	0.42
1:A:579:GLU:HB3	1:A:582:ARG:HH12	1.83	0.42
1:B:63:PHE:CD1	1:B:64:LEU:HD23	2.54	0.42
1:B:577:LEU:HD23	1:B:577:LEU:HA	1.83	0.42
1:A:33:LEU:HD21	1:A:102:LEU:HG	2.01	0.42
1:A:244:VAL:HG11	1:A:317:TYR:HB3	2.01	0.42
1:B:118:ILE:CD1	1:B:551:GLY:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ALA:HB2	1:B:474:VAL:CG2	2.49	0.42
1:B:387:ALA:C	1:B:389:GLU:N	2.76	0.42
1:B:414:LYS:NZ	1:B:422:ASP:OD2	2.33	0.42
1:A:38:LEU:CD2	1:A:53:SER:HB3	2.49	0.42
1:B:217:PHE:CE1	1:B:221:HIS:CE1	3.08	0.42
1:A:286:ALA:HA	1:A:474:VAL:CG1	2.49	0.42
1:B:161:ARG:HH11	1:B:161:ARG:HG2	1.85	0.42
1:A:295:HIS:CE1	1:A:490:ASP:C	2.97	0.42
1:B:55:LEU:HD23	1:B:180:SER:HB3	2.00	0.42
1:B:214:ALA:O	1:B:218:LEU:HG	2.19	0.42
1:B:40:VAL:HG21	1:B:109:THR:OG1	2.20	0.42
1:B:44:PRO:HG3	1:B:202:GLN:NE2	2.34	0.42
1:B:557:ASP:OD1	1:B:561:GLU:N	2.52	0.42
1:A:102:LEU:HD23	1:A:102:LEU:HA	1.87	0.42
1:A:454:PRO:HG2	1:A:468:HIS:NE2	2.35	0.42
1:A:95:THR:HG21	1:A:146:LEU:HA	2.01	0.41
1:A:135:TRP:N	1:A:135:TRP:CD1	2.86	0.41
1:A:233:LEU:HD12	1:A:239:PRO:HD3	2.02	0.41
1:B:178:PHE:CA	5:B:604:LMT:H81	2.46	0.41
1:A:20:HIS:HB3	5:A:605:LMT:H3'	2.02	0.41
1:A:48:ALA:HA	1:A:51:ILE:HD12	2.02	0.41
1:A:61:PHE:HE1	1:A:101:LEU:HD11	1.84	0.41
1:A:79:ILE:HG23	1:A:80:VAL:N	2.35	0.41
1:A:281:GLU:HG3	1:A:428:ASN:HB2	2.02	0.41
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.80	0.41
1:A:493:ASP:HB3	1:A:518:ILE:CG2	2.47	0.41
1:A:509:ALA:HA	1:A:512:TYR:CZ	2.56	0.41
1:A:135:TRP:HA	1:A:138:MET:CB	2.44	0.41
1:A:234:VAL:HG22	1:A:352:PRO:HG2	2.02	0.41
1:A:272:TYR:O	1:A:275:PHE:CD2	2.73	0.41
1:B:290:ILE:HD13	1:B:519:PHE:CE1	2.55	0.41
1:A:246:TYR:OH	1:A:311:TYR:O	2.32	0.41
1:B:66:PHE:CD1	5:B:604:LMT:H22	2.56	0.41
1:B:160:LEU:C	1:B:161:ARG:HD2	2.46	0.41
1:B:195:PHE:CZ	1:B:239:PRO:HG3	2.55	0.41
1:B:372:ASP:OD2	1:B:423:VAL:HG12	2.19	0.41
1:B:416:TYR:CD1	1:B:416:TYR:C	2.97	0.41
4:B:602:QSR:O9	4:B:602:QSR:O1	2.39	0.41
1:A:20:HIS:HB3	5:A:605:LMT:C3'	2.51	0.41
1:A:104:ASP:HA	1:A:107:VAL:HG22	2.02	0.41
1:A:15:MET:CE	1:A:86:MET:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD22	1:A:120:TRP:CZ2	2.56	0.41
1:B:158:GLN:HG2	1:B:159:LYS:HG2	2.03	0.41
1:B:163:LEU:O	1:B:164:THR:C	2.64	0.41
1:B:527:TRP:CZ3	1:B:576:VAL:HG12	2.56	0.41
1:A:15:MET:HE3	1:A:15:MET:HB3	1.89	0.41
1:B:43:TRP:NE1	1:B:50:ARG:HE	2.18	0.41
1:B:162:SER:O	1:B:166:ARG:N	2.54	0.41
1:B:203:ARG:HD2	1:B:240:GLU:OE2	2.21	0.41
1:B:223:LEU:HA	1:B:224:LEU:HA	1.71	0.41
1:A:82:SER:O	1:A:85:LEU:N	2.53	0.41
1:A:87:ARG:CZ	1:A:157:TRP:CD1	3.04	0.41
1:A:448:THR:OG1	1:A:491:HIS:HE1	2.04	0.41
1:A:501:ARG:HH21	1:A:517:ASP:CG	2.29	0.41
1:B:50:ARG:CZ	4:B:603:QSR:O11	2.69	0.41
1:A:516:GLN:OE1	1:A:524:ARG:N	2.34	0.40
1:B:344:PHE:CE2	1:B:378:GLN:HB3	2.56	0.40
1:B:356:GLN:O	1:B:360:SER:HB3	2.21	0.40
1:A:52:TYR:CD2	1:A:199:ILE:HG23	2.56	0.40
1:A:296:MET:HE2	1:A:539:THR:HG21	2.03	0.40
1:B:264:LEU:O	1:B:396:TRP:HA	2.21	0.40
1:A:271:ASN:ND2	1:A:455:LEU:HG	2.37	0.40
1:A:543:MET:HG2	1:A:555:THR:HG23	2.03	0.40
1:B:37:TYR:CE1	1:B:105:SER:HA	2.56	0.40
1:B:516:GLN:HE21	1:B:520:THR:HG21	1.87	0.40
1:B:266:THR:HA	1:B:448:THR:O	2.22	0.40
1:A:501:ARG:NH2	1:A:517:ASP:OD2	2.55	0.40
1:B:280:PRO:HD2	1:B:424:ASP:OD2	2.21	0.40
1:B:462:PHE:CZ	1:B:465:SER:HA	2.57	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	559/592 (94%)	526 (94%)	33 (6%)	0	100	100
1	B	557/592 (94%)	526 (94%)	25 (4%)	6 (1%)	11	29
All	All	1116/1184 (94%)	1052 (94%)	58 (5%)	6 (0%)	24	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	SER
1	B	244	VAL
1	B	391	ASN
1	B	166	ARG
1	B	163	LEU
1	B	160	LEU

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	465/518 (90%)	464 (100%)	1 (0%)	87	95
1	B	474/518 (92%)	474 (100%)	0	100	100
All	All	939/1036 (91%)	938 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	202	GLN
1	A	368	GLN
1	A	476	HIS

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Mol	Chain	Res	Type
1	A	525	HIS
1	A	569	GLN
1	B	245	GLN
1	B	428	ASN
1	B	483	GLN
1	B	525	HIS
1	B	554	GLN
1	B	575	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](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LMT	B	604	-	36,36,36	1.30	3 (8%)	47,47,47	1.23	4 (8%)
5	LMT	A	605	-	25,25,36	1.28	3 (12%)	36,36,47	1.66	6 (16%)
3	PO4	B	601	-	4,4,4	0.96	0	6,6,6	0.63	0
4	QSR	B	603	-	69,69,99	1.56	9 (13%)	75,81,111	1.25	8 (10%)
4	QSR	A	603	-	51,51,99	1.68	6 (11%)	57,63,111	1.63	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	QSR	A	604	-	26,26,99	1.65	4 (15%)	29,31,111	1.26	4 (13%)
4	QSR	B	602	-	66,66,99	1.56	9 (13%)	72,78,111	1.35	9 (12%)
3	PO4	A	602	-	4,4,4	0.93	0	6,6,6	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	B	604	-	-	9/21/61/61	0/2/2/2
5	LMT	A	605	-	-	5/10/50/61	0/2/2/2
4	QSR	B	603	-	-	46/80/80/110	-
4	QSR	A	604	-	-	15/28/28/110	-
4	QSR	A	603	-	-	36/61/61/110	-
4	QSR	B	602	-	-	45/77/77/110	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	QSR	O14-C35	4.95	1.47	1.33
4	A	603	QSR	O16-C46	4.86	1.48	1.34
4	B	603	QSR	O2-C14	4.74	1.47	1.34
4	A	604	QSR	O2-C14	4.71	1.47	1.34
4	B	603	QSR	C44-C43	4.69	1.58	1.31
4	B	602	QSR	C70-C69	4.64	1.58	1.31
4	B	602	QSR	O16-C46	4.54	1.47	1.34
4	A	604	QSR	O3-C17	4.53	1.46	1.33
4	B	603	QSR	O3-C17	4.46	1.46	1.33
4	B	603	QSR	C55-C54	4.19	1.55	1.31
4	A	603	QSR	O2-C14	4.16	1.44	1.35
4	B	603	QSR	O14-C35	4.11	1.45	1.33
4	A	603	QSR	O3-C17	4.06	1.45	1.33
4	A	603	QSR	C55-C54	4.05	1.54	1.31
4	B	602	QSR	O3-C17	3.91	1.44	1.33
5	B	604	LMT	O5B-C1B	3.88	1.51	1.41
4	B	602	QSR	C55-C54	3.87	1.53	1.31
4	B	602	QSR	O14-C35	3.77	1.44	1.33
4	B	603	QSR	O16-C46	3.37	1.43	1.34
5	B	604	LMT	O5'-C1'	3.23	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	QSR	O2-C14	3.22	1.43	1.34
5	A	605	LMT	O5'-C1'	3.04	1.49	1.41
5	A	605	LMT	O5B-C1B	3.03	1.49	1.41
5	B	604	LMT	C3B-C2B	-2.82	1.45	1.52
4	A	604	QSR	C13-C14	2.67	1.58	1.50
4	A	603	QSR	C47-C46	2.61	1.58	1.50
4	B	602	QSR	O2-C15	-2.52	1.40	1.46
4	B	602	QSR	C47-C46	2.51	1.58	1.50
4	B	603	QSR	C13-C14	2.44	1.57	1.50
5	A	605	LMT	C3B-C2B	-2.27	1.46	1.52
4	A	604	QSR	C18-C17	2.25	1.57	1.50
4	B	603	QSR	C18-C17	2.16	1.57	1.50
4	B	603	QSR	C36-C35	2.09	1.56	1.50
4	B	602	QSR	C18-C17	2.03	1.56	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	QSR	O2-C14-C13	6.08	121.92	111.09
4	A	603	QSR	O16-C46-C47	4.55	121.32	111.48
5	A	605	LMT	O5B-C5B-C4B	4.31	117.47	109.70
4	B	602	QSR	O3-C17-C18	4.28	124.90	111.83
4	A	603	QSR	O14-C35-C36	4.26	124.08	111.15
5	A	605	LMT	C3B-C4B-C5B	4.21	117.86	110.23
5	A	605	LMT	C1B-O1B-C4'	-4.11	108.25	117.98
4	B	602	QSR	O2-C14-C13	3.86	119.83	111.48
4	B	603	QSR	O2-C14-C13	3.80	119.71	111.48
4	B	603	QSR	C33-O16-C46	3.65	126.53	117.80
5	B	604	LMT	O2B-C2B-C3B	-3.40	102.35	110.38
4	A	604	QSR	O2-C14-C13	3.33	118.68	111.48
4	A	603	QSR	O3-C17-C18	3.19	121.58	111.83
4	B	602	QSR	O16-C46-C47	3.18	118.36	111.48
4	B	602	QSR	O3-C17-O4	-3.07	115.96	123.63
4	B	603	QSR	C48-C47-C46	-2.92	102.99	113.69
4	A	604	QSR	O3-C17-C18	2.87	120.59	111.83
5	B	604	LMT	O5B-C1B-C2B	2.78	116.08	110.37
5	A	605	LMT	O5'-C5'-C4'	2.71	115.33	109.72
4	B	602	QSR	O14-C35-C36	2.68	119.30	111.15
4	B	602	QSR	C16-O3-C17	-2.65	107.45	117.12
5	B	604	LMT	C1B-O5B-C5B	2.62	118.84	113.72
4	A	603	QSR	C34-C33-C32	-2.62	105.69	111.78
5	A	605	LMT	C2'-C3'-C4'	2.58	115.55	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	LMT	O1B-C1B-C2B	2.38	113.95	108.09
4	B	603	QSR	O14-C35-C36	2.32	118.91	111.83
4	A	603	QSR	O2-C14-O1	-2.28	118.60	122.99
4	B	603	QSR	C42-C43-C44	-2.25	107.97	124.83
4	A	604	QSR	C28-C15-C16	-2.24	106.57	111.78
4	B	602	QSR	C71-C70-C69	-2.20	108.32	124.83
5	B	604	LMT	C1B-O1B-C4'	-2.18	112.82	117.98
4	B	603	QSR	O16-C46-C47	2.14	116.12	111.48
4	B	603	QSR	O16-C33-C32	2.10	115.86	108.34
4	B	602	QSR	C37-C36-C35	-2.09	104.20	114.11
4	A	604	QSR	O3-C17-O4	-2.07	118.45	123.63
4	B	603	QSR	O3-C17-C18	2.06	118.13	111.83
4	A	603	QSR	O2-C15-C16	2.03	115.63	108.34
4	B	602	QSR	O2-C14-O1	-2.00	119.02	123.70

There are no chirality outliers.

All (156) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	QSR	C28-O5-P1-O6
4	A	603	QSR	C28-O5-P1-O8
4	A	603	QSR	O1-C14-O2-C15
4	A	603	QSR	C13-C14-O2-C15
4	A	603	QSR	C32-O13-P2-O10
4	A	603	QSR	C32-O13-P2-O11
4	A	603	QSR	C32-O13-P2-O12
4	A	603	QSR	O17-C46-O16-C33
4	A	603	QSR	C47-C46-O16-C33
4	A	603	QSR	O8-C29-C30-C31
4	A	604	QSR	C28-O5-P1-O7
4	A	604	QSR	C28-O5-P1-O8
4	B	602	QSR	C28-O5-P1-O6
4	B	602	QSR	C28-O5-P1-O8
4	B	602	QSR	C29-O8-P1-O5
4	B	602	QSR	O1-C14-O2-C15
4	B	602	QSR	C32-O13-P2-O10
4	B	602	QSR	C32-O13-P2-O11
4	B	602	QSR	C32-O13-P2-O12
4	B	602	QSR	C33-C32-O13-P2
4	B	602	QSR	O8-C29-C30-C31
4	B	603	QSR	C28-O5-P1-O6
4	B	603	QSR	O1-C14-O2-C15

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Mol	Chain	Res	Type	Atoms
4	B	603	QSR	C13-C14-O2-C15
4	B	603	QSR	C31-O10-P2-O12
4	B	603	QSR	C31-O10-P2-O13
4	B	603	QSR	C32-O13-P2-O10
4	B	603	QSR	C32-O13-P2-O11
4	B	603	QSR	C32-O13-P2-O12
4	B	603	QSR	C30-C31-O10-P2
4	B	603	QSR	O17-C46-O16-C33
4	B	603	QSR	C47-C46-O16-C33
5	A	605	LMT	C2'-C1'-O1'-C1
5	B	604	LMT	O5B-C1B-O1B-C4'
4	A	603	QSR	O15-C35-O14-C34
4	B	602	QSR	O15-C35-O14-C34
4	A	603	QSR	C36-C35-O14-C34
4	B	602	QSR	C36-C35-O14-C34
4	B	602	QSR	C13-C14-O2-C15
4	B	602	QSR	C53-C54-C55-C09
4	B	602	QSR	C47-C46-O16-C33
4	A	603	QSR	C30-C29-O8-P1
4	B	603	QSR	C30-C29-O8-P1
5	B	604	LMT	O5B-C5B-C6B-O6B
4	B	603	QSR	C53-C54-C55-C09
5	A	605	LMT	C4'-C5'-C6'-O6'
4	B	602	QSR	O17-C46-O16-C33
4	A	604	QSR	C18-C17-O3-C16
4	B	603	QSR	C18-C17-O3-C16
5	B	604	LMT	C4B-C5B-C6B-O6B
4	A	603	QSR	O8-C29-C30-O9
4	B	602	QSR	O8-C29-C30-O9
4	B	603	QSR	O8-C29-C30-O9
4	A	604	QSR	O4-C17-O3-C16
4	B	603	QSR	O4-C17-O3-C16
5	A	605	LMT	O5'-C5'-C6'-O6'
4	B	602	QSR	C50-C51-C52-C53
4	B	603	QSR	C36-C35-O14-C34
5	B	604	LMT	C2'-C1'-O1'-C1
4	A	603	QSR	C33-C32-O13-P2
4	B	602	QSR	C30-C29-O8-P1
4	A	603	QSR	C51-C52-C53-C54
4	B	603	QSR	O15-C35-O14-C34
4	B	602	QSR	C68-C69-C70-C71
4	B	602	QSR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	B	603	QSR	C47-C48-C49-C50
4	B	602	QSR	C48-C49-C50-C51
4	B	602	QSR	C20-C21-C22-C67
4	B	603	QSR	C50-C51-C52-C53
4	B	603	QSR	C51-C52-C53-C54
4	B	603	QSR	C42-C43-C44-C01
4	B	603	QSR	C11-C10-C9-C8
4	A	603	QSR	C48-C49-C50-C51
5	B	604	LMT	C1-C2-C3-C4
4	A	603	QSR	C23-C09-C55-C54
4	B	603	QSR	C55-C09-C23-C24
4	B	603	QSR	C39-C40-C41-C42
4	B	603	QSR	C46-C47-C48-C49
4	B	603	QSR	C11-C12-C13-C14
4	B	603	QSR	O8-C29-C30-C31
4	B	602	QSR	C28-C15-C16-O3
4	A	604	QSR	C15-C28-O5-P1
4	A	604	QSR	C28-O5-P1-O6
4	B	602	QSR	C70-C71-C72-C73
4	A	604	QSR	C17-C18-C19-C20
4	B	602	QSR	C21-C22-C67-C68
4	B	603	QSR	C44-C01-C02-C03
4	B	602	QSR	C71-C72-C73-C74
4	B	603	QSR	C7-C8-C9-C10
4	B	603	QSR	C01-C02-C03-C04
4	B	603	QSR	O3-C17-C18-C19
4	B	603	QSR	C28-C15-C16-O3
4	A	604	QSR	C7-C8-C9-C10
4	B	603	QSR	C35-C36-C37-C38
4	A	604	QSR	C20-C21-C22-C67
4	B	602	QSR	O2-C15-C16-O3
4	B	603	QSR	C09-C23-C24-C25
4	A	604	QSR	C11-C12-C13-C14
5	B	604	LMT	C4-C5-C6-C7
5	B	604	LMT	O5'-C1'-O1'-C1
4	A	603	QSR	O13-C32-C33-C34
4	A	604	QSR	C18-C19-C20-C21
5	B	604	LMT	C5-C6-C7-C8
4	A	603	QSR	O2-C15-C16-O3
4	B	602	QSR	C19-C20-C21-C22
4	B	603	QSR	C9-C10-C11-C12
4	A	603	QSR	C18-C17-O3-C16

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Mol	Chain	Res	Type	Atoms
4	A	604	QSR	C10-C11-C12-C13
4	A	603	QSR	O4-C17-O3-C16
4	B	602	QSR	C18-C19-C20-C21
4	A	604	QSR	O2-C15-C28-O5
5	A	605	LMT	O5'-C1'-O1'-C1
4	B	603	QSR	O2-C15-C16-O3
4	A	603	QSR	C28-C15-C16-O3
4	B	603	QSR	C52-C53-C54-C55
4	B	602	QSR	C7-C8-C9-C10
5	B	604	LMT	C9-C10-C11-C12
4	A	603	QSR	C28-O5-P1-O7
4	A	603	QSR	C29-O8-P1-O5
4	A	603	QSR	C29-O8-P1-O6
4	A	603	QSR	C29-O8-P1-O7
4	B	602	QSR	C28-O5-P1-O7
4	B	602	QSR	C29-O8-P1-O6
4	B	603	QSR	C28-O5-P1-O8
4	B	603	QSR	C31-O10-P2-O11
4	B	603	QSR	C10-C11-C12-C13
4	A	604	QSR	C16-C15-C28-O5
4	B	602	QSR	C52-C53-C54-C55
4	A	603	QSR	C17-C18-C19-C20
4	B	602	QSR	C11-C12-C13-C14
4	B	602	QSR	O4-C17-O3-C16
4	B	602	QSR	O14-C35-C36-C37
4	B	602	QSR	C18-C17-O3-C16
4	B	602	QSR	C47-C48-C49-C50
4	A	603	QSR	C47-C48-C49-C50
4	B	603	QSR	C32-C33-O16-C46
4	A	603	QSR	C16-C15-C28-O5
4	B	603	QSR	O4-C17-C18-C19
4	A	604	QSR	C11-C10-C9-C8
4	B	603	QSR	O14-C35-C36-C37
4	A	603	QSR	C18-C19-C20-C21
4	B	602	QSR	O15-C35-C36-C37
4	B	602	QSR	C67-C68-C69-C70
5	A	605	LMT	C3'-C4'-O1B-C1B
4	B	603	QSR	C02-C01-C44-C43
4	A	603	QSR	O16-C46-C47-C48
4	B	602	QSR	O16-C46-C47-C48
4	B	602	QSR	C10-C11-C12-C13
4	A	603	QSR	C29-C30-C31-O10

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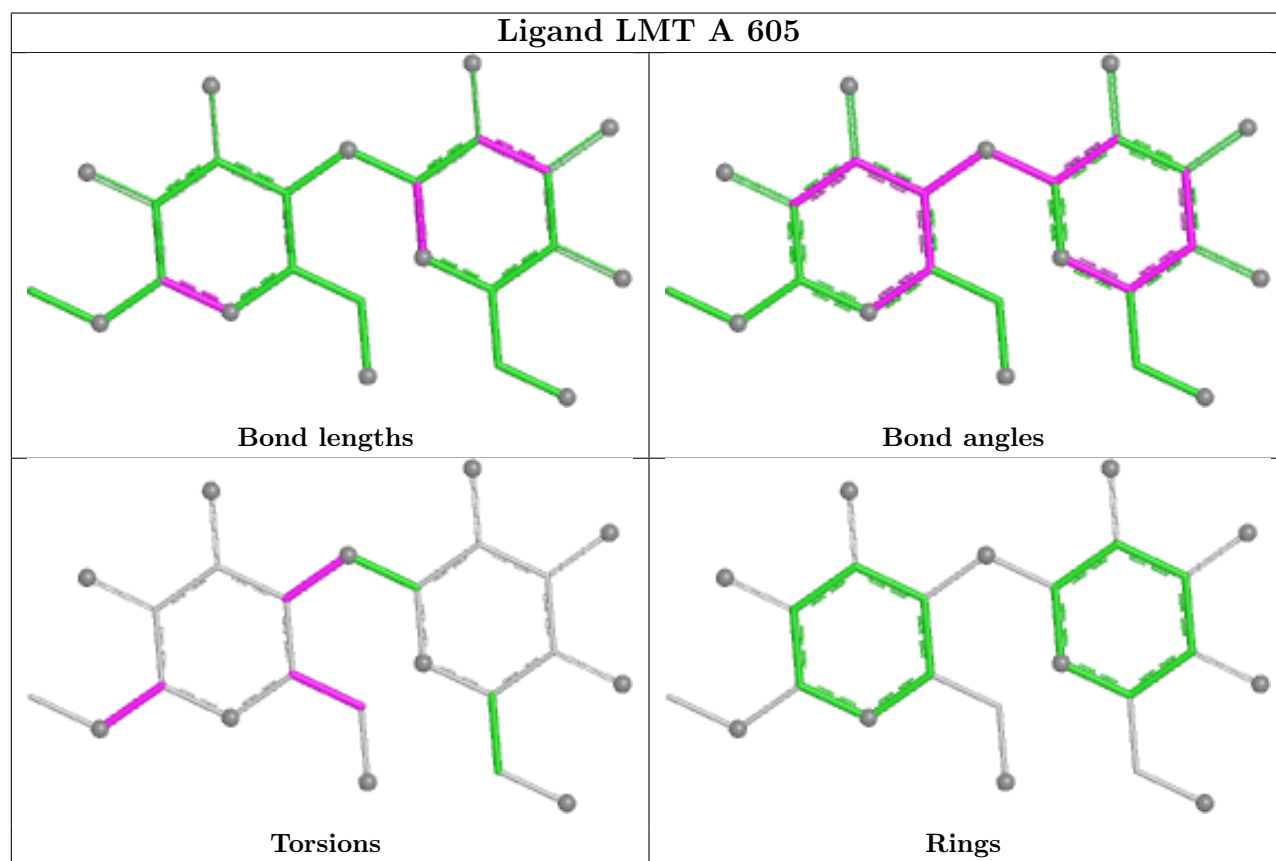
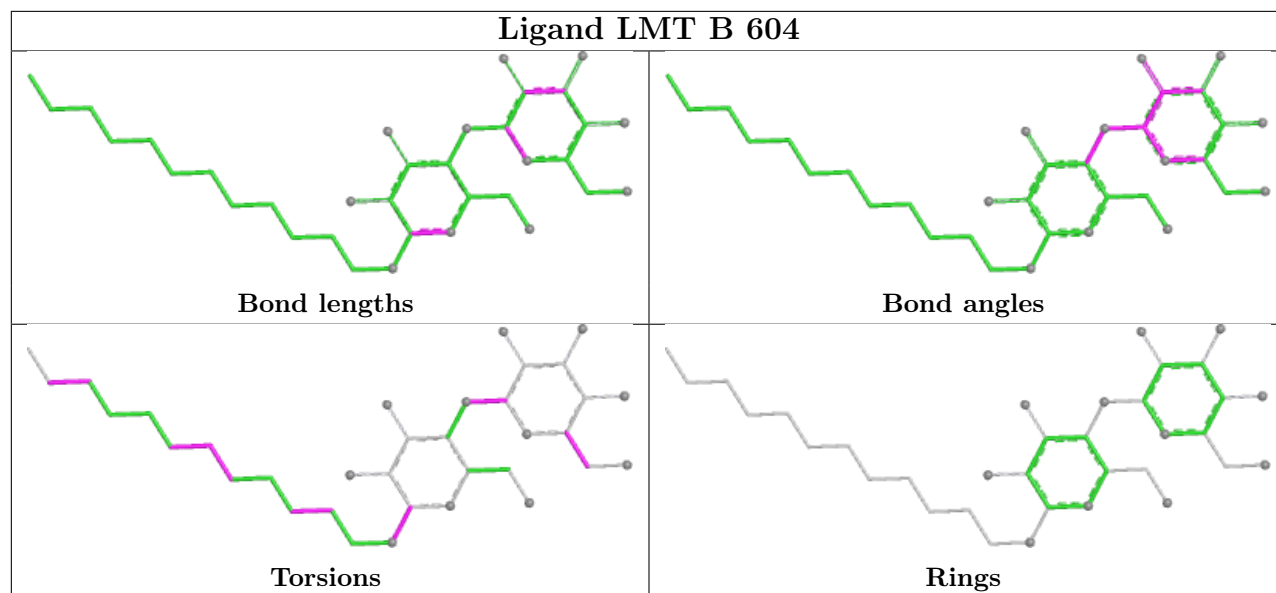
Mol	Chain	Res	Type	Atoms
4	A	603	QSR	C49-C50-C51-C52
4	B	602	QSR	C12-C13-C14-O2
4	A	603	QSR	O17-C46-C47-C48
4	B	602	QSR	O17-C46-C47-C48
4	B	602	QSR	O16-C33-C34-O14
4	A	603	QSR	O3-C17-C18-C19
4	B	603	QSR	C12-C13-C14-O2

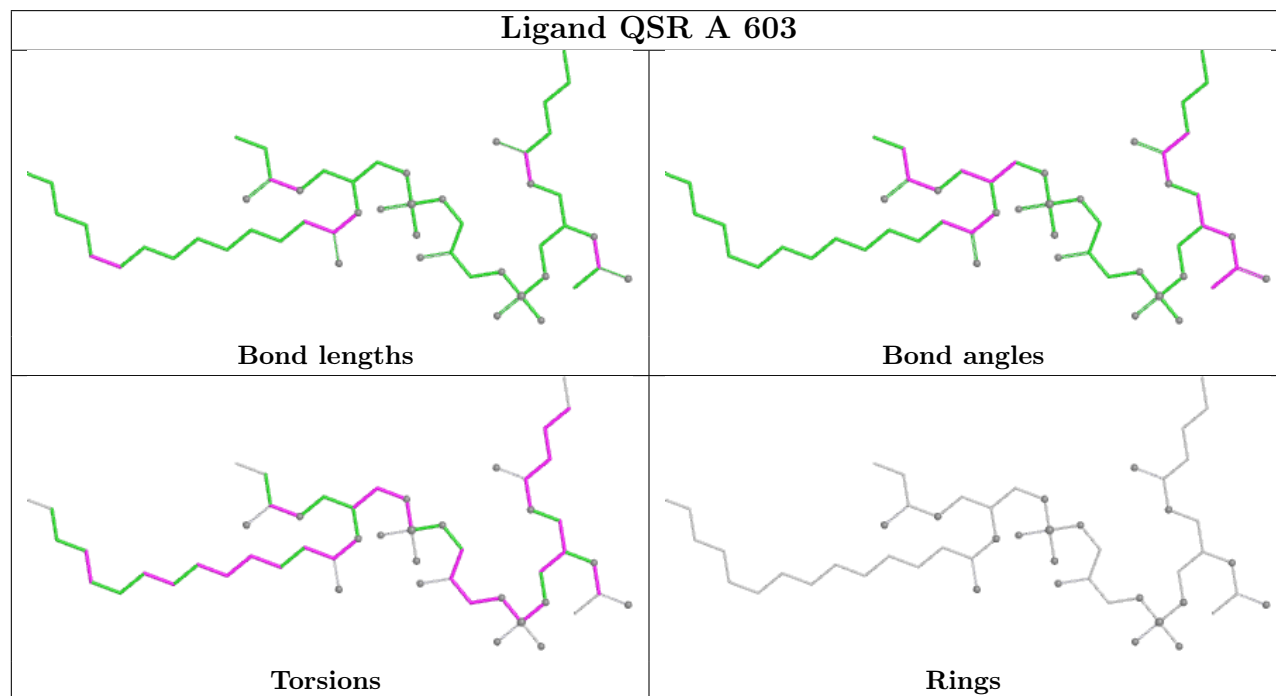
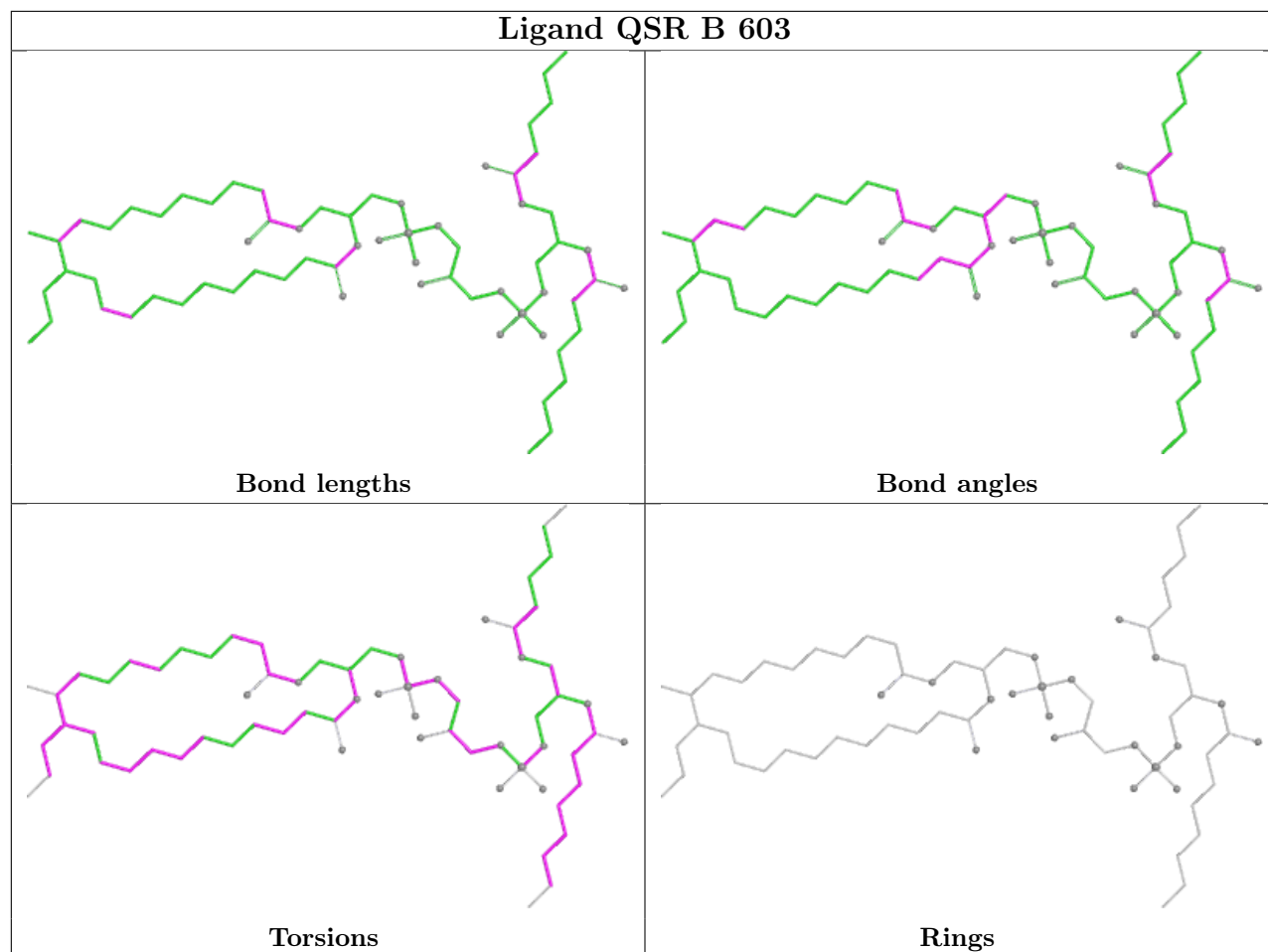
There are no ring outliers.

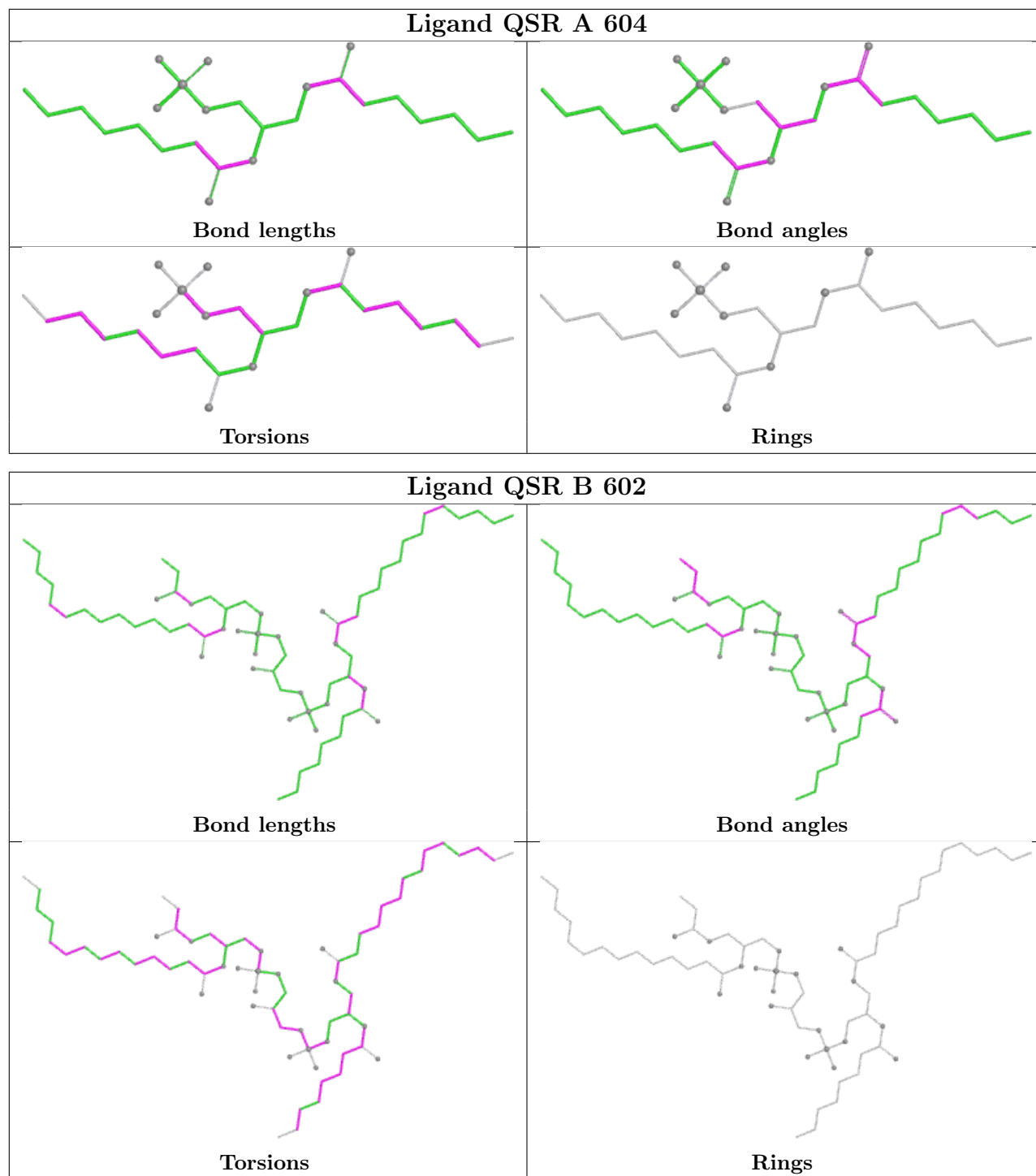
7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	604	LMT	8	0
5	A	605	LMT	5	0
3	B	601	PO4	1	0
4	B	603	QSR	4	0
4	A	603	QSR	1	0
4	B	602	QSR	1	0
3	A	602	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	569/592 (96%)	1.39	144 (25%)  	26, 62, 102, 124	0
1	B	565/592 (95%)	1.13	95 (16%)  	28, 56, 84, 108	0
All	All	1134/1184 (95%)	1.26	239 (21%)  	26, 57, 96, 124	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	ASN	10.0
1	A	387	ALA	9.9
1	A	209	SER	9.0
1	A	35	SER	8.9
1	A	240	GLU	8.7
1	A	203	ARG	8.1
1	A	34	GLY	8.0
1	B	411	ASN	7.9
1	A	31	THR	7.7
1	B	122	LEU	7.2
1	A	134	ASP	7.1
1	A	132	ALA	7.0
1	A	126	PRO	7.0
1	A	113	LEU	6.7
1	A	210	TYR	6.2
1	A	407	SER	5.8
1	A	205	ASN	5.7
1	A	32	LEU	5.6
1	A	551	GLY	5.5
1	A	133	ARG	5.5
1	A	37	TYR	5.4
1	B	125	ASN	5.2
1	A	411	ASN	5.1
1	B	386	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	585	ALA	5.0
1	A	242	VAL	5.0
1	A	39	PHE	5.0
1	B	413	VAL	4.9
1	A	566	GLN	4.9
1	A	124	ILE	4.9
1	B	245	GLN	4.9
1	B	404	ILE	4.8
1	B	80	VAL	4.8
1	A	565	ASP	4.8
1	A	8	TYR	4.8
1	B	110	ARG	4.7
1	A	211	PRO	4.6
1	B	134	ASP	4.6
1	A	484	ARG	4.6
1	B	564	LYS	4.5
1	B	487	VAL	4.5
1	A	80	VAL	4.4
1	A	16	VAL	4.4
1	B	151	LEU	4.4
1	B	234	VAL	4.4
1	A	550	ASN	4.3
1	A	206	LEU	4.3
1	B	570	LEU	4.3
1	A	139	PHE	4.3
1	B	197	ARG	4.3
1	A	568	PRO	4.2
1	B	111	PHE	4.2
1	B	163	LEU	4.2
1	A	122	LEU	4.1
1	A	386	TYR	4.0
1	B	232	ARG	4.0
1	A	14	GLN	4.0
1	A	135	TRP	4.0
1	A	163	LEU	4.0
1	A	549	ASN	4.0
1	A	563	ILE	3.9
1	B	387	ALA	3.9
1	B	42	ASP	3.9
1	A	197	ARG	3.9
1	A	55	LEU	3.9
1	A	226	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	142	VAL	3.9
1	B	549	ASN	3.8
1	A	7	ARG	3.8
1	A	207	PRO	3.8
1	A	238	ASN	3.8
1	B	571	SER	3.8
1	B	568	PRO	3.8
1	B	227	GLN	3.7
1	A	137	LEU	3.7
1	B	533	GLY	3.7
1	A	586	ASN	3.6
1	B	550	ASN	3.6
1	B	226	ALA	3.6
1	B	238	ASN	3.5
1	B	243	SER	3.5
1	A	136	GLN	3.5
1	A	112	HIS	3.5
1	A	415	ARG	3.5
1	B	7	ARG	3.5
1	B	274	ARG	3.4
1	B	563	ILE	3.4
1	A	76	LEU	3.4
1	B	229	TYR	3.3
1	A	254	ARG	3.3
1	A	416	TYR	3.3
1	B	236	GLN	3.2
1	B	579	GLU	3.2
1	B	323	SER	3.2
1	A	125	ASN	3.2
1	B	403	ASN	3.2
1	A	42	ASP	3.2
1	A	193	ALA	3.2
1	B	57	ILE	3.2
1	B	462	PHE	3.2
1	A	291	ASP	3.1
1	A	585	ALA	3.1
1	A	237	GLY	3.1
1	B	412	PHE	3.1
1	A	84	ARG	3.1
1	B	137	LEU	3.1
1	B	478	PRO	3.1
1	A	170	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	MET	3.1
1	A	306	ILE	3.0
1	A	322	LEU	3.0
1	A	229	TYR	3.0
1	A	569	GLN	3.0
1	B	288	GLN	3.0
1	B	155	TRP	3.0
1	B	574	LEU	3.0
1	A	247	PRO	3.0
1	B	139	PHE	3.0
1	A	45	THR	2.9
1	A	564	LYS	2.9
1	B	161	ARG	2.9
1	A	51	ILE	2.9
1	B	369	THR	2.9
1	A	117	PRO	2.9
1	B	209	SER	2.9
1	B	582	ARG	2.9
1	A	57	ILE	2.9
1	A	15	MET	2.9
1	B	201	MET	2.9
1	B	486	ASN	2.9
1	B	121	GLU	2.8
1	B	135	TRP	2.8
1	A	146	LEU	2.8
1	A	412	PHE	2.8
1	B	47	LEU	2.8
1	B	120	TRP	2.8
1	B	124	ILE	2.8
1	A	371	SER	2.8
1	A	208	LEU	2.8
1	B	85	LEU	2.8
1	B	86	MET	2.8
1	A	151	LEU	2.8
1	B	178	PHE	2.8
1	B	195	PHE	2.8
1	A	230	GLN	2.7
1	A	233	LEU	2.7
1	A	405	ASP	2.7
1	A	138	MET	2.7
1	A	160	LEU	2.7
1	B	165	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	2.7
1	B	102	LEU	2.7
1	A	26	ASN	2.7
1	A	108	PHE	2.7
1	A	38	LEU	2.6
1	A	235	GLU	2.6
1	B	136	GLN	2.6
1	B	336	GLN	2.6
1	B	101	LEU	2.6
1	A	442	ASN	2.6
1	A	326	THR	2.6
1	B	212	MET	2.6
1	B	410	LYS	2.6
1	A	195	PHE	2.6
1	A	363	SER	2.6
1	B	138	MET	2.6
1	B	117	PRO	2.6
1	A	162	SER	2.5
1	A	529	THR	2.5
1	A	390	ASP	2.5
1	B	167	ARG	2.5
1	A	22	PHE	2.5
1	A	41	ALA	2.5
1	A	518	ILE	2.5
1	B	220	LYS	2.5
1	A	202	GLN	2.5
1	A	553	TYR	2.5
1	B	153	ALA	2.5
1	B	287	GLU	2.4
1	A	483	GLN	2.4
1	A	204	ALA	2.4
1	A	140	ILE	2.4
1	A	150	MET	2.4
1	A	409	GLN	2.4
1	A	9	ARG	2.4
1	A	421	SER	2.4
1	A	365	PRO	2.4
1	A	420	ALA	2.4
1	B	437	ALA	2.4
1	B	8	TYR	2.3
1	A	72	ILE	2.3
1	A	77	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	200	THR	2.3
1	B	235	GLU	2.3
1	A	19	GLY	2.3
1	A	74	PHE	2.3
1	A	33	LEU	2.3
1	B	96	ALA	2.3
1	A	10	GLU	2.3
1	A	581	LYS	2.3
1	B	81	MET	2.3
1	A	231	ARG	2.3
1	A	355	ARG	2.3
1	A	245	GLN	2.3
1	B	147	LEU	2.3
1	A	241	ALA	2.2
1	B	449	ALA	2.2
1	A	389	GLU	2.2
1	A	239	PRO	2.2
1	A	249	SER	2.2
1	A	408	ASN	2.2
1	A	172	PRO	2.2
1	B	248	LEU	2.2
1	B	58	VAL	2.2
1	B	190	TRP	2.2
1	A	275	PHE	2.2
1	B	79	ILE	2.2
1	A	366	ALA	2.2
1	B	441	ASP	2.2
1	B	239	PRO	2.1
1	A	29	LEU	2.1
1	A	168	HIS	2.1
1	A	364	MET	2.1
1	A	66	PHE	2.1
1	B	170	ALA	2.1
1	A	216	ARG	2.1
1	A	109	THR	2.1
1	A	497	THR	2.1
1	A	552	HIS	2.1
1	B	534	SER	2.1
1	A	92	ILE	2.1
1	B	123	VAL	2.1
1	A	157	TRP	2.0
1	A	492	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	77	THR	2.0
1	A	47	LEU	2.0
1	A	89	LEU	2.0
1	B	224	LEU	2.0
1	A	36	ARG	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](#)

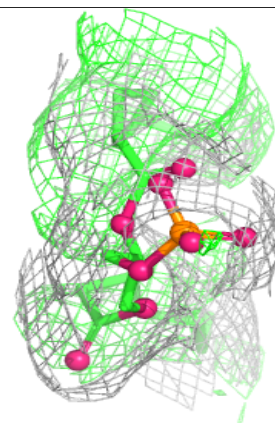
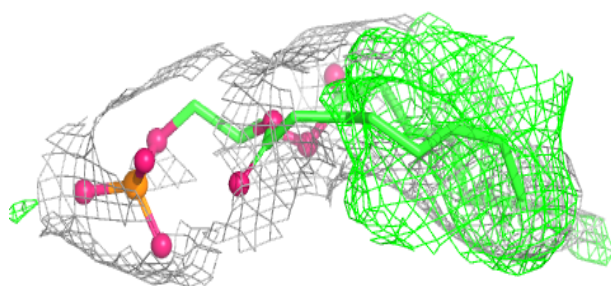
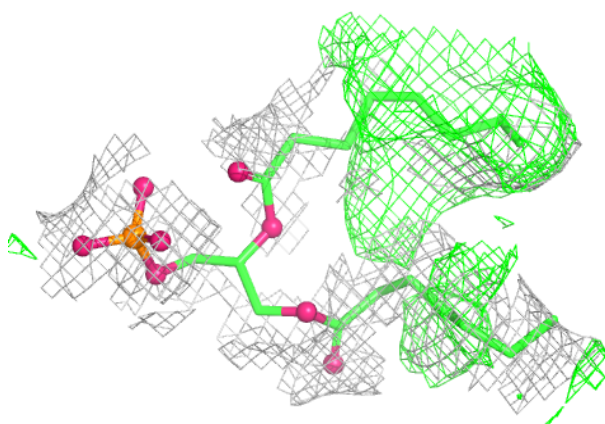
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	QSR	A	604	27/100	0.57	0.28	76,88,95,96	0
5	LMT	A	605	24/35	0.69	0.20	96,105,113,123	0
3	PO4	B	601	5/5	0.74	0.32	81,81,83,86	0
4	QSR	A	603	52/100	0.78	0.23	68,90,107,115	0
2	CA	A	601	1/1	0.81	0.23	86,86,86,86	0
4	QSR	B	602	67/100	0.81	0.24	47,66,82,88	0
3	PO4	A	602	5/5	0.81	0.46	86,93,94,98	0
4	QSR	B	603	70/100	0.83	0.20	48,68,79,94	0
5	LMT	B	604	35/35	0.84	0.16	56,75,89,92	0

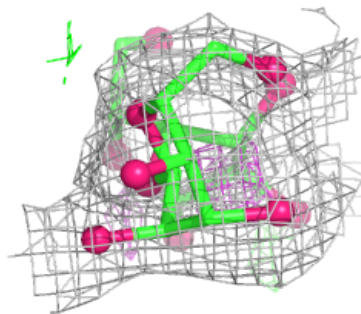
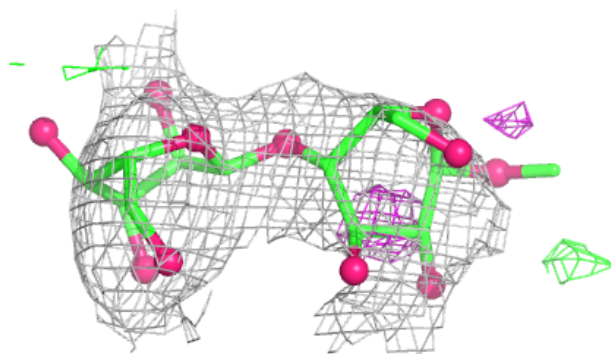
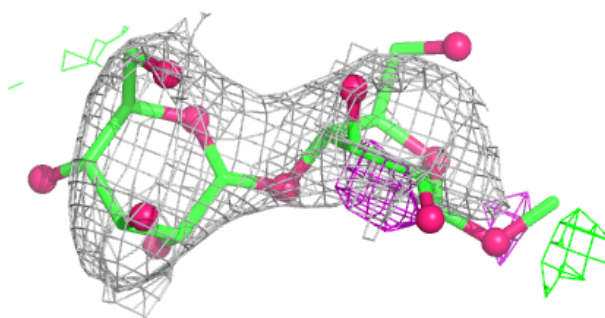
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QSR A 604:

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

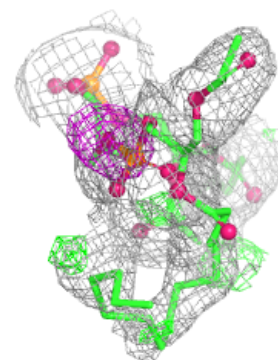
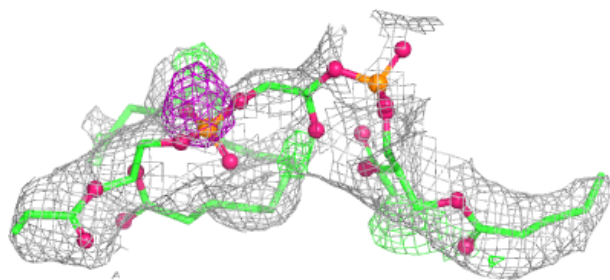
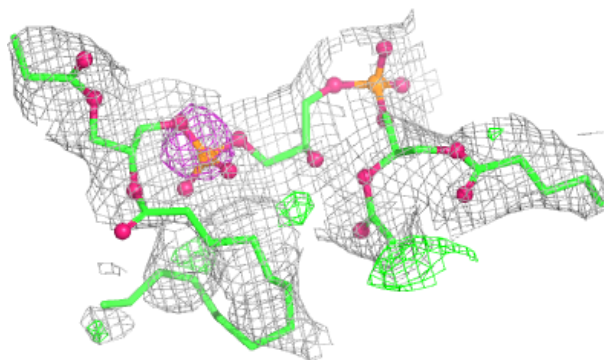
**Electron density around LMT A 605:**

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

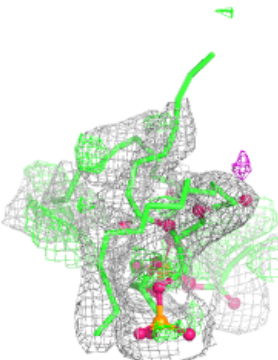
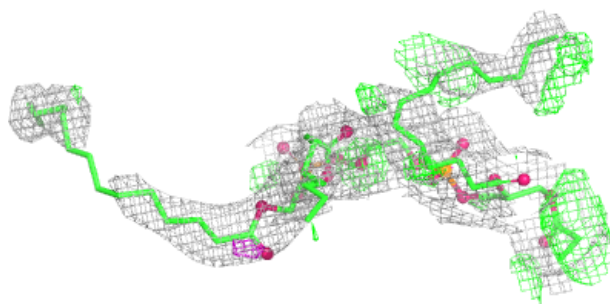
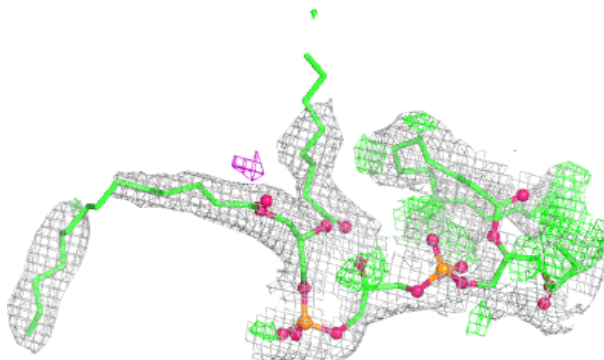


Electron density around QSR A 603:

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

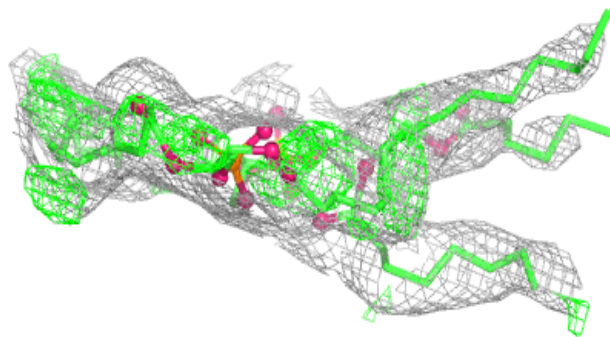
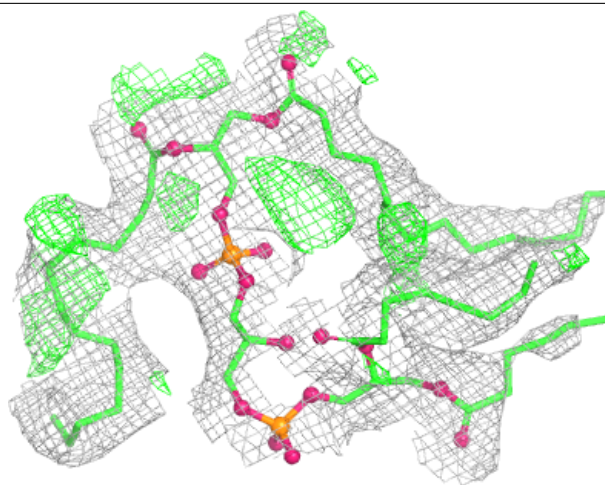
**Electron density around QSR B 602:**

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



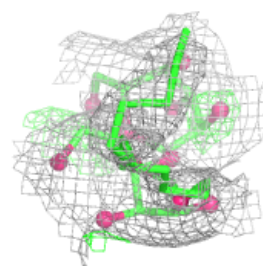
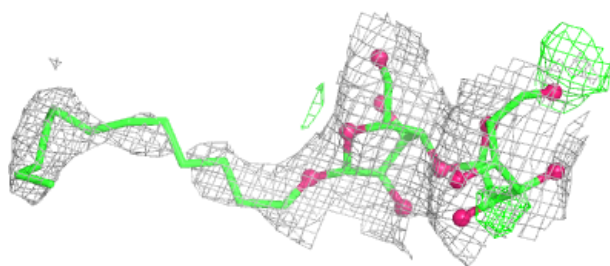
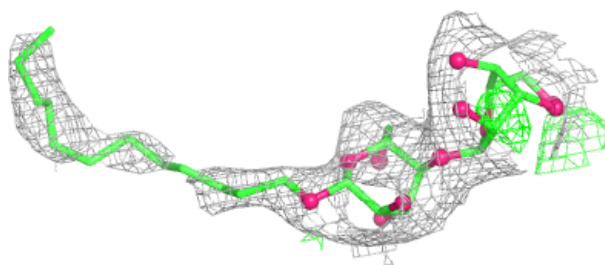
Electron density around QSR B 603:

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



Electron density around LMT B 604:

$2mF_o-DF_c$ (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.