



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 07:54 PM UTC

PDB ID : 4MDT / pdb_00004mdt
Title : Structure of LpxC bound to the reaction product UDP-(3-O-(R-3-hydroxymyristoyl))-glucosamine
Authors : Clayton, G.M.; Klein, D.J.; Rickert, K.W.; Patel, S.B.; Kornienko, M.; Zugay-Murphy, J.; Reid, J.C.; Tummala, S.; Sharma, S.; Singh, S.B.; Miesel, L.; Lumb, K.J.; Soisson, S.M.
Deposited on : 2013-08-23
Resolution : 2.59 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](#) ①) 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

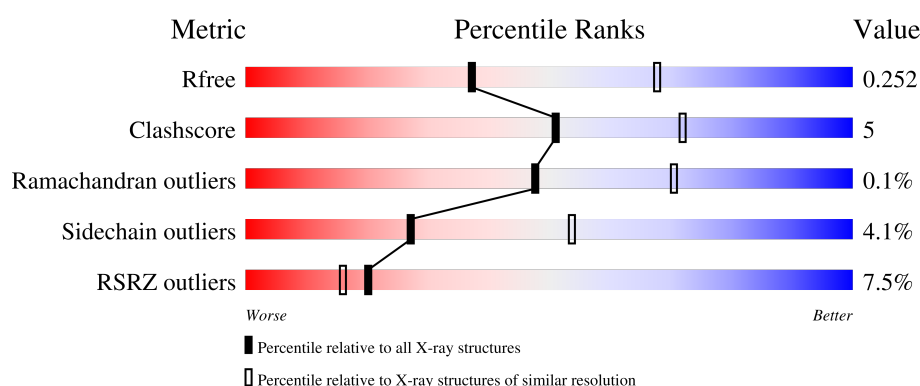
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	305	85% 12% ..
1	B	305	% 79% 18% ..
1	C	305	14% 79% 17% ..
1	D	305	14% 74% 19% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	D	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9746 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 UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2356	1497	408	438	13			
1	B	300	Total	C	N	O	S	0	0	0
			2356	1497	408	438	13			
1	C	299	Total	C	N	O	S	0	0	0
			2350	1494	407	436	13			
1	D	293	Total	C	N	O	S	0	0	0
			2299	1457	399	431	12			

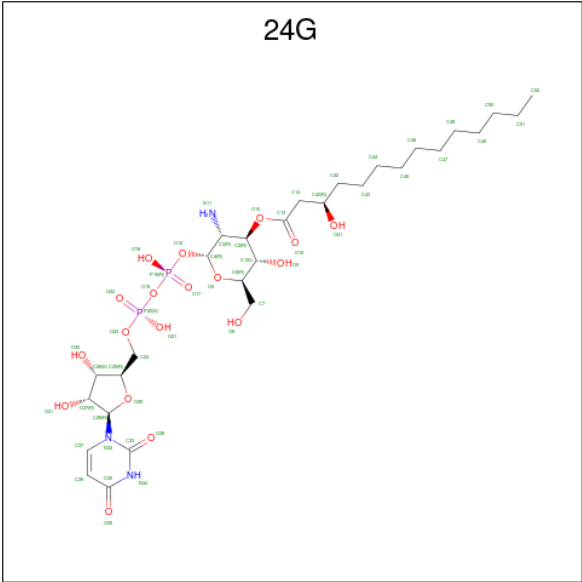
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	SER	CYS	engineered mutation	UNP K0BGQ2
B	125	SER	CYS	engineered mutation	UNP K0BGQ2
C	125	SER	CYS	engineered mutation	UNP K0BGQ2
D	125	SER	CYS	engineered mutation	UNP K0BGQ2

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

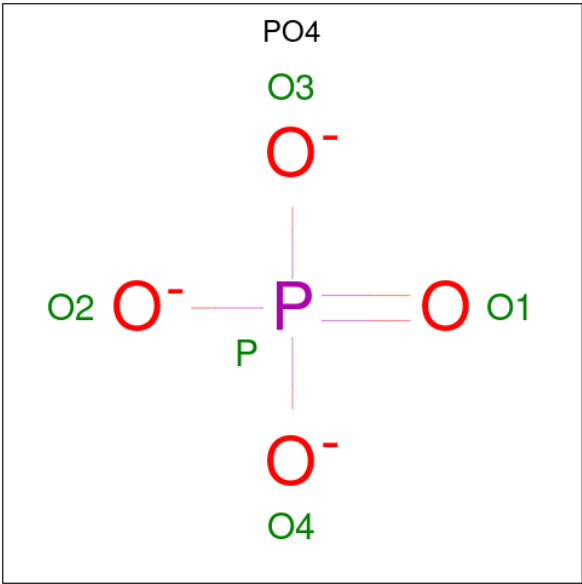
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is uridine-5'-diphosphate-3-O-(R-3-hydroxymyristoyl)-glucosamine (CCD ID: 24G) (formula: C₂₉H₅₁N₃O₁₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			52	29	3	18	2		
3	B	1	Total	C	N	O	P	0	0
			52	29	3	18	2		
3	C	1	Total	C	N	O	P	0	0
			52	29	3	18	2		
3	D	1	Total	C	N	O	P	0	0
			52	29	3	18	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is water.

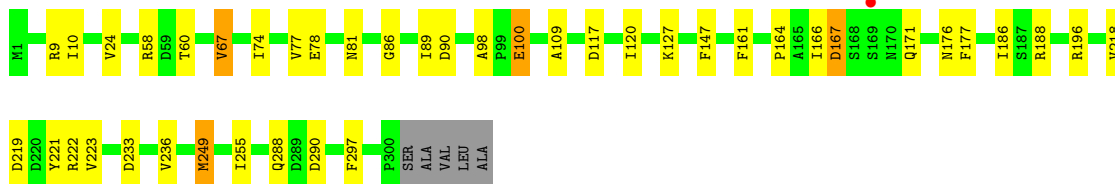
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	55	Total	O	0	0
			55	55		
5	C	17	Total	O	0	0
			17	17		
5	D	20	Total	O	0	0
			20	20		

3 Residue-property plots

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.

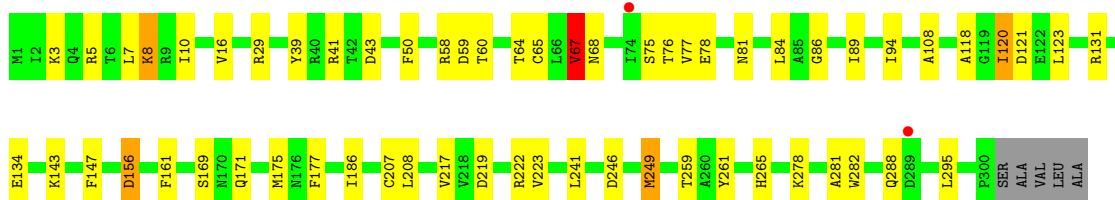
- Molecule 1: UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase

Chain A: 



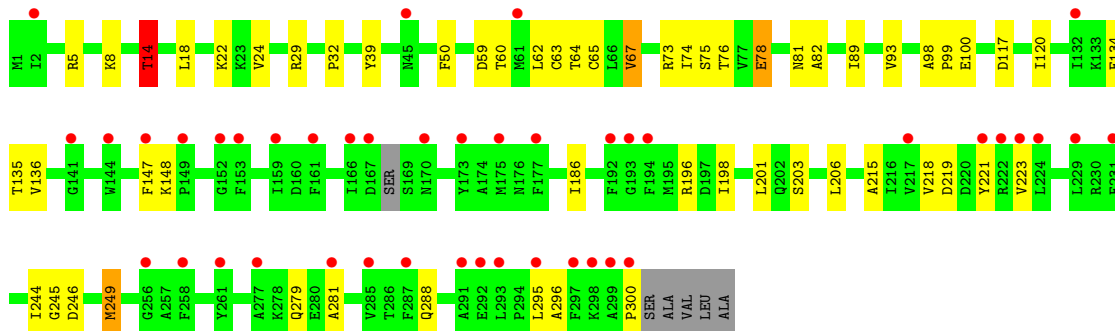
- Molecule 1: UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase

Chain B: 

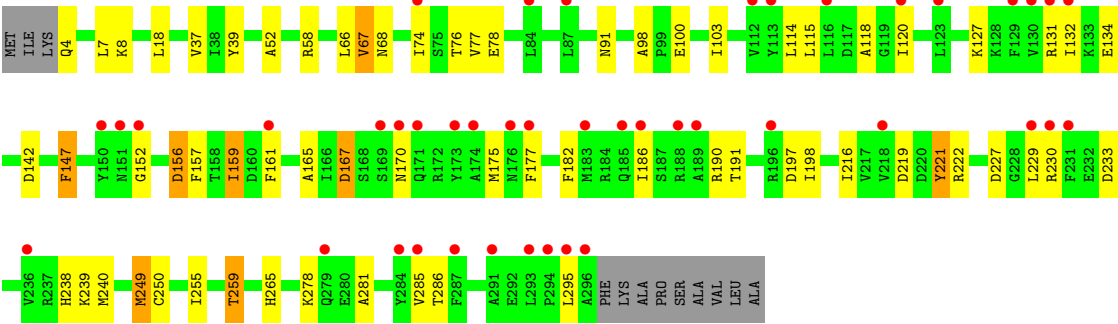
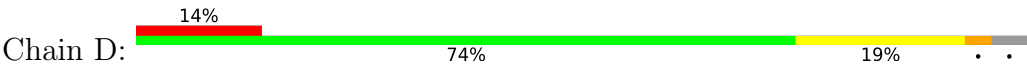


- Molecule 1: UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase

Chain C: 



- Molecule 1: UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosamine deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.97Å 103.52Å 103.97Å 90.00° 103.96° 90.00°	Depositor
Resolution (Å)	50.45 – 2.59 50.45 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.45-2.59) 95.9 (50.45-2.59)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.58Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.7, BUSTER 2.9.7	Depositor
R, R_{free}	0.197 , 0.240 0.205 , 0.252	Depositor DCC
R_{free} test set	2646 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9746	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PO4, 24G

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	0.87	1/2404 (0.0%)	1.37	13/3255 (0.4%)
1	B	0.87	1/2404 (0.0%)	1.37	14/3255 (0.4%)
1	C	0.84	1/2397 (0.0%)	1.37	10/3244 (0.3%)
1	D	0.85	2/2345 (0.1%)	1.41	17/3177 (0.5%)
All	All	0.86	5/9550 (0.1%)	1.38	54/12931 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	249	MET	SD-CE	-7.89	1.59	1.79
1	B	249	MET	SD-CE	-7.47	1.60	1.79
1	D	249	MET	SD-CE	-5.94	1.64	1.79
1	D	233	ASP	CA-C	5.58	1.60	1.52
1	A	249	MET	SD-CE	-5.24	1.66	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ILE	N-CA-C	8.80	119.36	110.82
1	A	219	ASP	CA-CB-CG	8.75	121.35	112.60
1	A	186	ILE	N-CA-C	8.29	118.69	111.56
1	D	167	ASP	CA-CB-CG	7.79	120.39	112.60
1	B	186	ILE	N-CA-C	7.47	118.50	111.48
1	A	74	ILE	N-CA-CB	7.38	121.94	112.34
1	A	78	GLU	N-CA-C	7.35	119.29	111.28
1	D	78	GLU	N-CA-C	7.33	118.96	110.97
1	C	219	ASP	CA-CB-CG	7.12	119.72	112.60
1	B	78	GLU	N-CA-C	6.97	119.48	111.11
1	C	78	GLU	N-CA-C	6.88	118.77	111.28
1	A	117	ASP	CA-CB-CG	6.77	119.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	ILE	N-CA-C	6.52	117.27	110.62
1	D	221	TYR	N-CA-C	6.34	121.41	113.43
1	B	208	LEU	N-CA-C	6.32	118.17	111.28
1	A	100	GLU	N-CA-C	6.19	118.48	109.07
1	A	290	ASP	CA-CB-CG	6.12	118.72	112.60
1	D	216	ILE	N-CA-C	-6.06	100.89	108.89
1	A	176	ASN	N-CA-C	-5.91	99.57	108.96
1	C	117	ASP	CA-CB-CG	5.80	118.40	112.60
1	D	229	LEU	N-CA-C	5.77	118.88	109.59
1	B	68	ASN	CA-CB-CG	5.72	118.32	112.60
1	D	250	CYS	N-CA-C	-5.65	106.55	113.50
1	D	161	PHE	CA-CB-CG	5.64	119.44	113.80
1	C	296	ALA	N-CA-C	5.59	117.06	111.07
1	A	60	THR	CA-C-N	5.58	128.02	120.65
1	A	60	THR	C-N-CA	5.58	128.02	120.65
1	B	156	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	186	ILE	N-CA-C	5.54	120.86	109.34
1	D	98	ALA	N-CA-C	5.50	113.08	108.13
1	B	219	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	156	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	161	PHE	N-CA-C	-5.43	100.05	108.90
1	D	197	ASP	CA-C-N	5.42	127.60	120.60
1	D	197	ASP	C-N-CA	5.42	127.60	120.60
1	D	219	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	68	ASN	CA-CB-CG	5.39	117.99	112.60
1	B	223	VAL	N-CA-C	-5.39	101.78	108.89
1	C	14	THR	CB-CA-C	5.39	118.53	109.48
1	B	77	VAL	CA-C-N	5.37	127.79	120.54
1	B	77	VAL	C-N-CA	5.37	127.79	120.54
1	B	222	ARG	N-CA-C	5.37	117.14	109.14
1	C	295	LEU	CA-C-N	5.30	127.33	120.44
1	C	295	LEU	C-N-CA	5.30	127.33	120.44
1	D	100	GLU	N-CA-C	5.28	117.28	108.99
1	B	67	VAL	CB-CA-C	5.27	118.02	110.33
1	B	60	THR	CA-C-N	5.25	127.58	120.44
1	B	60	THR	C-N-CA	5.25	127.58	120.44
1	C	73	ARG	N-CA-C	5.18	117.93	109.59
1	A	222	ARG	N-CA-C	5.11	116.76	109.14
1	A	167	ASP	CA-C-N	5.09	127.11	120.28
1	A	167	ASP	C-N-CA	5.09	127.11	120.28
1	D	142	ASP	CA-CB-CG	5.08	117.68	112.60
1	C	67	VAL	CB-CA-C	5.03	118.22	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2356	0	2337	20	0
1	B	2356	0	2337	25	0
1	C	2350	0	2331	27	0
1	D	2299	0	2267	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	52	0	49	0	0
3	B	52	0	49	1	0
3	C	52	0	49	3	0
3	D	52	0	49	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	2	0
5	A	61	0	0	0	0
5	B	55	0	0	0	0
5	C	17	0	0	0	0
5	D	20	0	0	0	0
All	All	9746	0	9468	99	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 5.

All (99) 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:B:81:ASN:HD21	1:B:249:MET:HE2	1.29	0.97
1:B:81:ASN:ND2	1:B:249:MET:HE2	2.00	0.75
1:B:39:TYR:HB2	1:B:50:PHE:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:GLU:HB2	1:D:281:ALA:HA	1.73	0.71
1:C:81:ASN:HD21	1:C:249:MET:CE	2.05	0.69
1:D:4:GLN:HB3	1:D:91:ASN:HD21	1.58	0.69
1:A:81:ASN:ND2	1:A:249:MET:HE2	2.07	0.69
1:C:81:ASN:HD21	1:C:249:MET:HE2	1.56	0.69
1:B:64:THR:HG21	1:B:246:ASP:OD1	1.94	0.68
1:A:89:ILE:HD11	1:A:120:ILE:HD12	1.74	0.67
1:B:8:LYS:HG2	1:B:121:ASP:HB2	1.77	0.65
1:A:81:ASN:HD21	1:A:249:MET:HE2	1.63	0.63
1:B:58:ARG:HB2	1:B:67:VAL:HG13	1.82	0.61
1:A:24:VAL:HG11	1:A:100:GLU:O	2.01	0.60
1:C:134:GLU:HB2	1:C:281:ALA:HA	1.84	0.60
1:A:166:ILE:HG22	1:A:171:GLN:HE21	1.68	0.58
1:B:84:LEU:HD11	1:B:94:ILE:HD11	1.85	0.58
1:C:64:THR:OG1	1:C:246:ASP:OD1	2.18	0.58
1:C:135:THR:HG23	1:C:148:LYS:HG2	1.85	0.57
1:A:58:ARG:HB2	1:A:67:VAL:HG13	1.87	0.57
1:D:191:THR:HA	1:D:238:HIS:CD2	2.39	0.57
1:B:39:TYR:OH	1:B:81:ASN:OD1	2.23	0.57
1:A:10:ILE:CD1	1:D:167:ASP:HB2	2.36	0.56
1:C:39:TYR:HB2	1:C:50:PHE:HB2	1.89	0.55
1:D:156:ASP:O	1:D:259:THR:HA	2.07	0.54
1:C:5:ARG:HH22	1:C:300:PRO:HD3	1.71	0.54
1:B:134:GLU:HB2	1:B:281:ALA:HA	1.89	0.54
1:C:29:ARG:HB2	1:C:93:VAL:HB	1.90	0.53
1:C:59:ASP:HB3	1:C:65:CYS:HB3	1.91	0.53
1:D:265:HIS:NE2	4:D:403:PO4:O3	2.35	0.53
1:B:64:THR:HG22	1:B:265:HIS:HB3	1.91	0.53
1:A:10:ILE:HD12	1:D:167:ASP:HB2	1.91	0.53
1:B:175:MET:HE3	1:B:177:PHE:HA	1.90	0.53
1:A:218:VAL:HG12	1:A:223:VAL:HA	1.91	0.52
1:D:58:ARG:HB2	1:D:67:VAL:HG13	1.92	0.52
1:C:82:ALA:HA	1:C:244:ILE:HG22	1.91	0.51
1:C:24:VAL:HG11	1:C:100:GLU:O	2.10	0.51
1:A:164:PRO:HG2	1:A:221:TYR:HA	1.93	0.50
1:C:24:VAL:HG13	1:C:98:ALA:HB3	1.94	0.50
1:D:66:LEU:HB2	1:D:74:ILE:HG23	1.94	0.50
1:B:169:SER:O	1:B:171:GLN:NE2	2.41	0.49
1:C:201:LEU:HB3	1:C:206:LEU:HB2	1.93	0.49
3:D:402:24G:N11	4:D:403:PO4:O4	2.46	0.49
1:C:218:VAL:HG12	1:C:223:VAL:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ARG:HD3	1:D:285:VAL:HG11	1.95	0.48
1:D:175:MET:HE1	1:D:177:PHE:HD1	1.78	0.48
1:B:86:GLY:HA2	1:B:177:PHE:HZ	1.78	0.48
1:B:108:ALA:HB2	1:B:241:LEU:HD21	1.96	0.48
1:D:7:LEU:HD21	1:D:115:LEU:HD23	1.96	0.48
1:D:157:PHE:CE2	1:D:159:ILE:HG23	2.49	0.47
1:D:165:ALA:HB2	1:D:222:ARG:HA	1.97	0.47
1:C:198:ILE:HG21	3:C:402:24G:H27	1.97	0.47
1:B:7:LEU:HD22	1:B:118:ALA:HB3	1.97	0.46
1:D:198:ILE:HG21	3:D:402:24G:H27	1.96	0.46
1:A:161:PHE:H	1:A:171:GLN:HE22	1.62	0.46
1:B:3:LYS:HB3	1:B:123:LEU:O	2.16	0.46
1:D:77:VAL:HG21	1:D:249:MET:HE1	1.97	0.46
1:A:109:ALA:HB2	1:A:188:ARG:HG2	1.97	0.46
1:B:89:ILE:HD11	1:B:120:ILE:HD12	1.98	0.46
1:C:62:LEU:HD11	1:C:206:LEU:HD13	1.98	0.45
1:A:86:GLY:HA2	1:A:177:PHE:HZ	1.81	0.45
1:B:278:LYS:HD3	1:B:281:ALA:HB2	1.98	0.45
1:D:152:GLY:H	1:D:255:ILE:HG23	1.81	0.45
1:B:41:ARG:HH21	1:B:43:ASP:CG	2.25	0.44
1:D:4:GLN:HG3	1:D:127:LYS:HA	1.97	0.44
1:B:59:ASP:HB3	1:B:65:CYS:HB3	1.99	0.44
1:A:24:VAL:HG13	1:A:98:ALA:HB3	1.99	0.44
1:D:18:LEU:HD21	3:D:402:24G:H40	2.00	0.44
1:C:78:GLU:O	1:C:245:GLY:HA3	2.18	0.44
1:C:89:ILE:HD11	1:C:120:ILE:HD12	1.99	0.44
1:D:157:PHE:HE2	1:D:159:ILE:HG23	1.83	0.44
1:C:39:TYR:OH	1:C:81:ASN:OD1	2.31	0.43
1:A:24:VAL:HG22	1:A:98:ALA:HB3	1.99	0.43
1:C:18:LEU:HD11	3:C:402:24G:H36	1.99	0.43
1:D:240:MET:HE3	1:D:240:MET:HB2	1.90	0.43
1:D:177:PHE:CE1	1:D:182:PHE:HB2	2.53	0.43
1:D:132:ILE:HG13	1:D:147:PHE:CD1	2.54	0.42
1:B:10:ILE:HG12	1:B:29:ARG:HG2	2.00	0.42
1:A:233:ASP:HB2	1:A:236:VAL:HG12	2.01	0.42
1:B:156:ASP:O	1:B:259:THR:HA	2.19	0.42
1:B:131:ARG:O	1:B:282:TRP:HA	2.20	0.42
1:D:37:VAL:HB	1:D:52:ALA:HB2	2.02	0.42
1:D:278:LYS:HD3	1:D:281:ALA:HB2	2.00	0.42
1:D:39:TYR:HB3	1:D:74:ILE:HD13	2.02	0.42
1:C:14:THR:HG23	1:D:227:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ILE:HG21	1:D:239:LYS:HG3	2.02	0.41
1:A:77:VAL:HG21	1:A:249:MET:HE3	2.03	0.41
1:B:217:VAL:HG21	3:B:402:24G:H30	2.01	0.41
1:C:74:ILE:HA	1:C:99:PRO:O	2.21	0.41
1:C:215:ALA:HB3	3:C:402:24G:H33	2.03	0.41
1:A:90:ASP:OD1	1:A:127:LYS:HG3	2.19	0.41
1:C:39:TYR:HB3	1:C:74:ILE:HD13	2.03	0.41
1:C:81:ASN:HD21	1:C:249:MET:HE3	1.81	0.41
1:B:261:TYR:CG	1:C:32:PRO:HG3	2.55	0.41
1:D:190:ARG:HE	1:D:230:ARG:HG3	1.85	0.41
1:A:24:VAL:HG22	1:A:98:ALA:CB	2.50	0.41
1:A:255:ILE:HG12	1:A:297:PHE:CE2	2.56	0.41
1:C:63:CYS:SG	1:C:75:SER:HB2	2.61	0.41
1:D:8:LYS:HB2	1:D:118:ALA:O	2.21	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	298/305 (98%)	286 (96%)	12 (4%)	0	100	100
1	B	298/305 (98%)	282 (95%)	16 (5%)	0	100	100
1	C	295/305 (97%)	271 (92%)	24 (8%)	0	100	100
1	D	291/305 (95%)	273 (94%)	17 (6%)	1 (0%)	36	58
All	All	1182/1220 (97%)	1112 (94%)	69 (6%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	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	251/254 (99%)	245 (98%)	6 (2%)	43	70
1	B	251/254 (99%)	239 (95%)	12 (5%)	23	47
1	C	250/254 (98%)	237 (95%)	13 (5%)	21	44
1	D	245/254 (96%)	235 (96%)	10 (4%)	27	54
All	All	997/1016 (98%)	956 (96%)	41 (4%)	27	54

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	67	VAL
1	A	147	PHE
1	A	167	ASP
1	A	196	ARG
1	A	288	GLN
1	B	5	ARG
1	B	8	LYS
1	B	16	VAL
1	B	67	VAL
1	B	75	SER
1	B	76	THR
1	B	120	ILE
1	B	143	LYS
1	B	147	PHE
1	B	207	CYS
1	B	288	GLN
1	B	295	LEU
1	C	8	LYS
1	C	14	THR
1	C	22	LYS
1	C	60	THR
1	C	67	VAL
1	C	76	THR

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Mol	Chain	Res	Type
1	C	136	VAL
1	C	147	PHE
1	C	196	ARG
1	C	203	SER
1	C	221	TYR
1	C	279	GLN
1	C	288	GLN
1	D	67	VAL
1	D	76	THR
1	D	114	LEU
1	D	120	ILE
1	D	147	PHE
1	D	159	ILE
1	D	170	ASN
1	D	221	TYR
1	D	259	THR
1	D	286	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	162	ASN
1	A	171	GLN
1	A	176	ASN
1	A	288	GLN
1	B	12	GLN
1	B	185	GLN
1	B	288	GLN
1	C	81	ASN
1	C	176	ASN
1	C	202	GLN
1	C	253	ASN
1	C	288	GLN
1	D	91	ASN
1	D	170	ASN
1	D	273	GLN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 4 are 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$
3	24G	C	402	-	53,54,54	1.11	5 (9%)	73,76,76	1.35	10 (13%)
4	PO4	B	403	2	4,4,4	1.78	1 (25%)	6,6,6	0.93	0
4	PO4	D	403	2	4,4,4	3.86	1 (25%)	6,6,6	1.70	1 (16%)
3	24G	A	402	-	53,54,54	1.08	5 (9%)	73,76,76	1.52	13 (17%)
3	24G	D	402	-	53,54,54	1.20	5 (9%)	73,76,76	1.18	8 (10%)
3	24G	B	402	-	53,54,54	0.99	5 (9%)	73,76,76	1.26	8 (10%)
4	PO4	A	403	2	4,4,4	2.09	1 (25%)	6,6,6	1.17	0
4	PO4	C	403	2	4,4,4	2.08	1 (25%)	6,6,6	1.58	1 (16%)

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
3	24G	D	402	-	-	13/41/78/78	0/3/3/3
3	24G	B	402	-	-	11/41/78/78	0/3/3/3
3	24G	C	402	-	-	11/41/78/78	0/3/3/3
3	24G	A	402	-	-	16/41/78/78	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	PO4	P-O1	7.40	1.67	1.50
4	A	403	PO4	P-O1	4.06	1.60	1.50
3	D	402	24G	P16-O17	3.90	1.64	1.50
3	D	402	24G	P20-O22	3.82	1.64	1.50
3	A	402	24G	P20-O22	3.79	1.64	1.50
3	C	402	24G	P20-O22	3.77	1.63	1.50
3	A	402	24G	P16-O17	3.72	1.63	1.50
3	C	402	24G	P16-O17	3.72	1.63	1.50
3	D	402	24G	P16-O19	3.57	1.63	1.59
4	C	403	PO4	P-O1	3.50	1.58	1.50
3	B	402	24G	P16-O17	3.48	1.62	1.50
3	B	402	24G	P20-O22	3.48	1.62	1.50
3	D	402	24G	P20-O19	3.47	1.63	1.59
3	C	402	24G	P16-O19	3.10	1.62	1.59
4	B	403	PO4	P-O1	2.87	1.57	1.50
3	C	402	24G	P20-O19	2.78	1.62	1.59
3	A	402	24G	P20-O19	2.51	1.62	1.59
3	D	402	24G	C36-C35	2.50	1.49	1.43
3	B	402	24G	P20-O19	2.23	1.61	1.59
3	A	402	24G	C36-C35	2.14	1.48	1.43
3	C	402	24G	C36-C35	2.10	1.48	1.43
3	A	402	24G	P16-O19	2.10	1.61	1.59
3	B	402	24G	C36-C35	2.01	1.48	1.43
3	B	402	24G	O10-C2	-2.01	1.41	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	24G	O19-P16-O17	-3.97	98.78	110.70
3	A	402	24G	O5-C4-O12	3.70	116.20	111.36
3	A	402	24G	O19-P20-O22	-3.69	99.61	110.70
3	C	402	24G	O39-C35-N34	3.63	124.53	119.27
3	A	402	24G	O19-P16-O17	-3.38	100.54	110.70
3	A	402	24G	O39-C35-C36	-3.36	119.36	125.16
3	B	402	24G	O18-P16-O19	3.33	116.27	107.27
3	B	402	24G	O21-P20-O19	3.31	116.23	107.27
3	C	402	24G	O39-C35-C36	-3.17	119.69	125.16
4	C	403	PO4	O4-P-O1	-3.14	99.86	110.95
3	A	402	24G	O39-C35-N34	3.13	123.81	119.27
3	B	402	24G	O19-P20-O22	-3.04	101.55	110.70
3	D	402	24G	O39-C35-N34	2.93	123.52	119.27
3	C	402	24G	O19-P20-O22	-2.90	101.99	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	24G	O5-C4-O12	2.89	115.15	111.36
3	D	402	24G	O19-P20-O22	-2.85	102.13	110.70
3	D	402	24G	O29-C28-N32	2.73	114.55	108.36
3	A	402	24G	C37-C36-C35	-2.69	116.10	119.53
3	C	402	24G	O18-P16-O19	2.64	114.40	107.27
3	A	402	24G	C2-O10-C13	-2.59	113.37	117.59
3	B	402	24G	O39-C35-N34	2.59	123.02	119.27
3	B	402	24G	O19-P16-O17	-2.58	102.94	110.70
3	D	402	24G	O5-C4-O12	2.58	114.74	111.36
3	A	402	24G	O21-P20-O23	2.56	119.19	107.57
3	B	402	24G	C37-C36-C35	-2.55	116.27	119.53
4	D	403	PO4	O4-P-O3	-2.55	99.97	107.91
3	D	402	24G	O39-C35-C36	-2.49	120.88	125.16
3	A	402	24G	O10-C2-C1	2.49	113.47	107.76
3	A	402	24G	O18-P16-O12	2.46	116.72	106.70
3	D	402	24G	O21-P20-O19	2.45	113.89	107.27
3	C	402	24G	C37-C36-C35	-2.42	116.44	119.53
3	B	402	24G	O39-C35-C36	-2.37	121.07	125.16
3	A	402	24G	O12-C4-C3	2.33	112.61	108.40
3	B	402	24G	C2-C3-N11	-2.23	106.30	110.92
3	D	402	24G	C37-C36-C35	-2.20	116.72	119.53
3	C	402	24G	C36-C37-N32	2.16	125.35	121.84
3	A	402	24G	O18-P16-O19	2.15	113.09	107.27
3	A	402	24G	C36-C37-N32	2.13	125.30	121.84
3	C	402	24G	O21-P20-O19	2.11	112.97	107.27
3	D	402	24G	O18-P16-O19	2.09	112.92	107.27
3	C	402	24G	C26-C27-C28	2.03	105.30	101.46

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	24G	O23-C24-C25-O29
3	A	402	24G	C14-C40-C42-C43
3	A	402	24G	C24-O23-P20-O21
3	A	402	24G	C24-O23-P20-O22
3	A	402	24G	C24-O23-P20-O19
3	B	402	24G	O23-C24-C25-O29
3	C	402	24G	C14-C40-C42-C43
3	C	402	24G	C24-O23-P20-O21
3	C	402	24G	C24-O23-P20-O22
3	C	402	24G	C24-O23-P20-O19

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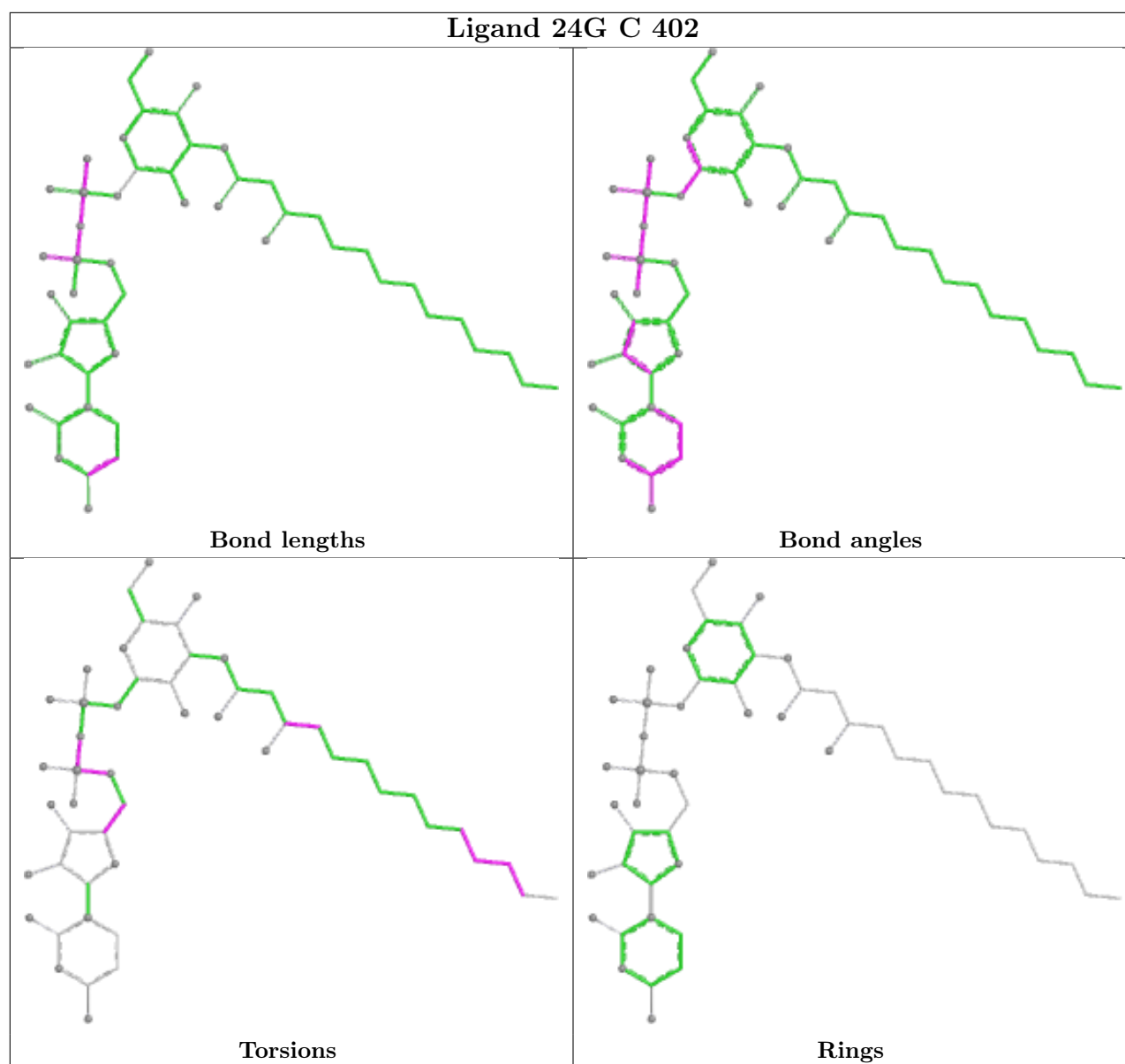
Mol	Chain	Res	Type	Atoms
3	D	402	24G	C14-C40-C42-C43
3	D	402	24G	C24-O23-P20-O21
3	D	402	24G	C24-O23-P20-O22
3	D	402	24G	C24-O23-P20-O19
3	D	402	24G	O23-C24-C25-O29
3	A	402	24G	O41-C40-C42-C43
3	D	402	24G	O41-C40-C42-C43
3	B	402	24G	O23-C24-C25-C26
3	A	402	24G	O23-C24-C25-C26
3	D	402	24G	C45-C46-C47-C48
3	D	402	24G	O23-C24-C25-C26
3	C	402	24G	O41-C40-C42-C43
3	A	402	24G	C48-C49-C50-C51
3	D	402	24G	C48-C49-C50-C51
3	A	402	24G	C47-C48-C49-C50
3	A	402	24G	P16-O19-P20-O22
3	C	402	24G	C48-C49-C50-C51
3	D	402	24G	C47-C48-C49-C50
3	B	402	24G	C14-C40-C42-C43
3	A	402	24G	C49-C50-C51-C52
3	B	402	24G	O5-C6-C7-O8
3	A	402	24G	C43-C44-C45-C46
3	B	402	24G	C48-C49-C50-C51
3	D	402	24G	P16-O19-P20-O21
3	D	402	24G	C49-C50-C51-C52
3	B	402	24G	O41-C40-C42-C43
3	C	402	24G	C49-C50-C51-C52
3	A	402	24G	C44-C45-C46-C47
3	C	402	24G	O23-C24-C25-O29
3	A	402	24G	O10-C13-C14-C40
3	C	402	24G	P16-O19-P20-O22
3	D	402	24G	P16-O19-P20-O22
3	B	402	24G	C13-C14-C40-C42
3	B	402	24G	C43-C44-C45-C46
3	B	402	24G	C47-C48-C49-C50
3	A	402	24G	P16-O19-P20-O21
3	A	402	24G	C45-C46-C47-C48
3	C	402	24G	C47-C48-C49-C50
3	C	402	24G	O23-C24-C25-C26
3	B	402	24G	O29-C28-N32-C37
3	B	402	24G	P16-O19-P20-O21

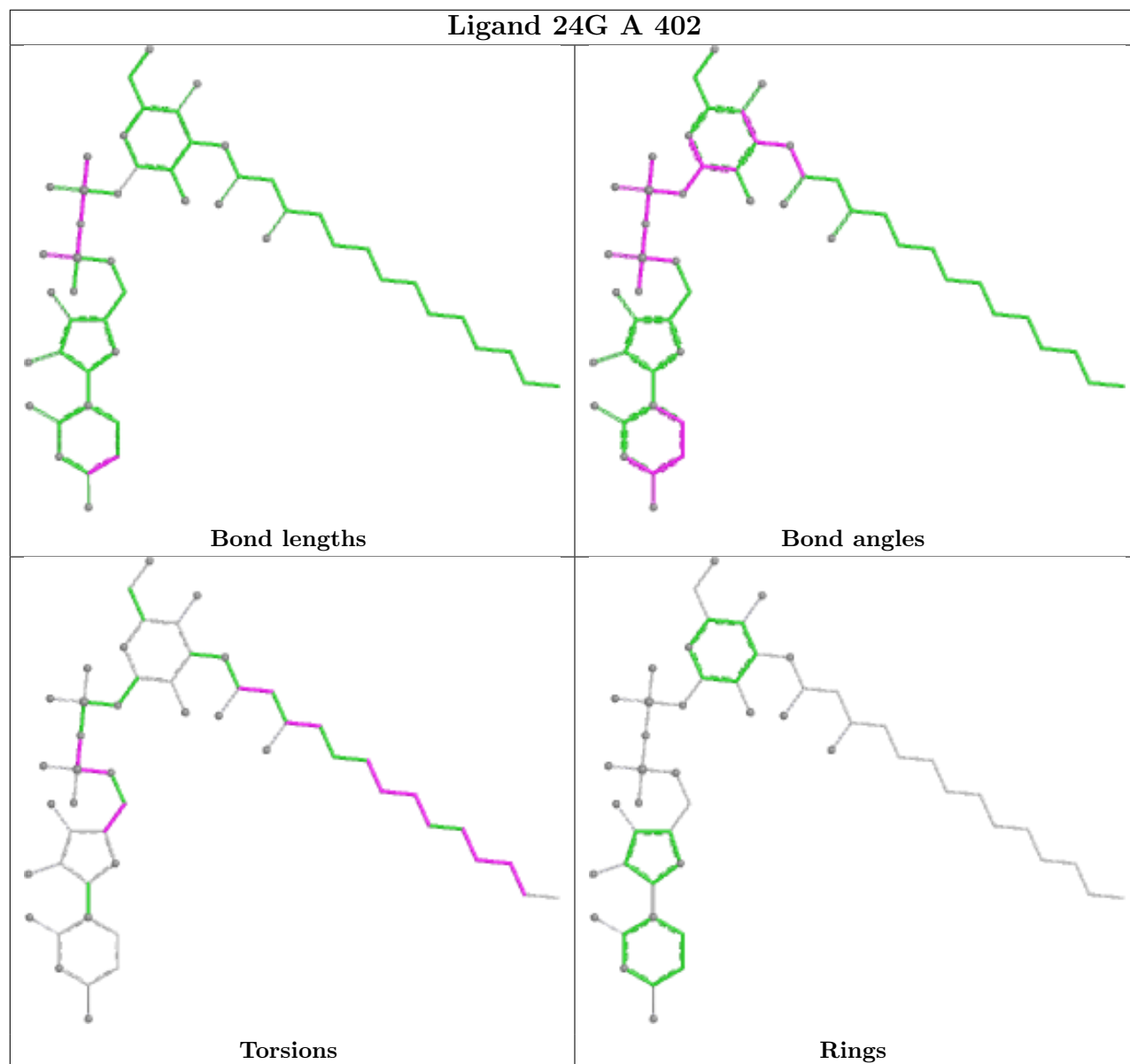
There are no ring outliers.

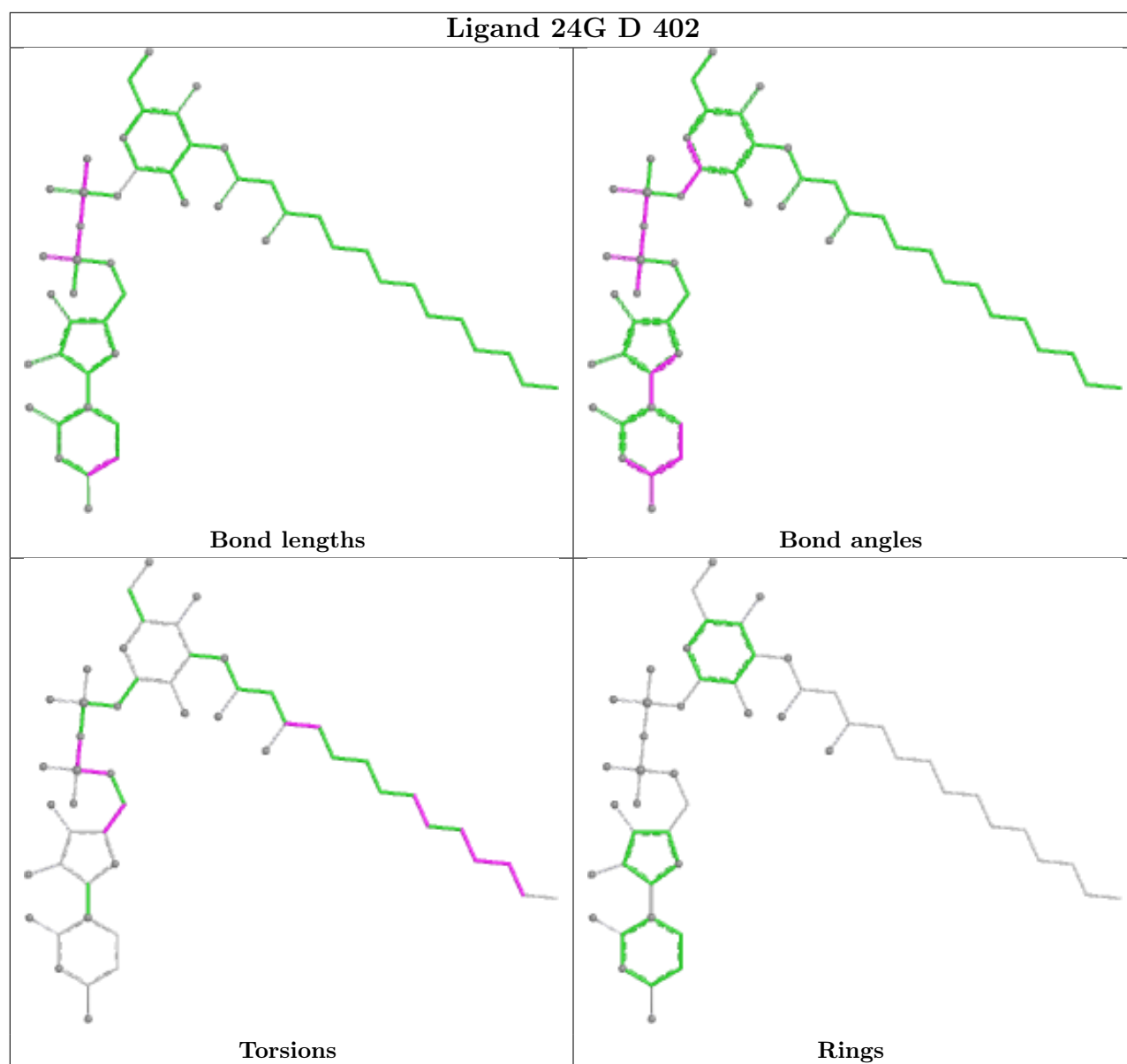
4 monomers are involved in 8 short contacts:

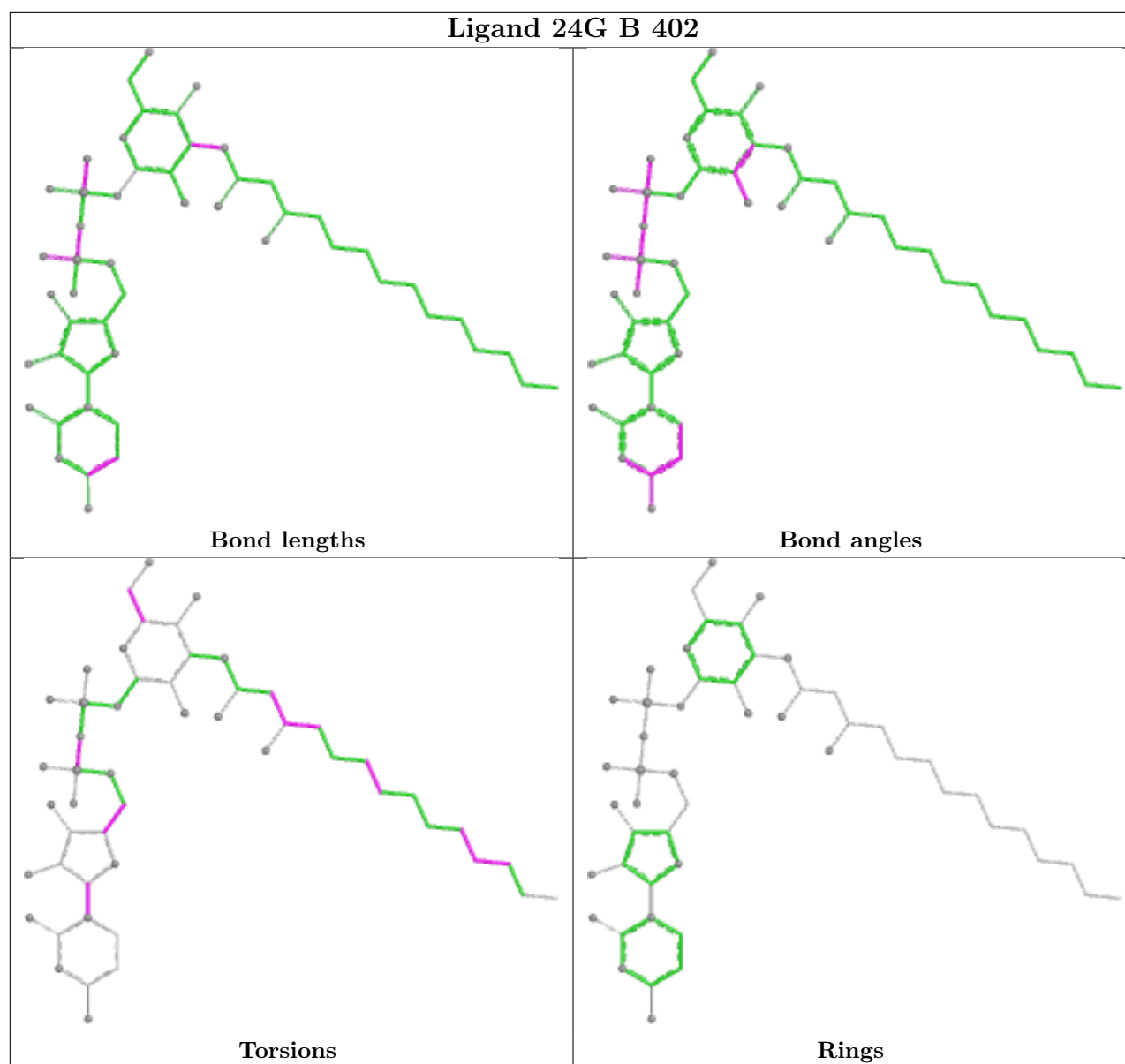
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	24G	3	0
4	D	403	PO4	2	0
3	D	402	24G	3	0
3	B	402	24G	1	0

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	300/305 (98%)	-0.06	1 (0%) 90 88	32, 46, 69, 90	0
1	B	300/305 (98%)	0.18	2 (0%) 84 82	32, 51, 75, 95	0
1	C	299/305 (98%)	1.01	43 (14%) 6 5	42, 72, 111, 148	0
1	D	293/305 (96%)	1.14	43 (14%) 6 4	44, 74, 117, 156	0
All	All	1192/1220 (97%)	0.56	89 (7%) 20 16	32, 59, 105, 156	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	293	LEU	5.1
1	C	300	PRO	4.3
1	D	113	TYR	4.3
1	D	296	ALA	4.0
1	D	295	LEU	3.9
1	C	287	PHE	3.6
1	C	297	PHE	3.5
1	D	236	VAL	3.3
1	D	170	ASN	3.3
1	D	177	PHE	3.2
1	C	298	LYS	3.2
1	C	293	LEU	3.1
1	C	217	VAL	3.1
1	D	152	GLY	3.1
1	D	285	VAL	3.1
1	D	185	GLN	3.1
1	D	171	GLN	3.0
1	D	287	PHE	3.0
1	C	221	TYR	3.0
1	D	186	ILE	3.0
1	C	224	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	291	ALA	3.0
1	D	196	ARG	2.9
1	C	223	VAL	2.9
1	C	295	LEU	2.9
1	C	141	GLY	2.9
1	C	161	PHE	2.8
1	D	183	MET	2.8
1	C	285	VAL	2.8
1	C	258	PHE	2.8
1	D	120	ILE	2.7
1	C	299	ALA	2.7
1	C	2	ILE	2.7
1	C	159	ILE	2.7
1	C	222	ARG	2.7
1	C	149	PRO	2.6
1	C	153	PHE	2.6
1	C	231	PHE	2.6
1	D	116	LEU	2.6
1	C	292	GLU	2.5
1	D	129	PHE	2.5
1	C	229	LEU	2.5
1	D	294	PRO	2.5
1	C	144	TRP	2.5
1	C	281	ALA	2.5
1	B	289	ASP	2.5
1	D	231	PHE	2.5
1	D	112	VAL	2.5
1	D	161	PHE	2.4
1	D	131	ARG	2.4
1	C	277	ALA	2.4
1	C	147	PHE	2.4
1	C	170	ASN	2.4
1	C	152	GLY	2.4
1	D	123	LEU	2.4
1	D	173	TYR	2.4
1	C	45	ASN	2.3
1	D	176	ASN	2.3
1	D	188	ARG	2.3
1	D	229	LEU	2.3
1	C	61	MET	2.3
1	C	173	TYR	2.3
1	D	132	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	175	MET	2.3
1	D	130	VAL	2.3
1	D	150	TYR	2.3
1	D	218	VAL	2.3
1	D	284	TYR	2.3
1	D	87	LEU	2.3
1	B	74	ILE	2.2
1	C	166	ILE	2.2
1	D	291	ALA	2.2
1	C	132	ILE	2.2
1	D	74	ILE	2.2
1	C	193	GLY	2.2
1	D	169	SER	2.2
1	D	84	LEU	2.2
1	C	167	ASP	2.2
1	D	151	ASN	2.1
1	C	256	GLY	2.1
1	D	230	ARG	2.1
1	D	189	ALA	2.1
1	C	177	PHE	2.1
1	C	194	PHE	2.1
1	D	279	GLN	2.1
1	C	261	TYR	2.1
1	D	174	ALA	2.0
1	C	192	PHE	2.0
1	A	169	SER	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](#)

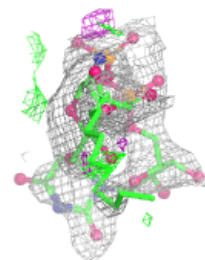
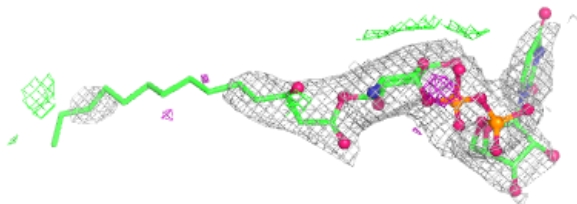
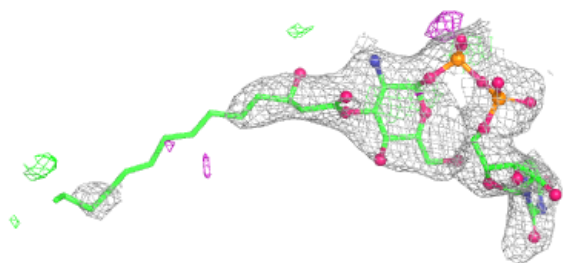
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	24G	C	402	52/52	0.82	0.18	97,105,132,132	0
3	24G	A	402	52/52	0.89	0.14	59,70,88,89	0
3	24G	D	402	52/52	0.90	0.14	55,83,90,92	0
4	PO4	D	403	5/5	0.94	0.08	42,48,52,57	0
4	PO4	C	403	5/5	0.96	0.07	62,67,68,70	0
3	24G	B	402	52/52	0.96	0.09	38,48,60,63	0
4	PO4	A	403	5/5	0.97	0.07	43,47,50,53	0
4	PO4	B	403	5/5	0.98	0.06	43,46,50,50	0
2	ZN	C	401	1/1	0.99	0.03	63,63,63,63	0
2	ZN	D	401	1/1	0.99	0.03	55,55,55,55	0
2	ZN	A	401	1/1	1.00	0.04	39,39,39,39	0
2	ZN	B	401	1/1	1.00	0.03	40,40,40,40	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.

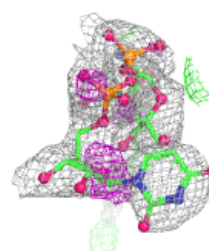
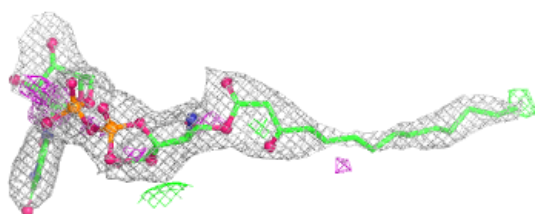
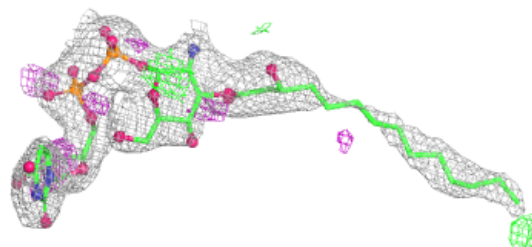
Electron density around 24G C 402:

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

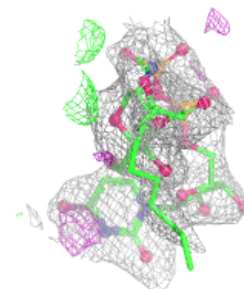
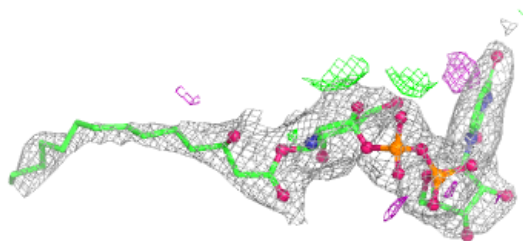


Electron density around 24G A 402:

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

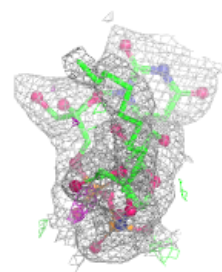
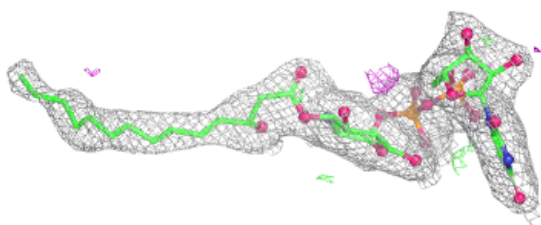
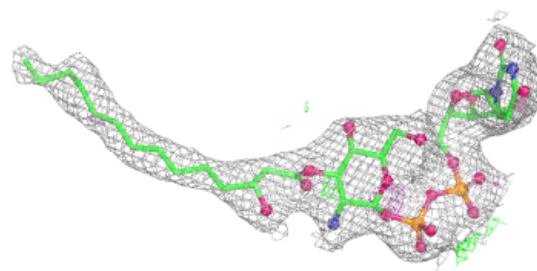
**Electron density around 24G D 402:**

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



Electron density around 24G B 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.