



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2025 – 11:06 am BST

PDB ID : 9G5F / pdb_00009g5f
Title : The structure of Aspergillus fumigatus UDP-GlcNAc pyrophosphorylase in complex with a fragment
Authors : Yan, K.
Deposited on : 2024-07-16
Resolution : 1.62 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

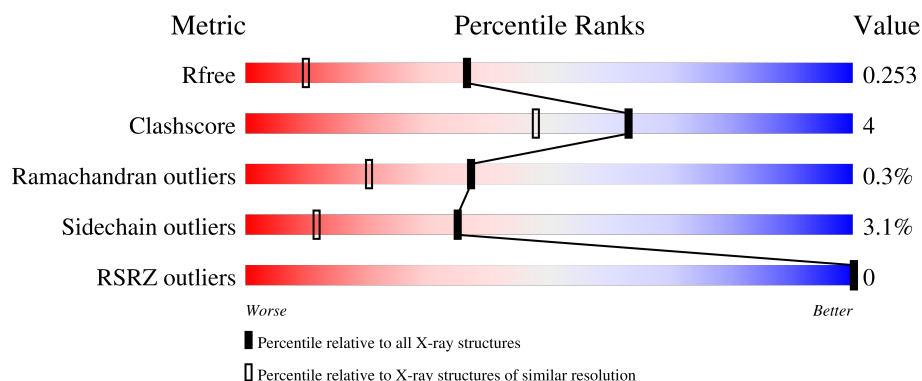
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 1.62 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}	164625	6077 (1.64-1.60)
Clashscore	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)
RSRZ outliers	164620	6075 (1.64-1.60)

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	484	 87% 10% ..
1	B	484	 87% 8% ..
2	C	484	 87% 8% ..
2	D	484	 85% 10% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15785 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-N-acetylglucosamine diphosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	473	Total	C	N	O	S	0	6	0
			3715	2375	633	694	13			
1	A	477	Total	C	N	O	S	0	7	0
			3743	2390	636	704	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP A0A229XUD0
A	26	GLY	-	expression tag	UNP A0A229XUD0

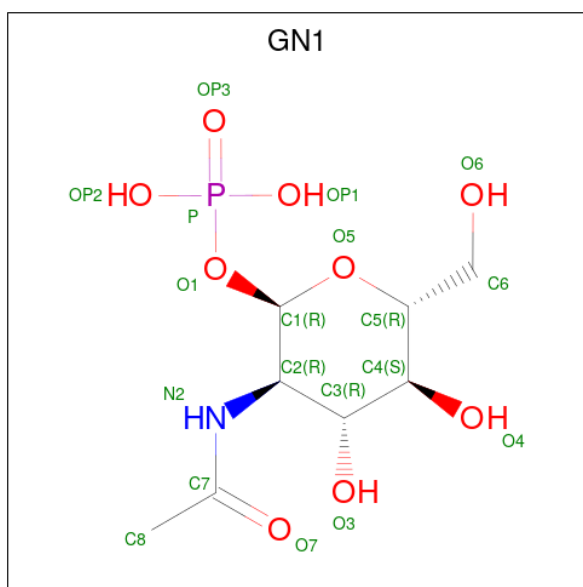
- Molecule 2 is a protein called UDP-N-acetylglucosamine diphosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	465	Total	C	N	O	S	0	4	0
			3634	2320	619	681	14			
2	D	466	Total	C	N	O	S	0	5	0
			3637	2321	618	684	14			

There are 2 discrepancies between the modelled and reference sequences:

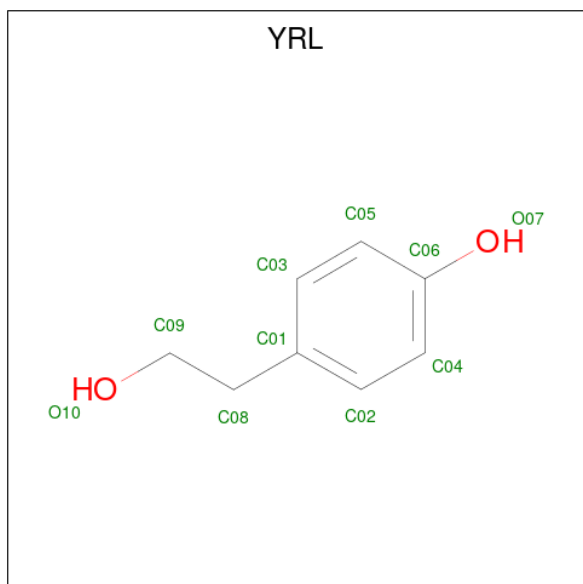
Chain	Residue	Modelled	Actual	Comment	Reference
C	26	GLY	-	expression tag	UNP A0A229XUD0
D	26	GLY	-	expression tag	UNP A0A229XUD0

- Molecule 3 is 2-acetamido-2-deoxy-1-O-phosphono-alpha-D-glucopyranose (CCD ID: GN1) (formula: C₈H₁₆NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
3	A	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

- Molecule 4 is 4-(2-hydroxyethyl)phenol (CCD ID: YRL) (formula: $C_8H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	8	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	8	2		
4	A	1	Total	C	O	0	0
			10	8	2		
4	A	1	Total	C	O	0	0
			10	8	2		
4	A	1	Total	C	O	0	0
			10	8	2		
4	D	1	Total	C	O	0	0
			10	8	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

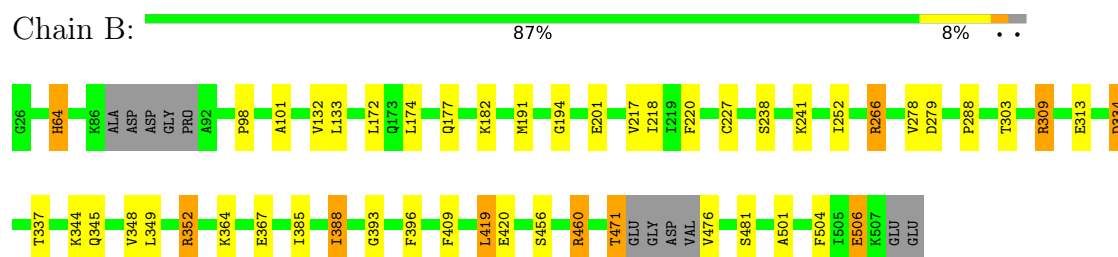
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	300	Total	O	0	0
			300	300		
6	A	294	Total	O	0	0
			294	294		
6	C	175	Total	O	0	0
			175	175		
6	D	187	Total	O	0	0
			187	187		

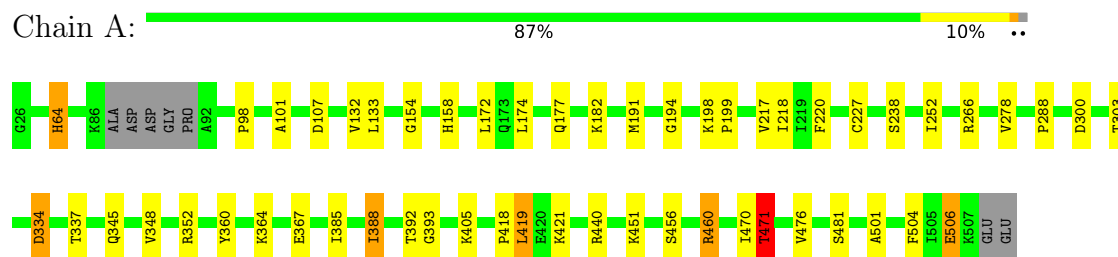
3 Residue-property plots [i](#)

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.

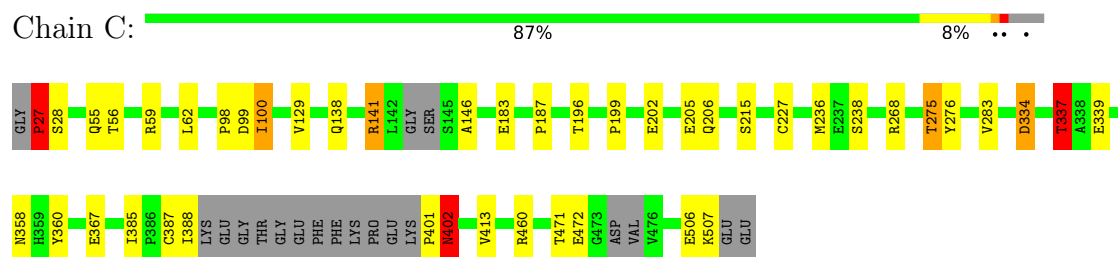
- Molecule 1: UDP-N-acetylglucosamine diphosphorylase



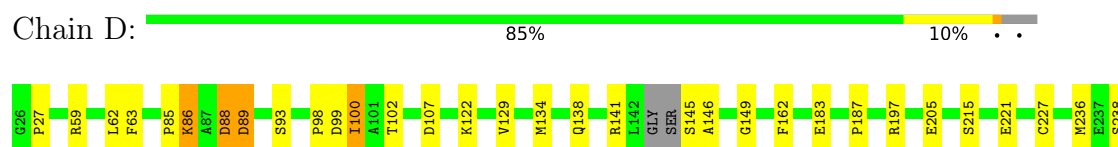
- Molecule 1: UDP-N-acetylglucosamine diphosphorylase

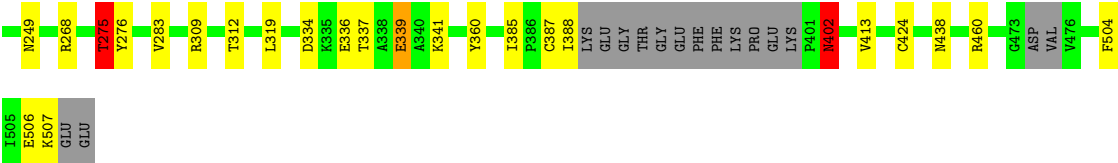


- Molecule 2: UDP-N-acetylglucosamine diphosphorylase



- Molecule 2: UDP-N-acetylglucosamine diphosphorylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.43Å 139.78Å 144.19Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	52.33 – 1.62 52.33 – 1.62	Depositor EDS
% Data completeness (in resolution range)	84.7 (52.33-1.62) 84.6 (52.33-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.209 , 0.247 0.217 , 0.253	Depositor DCC
R_{free} test set	11944 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15785	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: MG, YRL, YCM, GN1

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	0.65	0/3833	1.03	4/5174 (0.1%)
1	B	0.64	0/3801	1.02	4/5128 (0.1%)
2	C	0.61	0/3723	1.03	6/5030 (0.1%)
2	D	0.61	0/3729	0.99	3/5040 (0.1%)
All	All	0.63	0/15086	1.02	17/20372 (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	A	0	2
1	B	0	3
2	C	0	2
2	D	0	2
All	All	0	9

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	27	PRO	CA-N-CD	-8.19	100.53	112.00
2	C	337	THR	CA-CB-OG1	7.05	120.17	109.60
2	C	334	ASP	CB-CA-C	-6.75	95.48	110.19
2	C	275	THR	N-CA-CB	-5.97	100.19	111.00
2	C	183	GLU	CB-CG-CD	5.81	122.48	112.60
2	D	275	THR	N-CA-CB	-5.76	100.58	111.00
1	B	64	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	B	194	GLY	O-C-N	-5.62	116.15	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	158	HIS	CA-CB-CG	-5.45	108.35	113.80
2	C	358	ASN	CB-CA-C	5.42	118.53	110.62
1	A	64	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	A	194	GLY	O-C-N	-5.27	116.50	121.77
1	B	279	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	107	ASP	CB-CA-C	-5.06	101.65	110.09
2	D	183	GLU	CB-CG-CD	5.03	121.14	112.60
2	D	249	ASN	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ARG	Sidechain
1	A	460	ARG	Sidechain
1	B	266	ARG	Sidechain
1	B	352	ARG	Sidechain
1	B	460	ARG	Sidechain
2	C	460[A]	ARG	Sidechain
2	C	460[B]	ARG	Sidechain
2	D	460[A]	ARG	Sidechain
2	D	460[B]	ARG	Sidechain

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	3743	0	3728	34	0
1	B	3715	0	3717	32	0
2	C	3634	0	3609	21	0
2	D	3637	0	3597	30	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
4	A	30	0	27	0	0
4	B	20	0	19	1	0
4	D	10	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	294	0	0	4	0
6	B	300	0	0	2	0
6	C	175	0	0	2	0
6	D	187	0	0	5	0
All	All	15785	0	14706	116	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 4.

All (116) 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:266:ARG:NH1	1:A:367:GLU:OE1	1.96	0.96
1:A:266:ARG:HH12	1:A:367:GLU:CD	1.82	0.87
2:C:334:ASP:HB2	2:C:337:THR:HG23	1.59	0.85
2:D:107:ASP:OD2	6:D:701:HOH:O	1.96	0.82
1:A:504:PHE:CZ	1:A:506[A]:GLU:HG3	2.16	0.81
2:D:275:THR:HG21	6:D:774:HOH:O	1.81	0.79
1:B:101:ALA:HB2	1:B:419:LEU:HD13	1.65	0.79
2:D:98:PRO:HB2	2:D:100:ILE:HD12	1.65	0.77
2:C:98:PRO:HB2	2:C:100:ILE:HD12	1.67	0.77
1:A:101:ALA:HB2	1:A:419:LEU:HD13	1.66	0.76
1:B:504:PHE:CZ	1:B:506[A]:GLU:HG3	2.22	0.74
1:A:300:ASP:OD1	6:A:701:HOH:O	2.07	0.72
1:A:481:SER:HB2	1:A:506[A]:GLU:HG2	1.70	0.71
1:B:172:LEU:HD11	1:B:288:PRO:HG3	1.74	0.69
1:B:481:SER:HB2	1:B:506[A]:GLU:HG2	1.74	0.69
1:A:172:LEU:HD11	1:A:288:PRO:HG3	1.74	0.68
1:A:227:CYS:HB3	1:A:385:ILE:HD13	1.78	0.65
4:B:602:YRL:H091	2:D:312:THR:HG21	1.79	0.65
2:C:202:GLU:O	2:C:206:GLN:HG2	1.96	0.65
1:B:227:CYS:HB3	1:B:385:ILE:HD13	1.78	0.64
2:C:205:GLU:HG3	6:C:603:HOH:O	1.98	0.62
1:B:64:HIS:HD2	6:B:957:HOH:O	1.86	0.57
2:C:385:ILE:H	2:C:402:ASN:HD22	1.51	0.57
1:B:64:HIS:HE1	6:D:734:HOH:O	1.88	0.56
1:A:64:HIS:HD2	6:A:963:HOH:O	1.88	0.56
1:B:101:ALA:HB2	1:B:419:LEU:CD1	2.36	0.55
2:D:334[B]:ASP:OD2	2:D:337:THR:OG1	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:GLN:HA	2:C:146:ALA:O	2.07	0.54
2:D:227:CYS:HB3	2:D:385:ILE:HD13	1.89	0.53
2:D:339:GLU:OE1	4:D:601:YRL:O07	2.25	0.53
2:C:236:MET:O	2:C:387:CYS:HB2	2.09	0.53
1:B:309:ARG:HH11	1:B:309:ARG:CG	2.22	0.53
1:A:470:ILE:O	1:A:471:THR:HG22	2.08	0.53
1:B:132:VAL:HG11	1:B:252:ILE:HD11	1.91	0.53
1:B:309:ARG:HH12	1:B:313:GLU:HG3	1.73	0.53
2:C:227:CYS:HB3	2:C:385:ILE:HD13	1.91	0.53
2:D:85:PRO:O	2:D:86:LYS:C	2.52	0.52
1:A:132:VAL:HG11	1:A:252:ILE:HD11	1.90	0.52
1:B:504:PHE:CZ	1:B:506[A]:GLU:CG	2.93	0.52
2:C:55:GLN:HE21	2:C:55:GLN:HA	1.75	0.50
2:C:401:PRO:HB2	6:C:745:HOH:O	2.11	0.50
2:D:27:PRO:HG3	2:D:63:PHE:CG	2.47	0.50
1:B:98:PRO:HG2	1:B:419:LEU:HD11	1.94	0.50
2:D:385:ILE:H	2:D:402:ASN:HD22	1.60	0.50
1:B:217:VAL:C	1:B:218:ILE:HD12	2.37	0.50
2:C:238:SER:HA	2:C:388:ILE:HD11	1.94	0.49
1:B:334:ASP:OD2	1:B:337:THR:HG23	2.13	0.49
1:A:504:PHE:CZ	1:A:506[A]:GLU:CG	2.93	0.49
2:D:236:MET:O	2:D:387:CYS:HB2	2.12	0.49
2:D:506:GLU:HG3	2:D:507:LYS:N	2.27	0.49
1:A:440:ARG:NH1	6:A:707:HOH:O	2.45	0.49
1:A:345:GLN:O	1:A:348:VAL:HG12	2.12	0.49
2:D:138:GLN:HE21	2:D:145:SER:N	2.11	0.48
1:A:154:GLY:O	1:A:451:LYS:HE2	2.13	0.48
1:A:98:PRO:HG2	1:A:419:LEU:HD11	1.94	0.48
2:D:238:SER:HA	2:D:388:ILE:HD11	1.94	0.48
1:A:334:ASP:OD2	1:A:337:THR:HG23	2.14	0.47
2:D:205:GLU:HG3	6:D:738:HOH:O	2.14	0.47
1:B:191:MET:HB2	1:B:220:PHE:CZ	2.49	0.47
1:B:309:ARG:CG	1:B:309:ARG:NH1	2.78	0.46
1:A:177:GLN:HG2	1:A:182:LYS:O	2.16	0.46
1:A:217:VAL:C	1:A:218:ILE:HD12	2.40	0.46
1:B:98:PRO:CG	1:B:419:LEU:HD11	2.47	0.45
1:B:309:ARG:NH1	1:B:313:GLU:HG3	2.31	0.45
2:C:506:GLU:HG3	2:C:507:LYS:N	2.32	0.45
2:D:138:GLN:HA	2:D:146:ALA:O	2.17	0.45
1:A:418:PRO:HG2	1:A:421:LYS:HG2	1.99	0.45
1:B:456:SER:O	1:B:460:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:THR:CB	1:A:501:ALA:HB3	2.47	0.45
1:B:201:GLU:OE1	2:D:309:ARG:HD3	2.18	0.44
2:D:88:ASP:O	2:D:89:ASP:CB	2.65	0.44
1:B:471:THR:OG1	1:B:501:ALA:HB3	2.17	0.44
1:A:345:GLN:CB	1:A:348:VAL:HG12	2.47	0.44
2:D:215:SER:O	2:D:268:ARG:NH2	2.49	0.44
1:B:345:GLN:O	1:B:348:VAL:HG12	2.16	0.44
1:B:177:GLN:HG2	1:B:182:LYS:O	2.18	0.44
2:D:360:TYR:CD1	2:D:360:TYR:C	2.95	0.44
1:A:191:MET:HB2	1:A:220:PHE:CZ	2.52	0.44
2:C:129:VAL:O	2:C:187:PRO:HD2	2.18	0.44
2:C:27:PRO:O	2:C:59:ARG:NH1	2.51	0.44
1:B:388:ILE:HG13	1:B:393:GLY:C	2.43	0.43
2:C:471:THR:C	2:C:472:GLU:HG3	2.42	0.43
2:D:141:ARG:NH2	2:D:438:ASN:OD1	2.51	0.43
2:D:385:ILE:O	2:D:402:ASN:ND2	2.52	0.43
1:A:392:THR:HG23	6:A:945:HOH:O	2.18	0.43
1:A:101:ALA:HB2	1:A:419:LEU:CD1	2.44	0.43
2:D:276:TYR:CE2	2:D:283:VAL:HG11	2.53	0.43
1:B:238:SER:HA	1:B:388:ILE:HD13	2.01	0.42
2:D:129:VAL:O	2:D:187:PRO:HD2	2.19	0.42
1:B:218:ILE:HD12	1:B:218:ILE:N	2.34	0.42
1:A:504:PHE:HZ	1:A:506[A]:GLU:HG3	1.77	0.42
2:C:360:TYR:CD1	2:C:360:TYR:C	2.96	0.42
2:C:276:TYR:CE2	2:C:283:VAL:HG11	2.55	0.42
1:B:349:LEU:O	1:B:352:ARG:NH1	2.41	0.42
2:D:59:ARG:NH1	6:D:703:HOH:O	2.36	0.42
2:D:334[B]:ASP:OD1	2:D:336:GLU:HB3	2.20	0.42
1:B:266:ARG:HD3	1:B:367:GLU:OE1	2.20	0.42
1:A:481:SER:CB	1:A:506[A]:GLU:HG2	2.44	0.42
2:C:215:SER:O	2:C:268:ARG:NH2	2.50	0.42
2:D:197:ARG:HD2	2:D:221:GLU:HG3	2.02	0.42
1:B:345:GLN:CB	1:B:348:VAL:HG12	2.50	0.42
1:A:98:PRO:CG	1:A:419:LEU:HD11	2.50	0.41
1:A:198:LYS:N	1:A:199:PRO:HD2	2.36	0.41
1:A:456:SER:O	1:A:460:ARG:HD3	2.20	0.41
2:C:196:THR:C	2:C:199:PRO:HD2	2.46	0.41
2:D:504:PHE:CZ	2:D:506:GLU:HB2	2.54	0.41
1:B:133:LEU:HD11	1:B:278:VAL:HB	2.02	0.41
1:A:388:ILE:HG13	1:A:393:GLY:C	2.46	0.41
2:C:141:ARG:HH21	2:C:141:ARG:CG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:385:ILE:N	2:C:402:ASN:HD22	2.16	0.41
2:D:102:THR:HA	2:D:424:CYS:O	2.21	0.41
2:D:149:GLY:HA3	2:D:162:PHE:CE2	2.56	0.41
1:A:133:LEU:HD11	1:A:278:VAL:HB	2.03	0.41
1:B:241:LYS:HE2	6:B:779:HOH:O	2.21	0.40
1:A:238:SER:HA	1:A:388:ILE:HD13	2.04	0.40
1:A:360:TYR:CD1	1:A:360:TYR:C	2.99	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	479/484 (99%)	465 (97%)	13 (3%)	1 (0%)	44	25
1	B	472/484 (98%)	463 (98%)	9 (2%)	0	100	100
2	C	461/484 (95%)	451 (98%)	9 (2%)	1 (0%)	44	25
2	D	463/484 (96%)	452 (98%)	7 (2%)	4 (1%)	14	3
All	All	1875/1936 (97%)	1831 (98%)	38 (2%)	6 (0%)	37	20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	89	ASP
2	C	402	ASN
2	D	86	LYS
2	D	402	ASN
2	D	88	ASP
1	A	471	THR

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	399/407 (98%)	388 (97%)	11 (3%)	38	14
1	B	397/407 (98%)	383 (96%)	14 (4%)	31	9
2	C	388/408 (95%)	375 (97%)	13 (3%)	32	10
2	D	387/408 (95%)	374 (97%)	13 (3%)	32	10
All	All	1571/1630 (96%)	1520 (97%)	51 (3%)	35	11

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	174	LEU
1	B	303	THR
1	B	309	ARG
1	B	334	ASP
1	B	344	LYS
1	B	364	LYS
1	B	388	ILE
1	B	396	PHE
1	B	419	LEU
1	B	420	GLU
1	B	471	THR
1	B	476	VAL
1	B	506[A]	GLU
1	B	506[B]	GLU
1	A	174	LEU
1	A	303	THR
1	A	334	ASP
1	A	364	LYS
1	A	388	ILE
1	A	405	LYS
1	A	419	LEU
1	A	471	THR
1	A	476	VAL
1	A	506[A]	GLU

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Mol	Chain	Res	Type
1	A	506[B]	GLU
2	C	27	PRO
2	C	28	SER
2	C	56	THR
2	C	62	LEU
2	C	99	ASP
2	C	100	ILE
2	C	141	ARG
2	C	275	THR
2	C	337	THR
2	C	339	GLU
2	C	367	GLU
2	C	402	ASN
2	C	413	VAL
2	D	62	LEU
2	D	93	SER
2	D	99[A]	ASP
2	D	99[B]	ASP
2	D	100	ILE
2	D	122	LYS
2	D	134	MET
2	D	275	THR
2	D	319	LEU
2	D	339	GLU
2	D	341	LYS
2	D	402	ASN
2	D	413	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	B	64	HIS
1	B	115	GLN
1	B	230	ASN
1	B	408	GLN
1	A	34	GLN
1	A	64	HIS
1	A	115	GLN
1	A	457	GLN
2	C	46	HIS
2	C	55	GLN

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Mol	Chain	Res	Type
2	C	207	HIS
2	C	222	GLN
2	C	320	GLN
2	C	402	ASN
2	D	55	GLN
2	D	207	HIS
2	D	320	GLN
2	D	359	HIS
2	D	402	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	YCM	A	277	1	7,9,10	0.49	0	4,10,12	0.57	0
1	YCM	B	277	1	7,9,10	0.53	0	4,10,12	0.47	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
1	YCM	A	277	1	-	2/6/8/10	-
1	YCM	B	277	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	277	YCM	SG-CD-CE-NZ2
1	A	277	YCM	SG-CD-CE-NZ2
1	A	277	YCM	SG-CD-CE-OZ1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 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	$\# Z > 2$
4	YRL	B	603	-	10,10,10	1.31	1 (10%)	12,12,12	0.66	0
4	YRL	D	601	-	10,10,10	1.61	1 (10%)	12,12,12	0.62	0
3	GN1	A	601	-	18,19,19	0.62	0	27,28,28	0.99	1 (3%)
4	YRL	A	603	-	10,10,10	1.94	1 (10%)	12,12,12	1.02	0
4	YRL	B	602	-	10,10,10	1.93	1 (10%)	12,12,12	0.56	0
3	GN1	B	601	-	18,19,19	0.56	0	27,28,28	0.99	1 (3%)
4	YRL	A	604	-	10,10,10	0.96	1 (10%)	12,12,12	0.75	0
4	YRL	A	602	-	10,10,10	1.49	1 (10%)	12,12,12	1.18	1 (8%)

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
4	YRL	B	603	-	-	0/3/3/3	0/1/1/1
4	YRL	D	601	-	-	0/3/3/3	0/1/1/1
3	GN1	A	601	-	-	2/10/31/31	0/1/1/1
4	YRL	A	603	-	-	1/3/3/3	0/1/1/1
4	YRL	B	602	-	-	1/3/3/3	0/1/1/1
3	GN1	B	601	-	-	2/10/31/31	0/1/1/1
4	YRL	A	604	-	-	0/3/3/3	0/1/1/1
4	YRL	A	602	-	-	0/3/3/3	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	YRL	C08-C01	-6.01	1.34	1.51
4	B	602	YRL	C08-C01	-5.65	1.35	1.51
4	D	601	YRL	C08-C01	-4.76	1.37	1.51
4	A	602	YRL	C08-C01	-4.42	1.38	1.51
4	B	603	YRL	C08-C01	-3.10	1.42	1.51
4	A	604	YRL	C08-C01	-2.45	1.44	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	GN1	C4-C3-C2	-2.90	106.09	110.34
3	B	601	GN1	C4-C3-C2	-2.78	106.27	110.34
4	A	602	YRL	C08-C01-C03	2.44	127.39	121.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

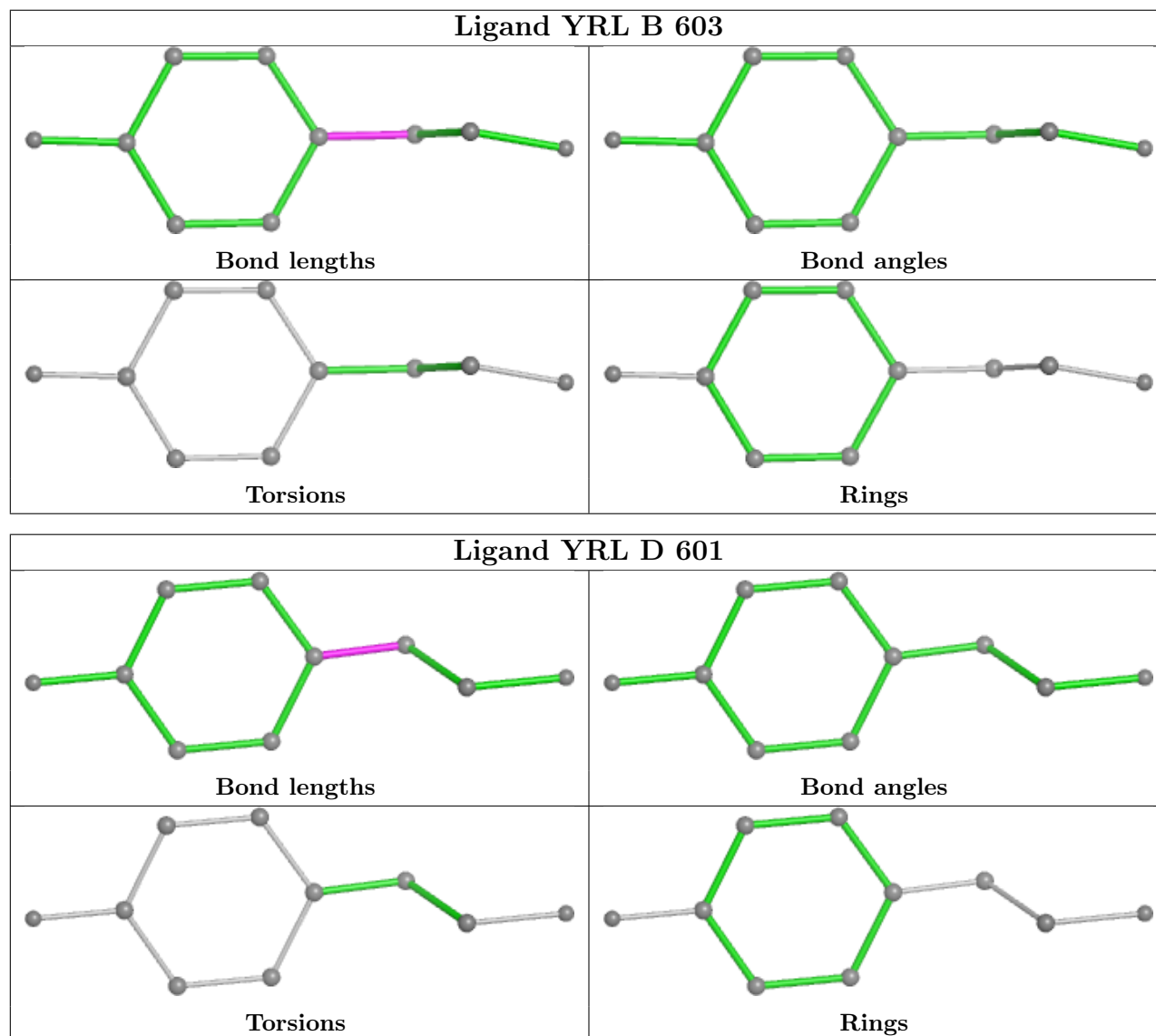
Mol	Chain	Res	Type	Atoms
4	B	602	YRL	C01-C08-C09-O10
4	A	603	YRL	C01-C08-C09-O10
3	B	601	GN1	C1-O1-P-OP2
3	A	601	GN1	C1-O1-P-OP2
3	B	601	GN1	C1-O1-P-OP3
3	A	601	GN1	C1-O1-P-OP3

There are no ring outliers.

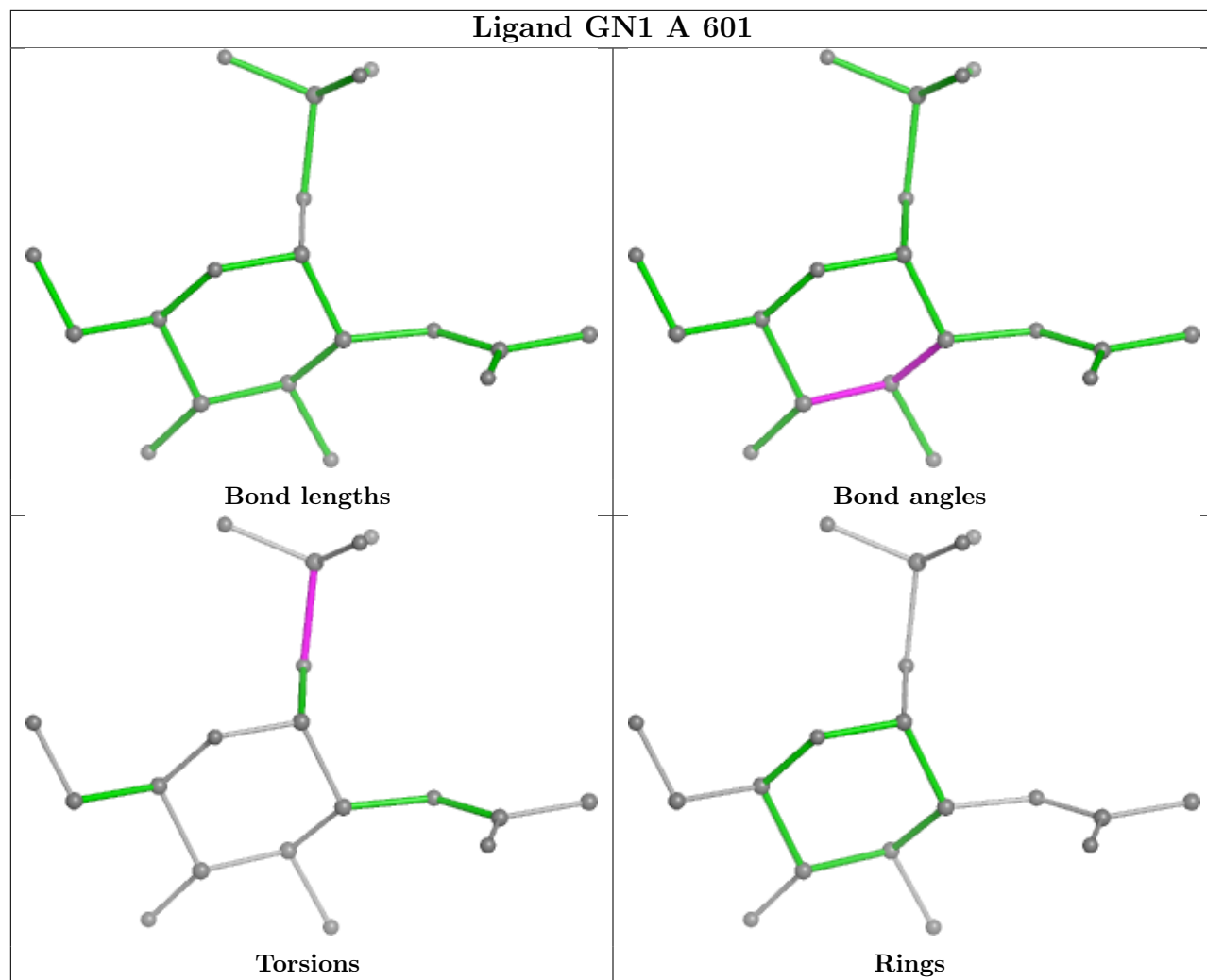
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	YRL	1	0
4	B	602	YRL	1	0

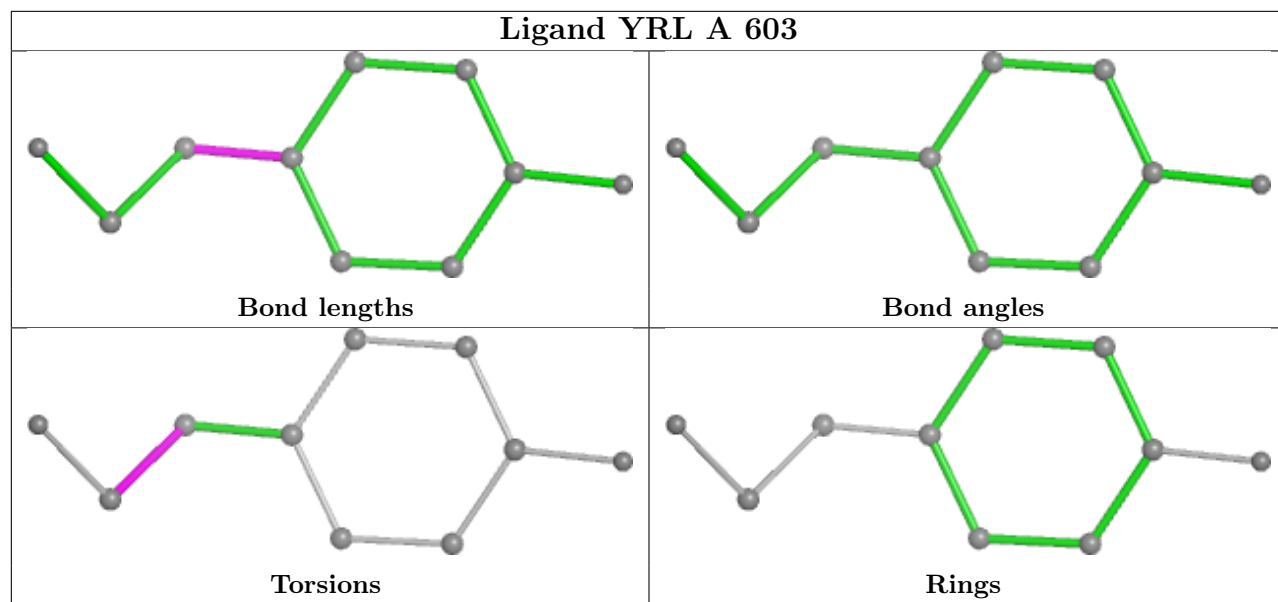
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



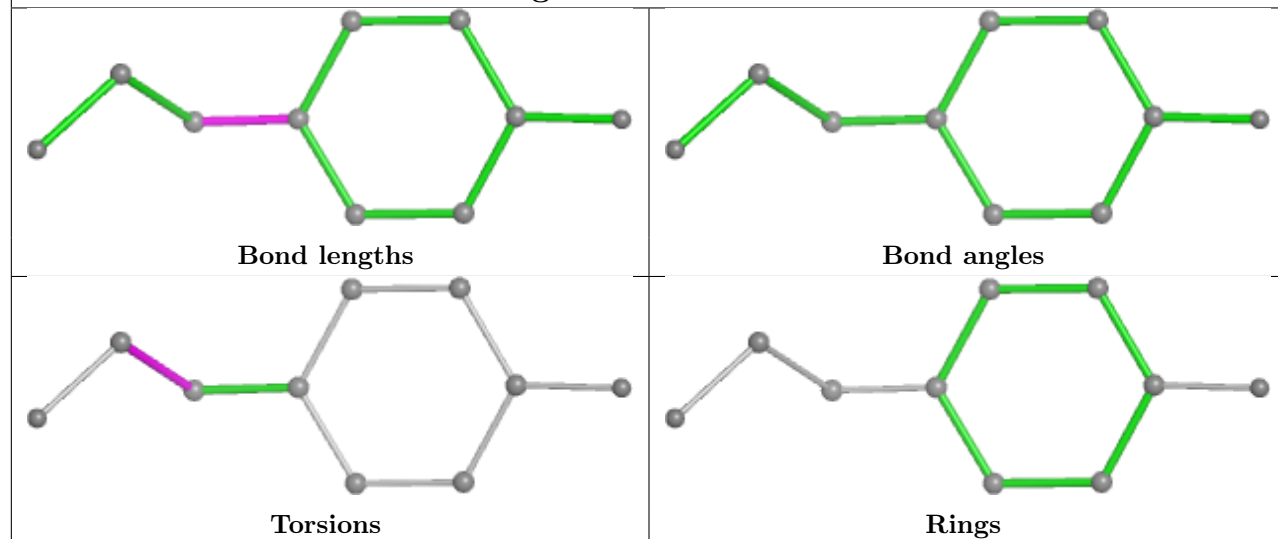
Ligand GN1 A 601



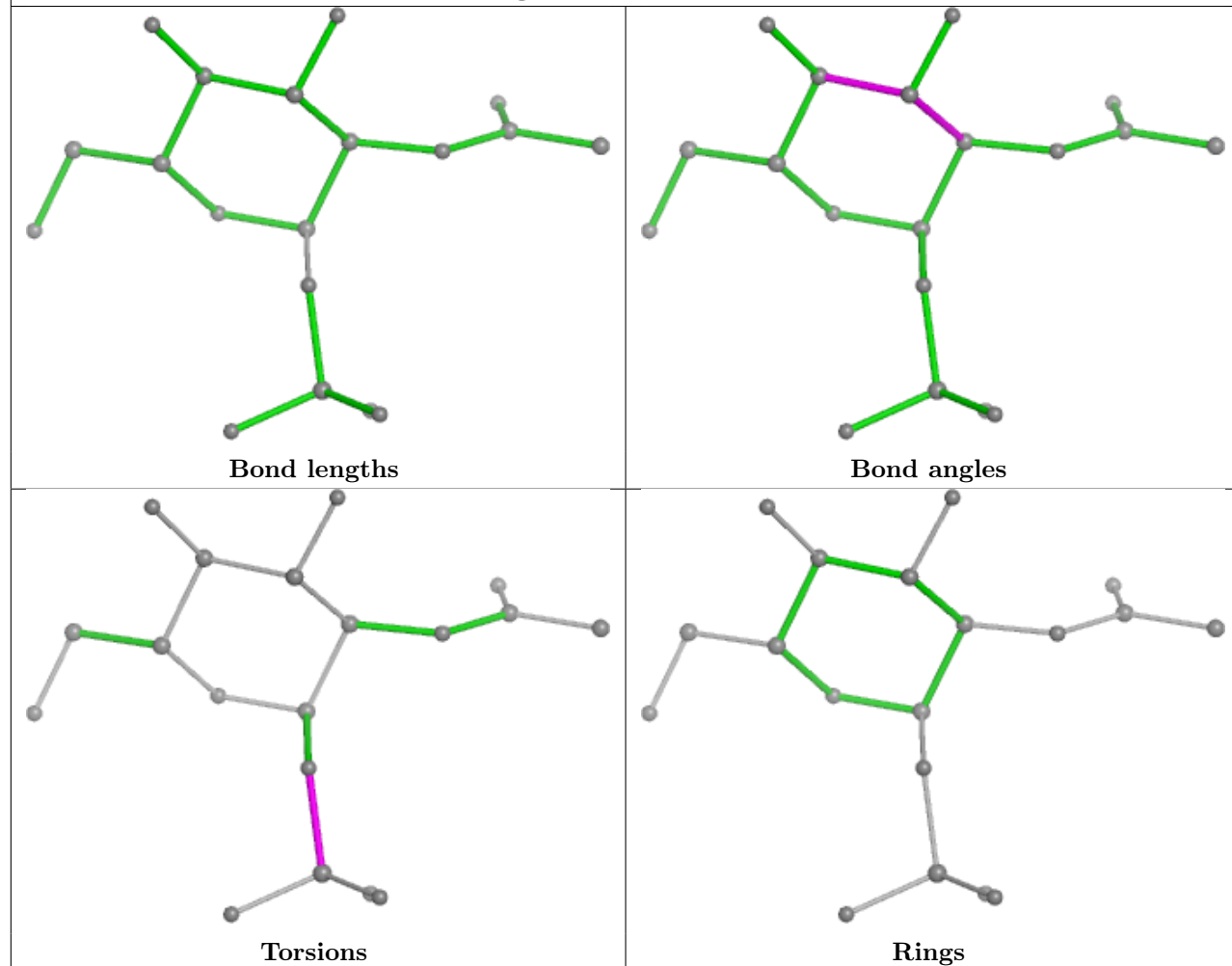
Ligand YRL A 603

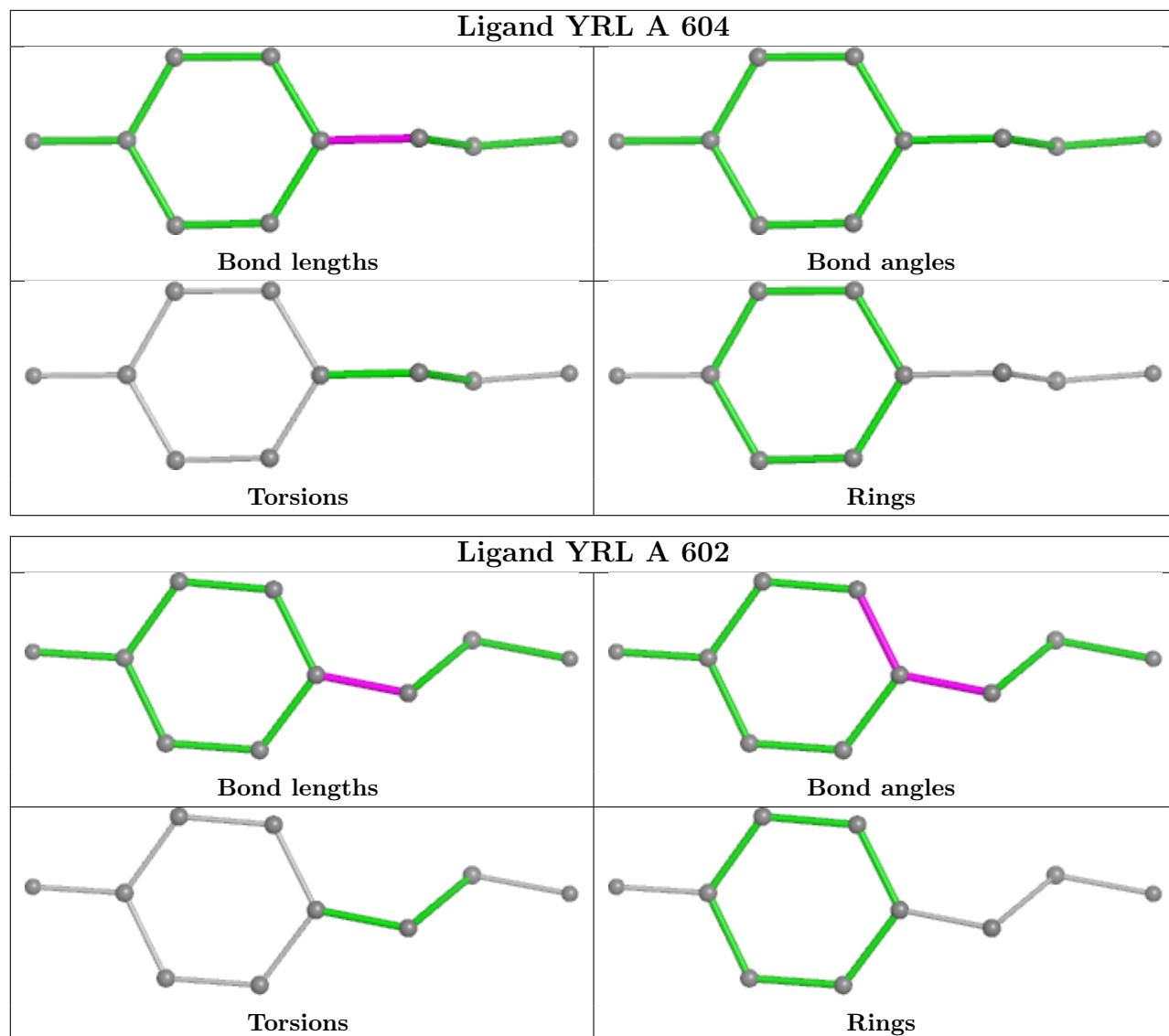


Ligand YRL B 602



Ligand GN1 B 601





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	476/484 (98%)	-0.74	0 100 100	17, 32, 64, 93	7 (1%)
1	B	472/484 (97%)	-0.75	0 100 100	16, 32, 60, 86	6 (1%)
2	C	465/484 (96%)	-0.61	0 100 100	19, 40, 75, 97	4 (0%)
2	D	466/484 (96%)	-0.60	0 100 100	18, 40, 77, 103	5 (1%)
All	All	1879/1936 (97%)	-0.67	0 100 100	16, 36, 71, 103	22 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	YCM	A	277	10/11	0.98	0.05	21,26,42,46	0
1	YCM	B	277	10/11	0.99	0.05	21,24,41,48	0

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

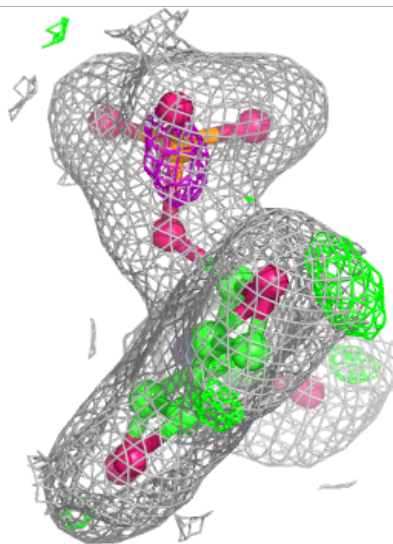
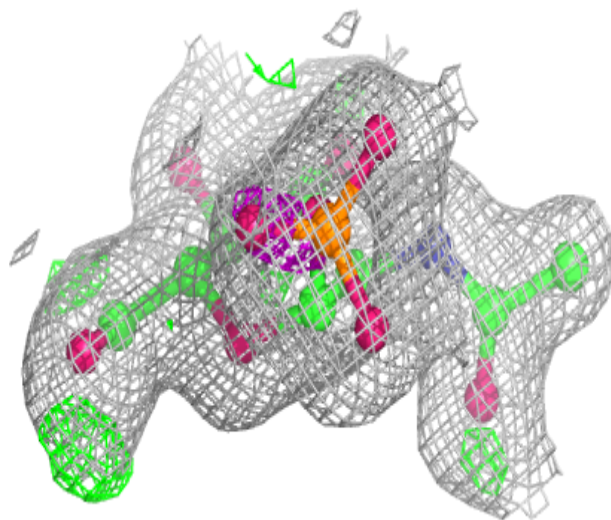
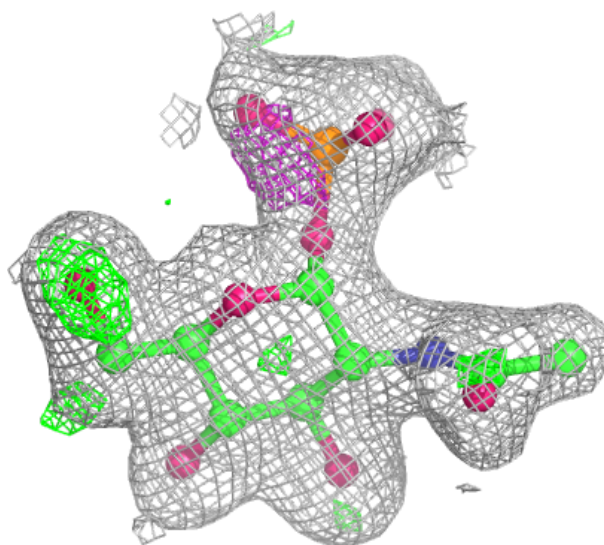
labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GN1	B	601	19/19	0.98	0.04	26,30,35,36	0
4	YRL	B	602	10/10	0.98	0.06	39,42,53,67	0
4	YRL	A	602	10/10	0.98	0.04	31,34,37,38	0
4	YRL	A	603	10/10	0.98	0.07	40,46,57,61	0
4	YRL	A	604	10/10	0.98	0.05	21,25,28,32	0
5	MG	B	604	1/1	0.98	0.07	48,48,48,48	0
5	MG	D	602	1/1	0.98	0.04	41,41,41,41	0
4	YRL	D	601	10/10	0.99	0.04	31,33,36,38	0
4	YRL	B	603	10/10	0.99	0.04	21,25,29,33	0
3	GN1	A	601	19/19	0.99	0.04	27,29,36,38	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.

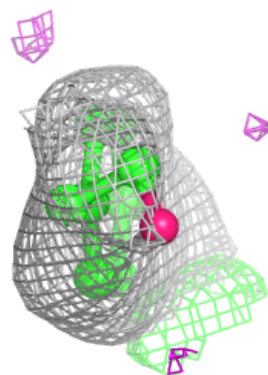
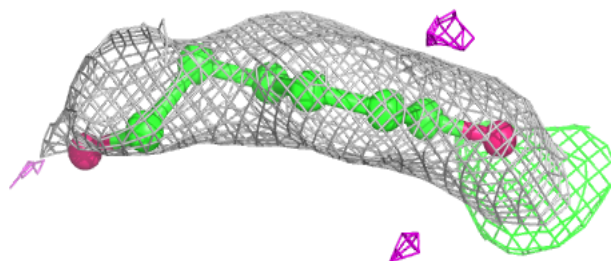
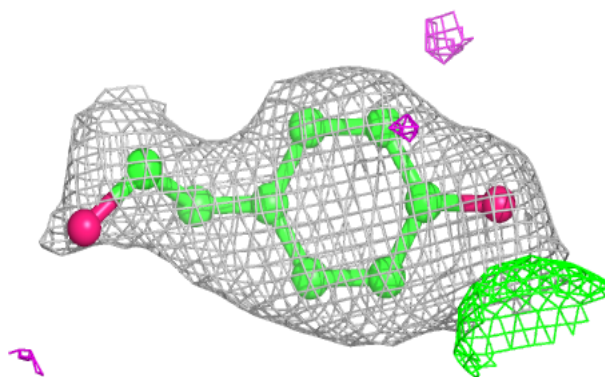
Electron density around GN1 B 601:

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

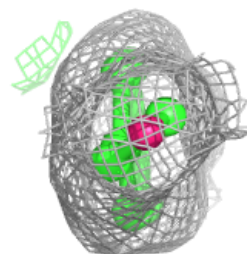
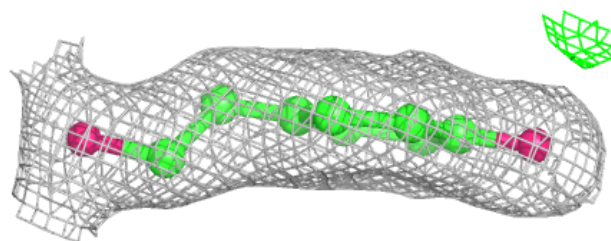
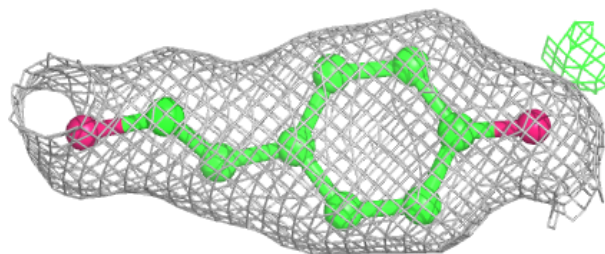


Electron density around YRL B 602:

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

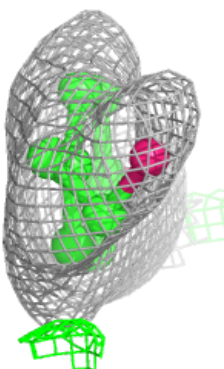
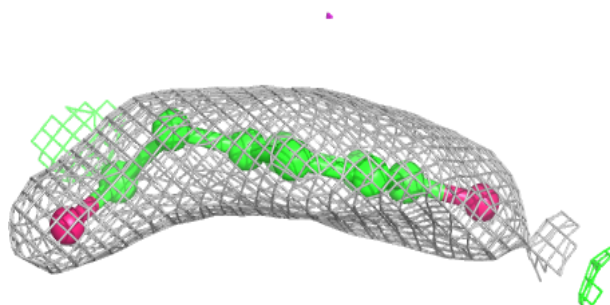
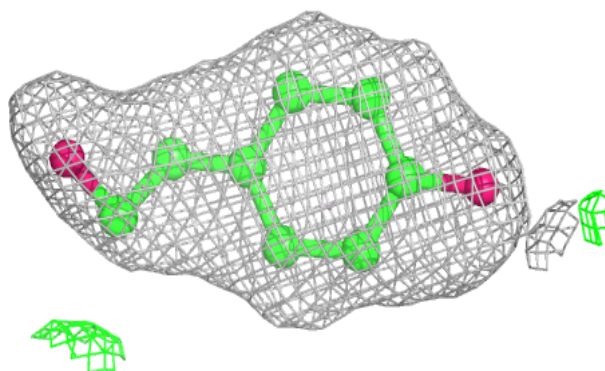
**Electron density around YRL A 602:**

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

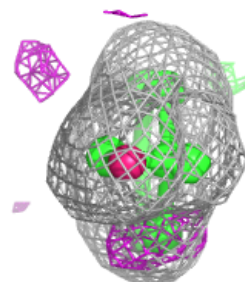
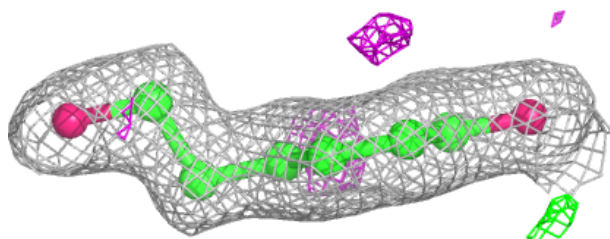
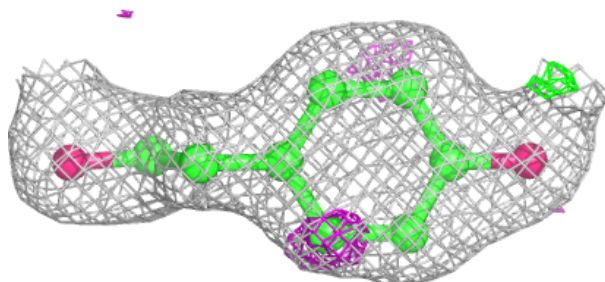


Electron density around YRL A 603:

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

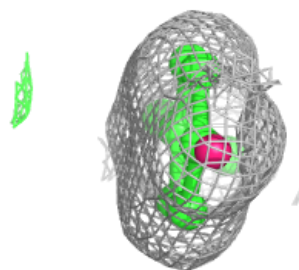
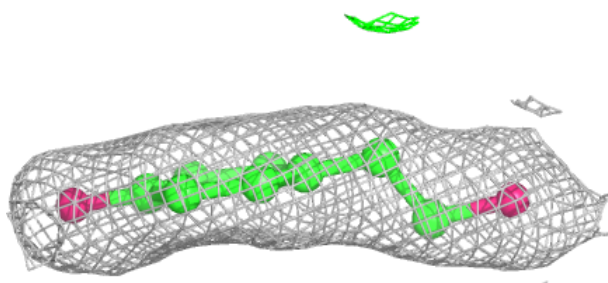
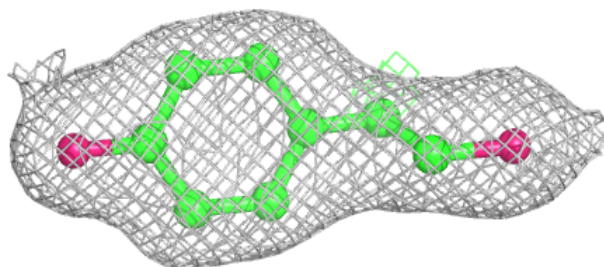
**Electron density around YRL A 604:**

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

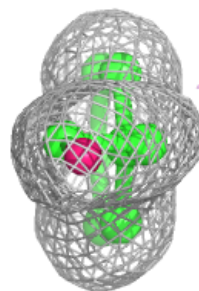
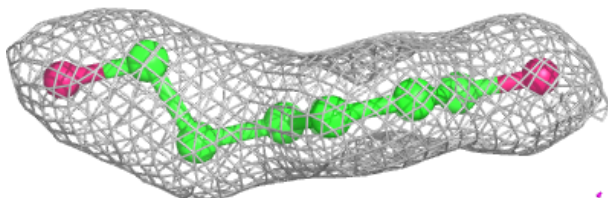
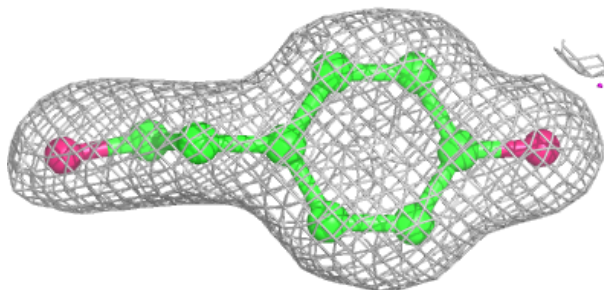


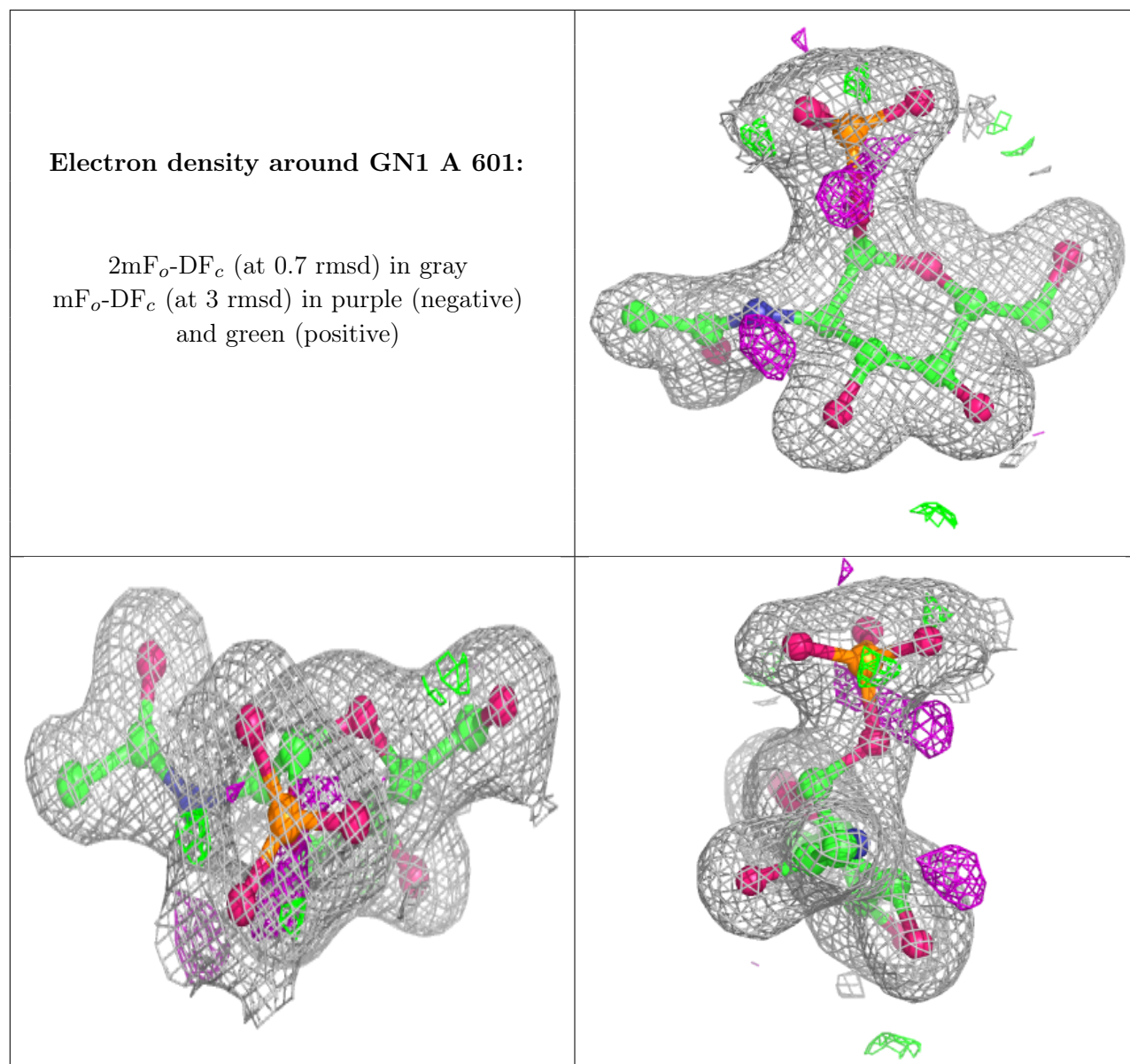
Electron density around YRL D 601:

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

**Electron density around YRL 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.