



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:16 AM UTC

PDB ID : 8BAY / pdb_00008bay
Title : Crystal Structure of IDH1 variant R132C S280F in complex with NADPH, Ca²⁺ and 3-butyl-2-oxoglutarate
Authors : Rabe, P.; Schofield, C.J.; Reinbold, R.; Brewitz, L.
Deposited on : 2022-10-12
Resolution : 2.35 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

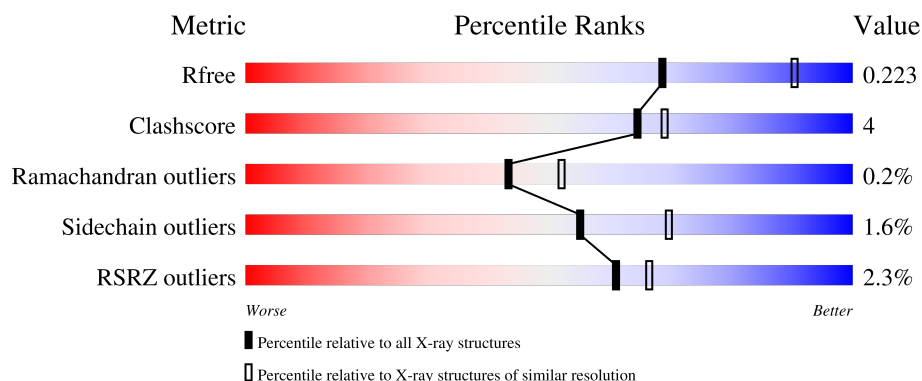
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	422	% 91% 7% .
1	B	422	5% 82% 13% .
1	C	422	2% 90% 8% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10159 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	2	0
			3223	2056	536	611	20			
1	B	407	Total	C	N	O	S	0	3	0
			3153	2007	524	603	19			
1	C	415	Total	C	N	O	S	0	5	0
			3298	2102	553	623	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	CYS	ARG	engineered mutation	UNP O75874
A	280	PHE	SER	engineered mutation	UNP O75874
A	415	LEU	-	expression tag	UNP O75874
A	416	GLU	-	expression tag	UNP O75874
A	417	HIS	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
B	132	CYS	ARG	engineered mutation	UNP O75874
B	280	PHE	SER	engineered mutation	UNP O75874
B	415	LEU	-	expression tag	UNP O75874
B	416	GLU	-	expression tag	UNP O75874
B	417	HIS	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
C	132	CYS	ARG	engineered mutation	UNP O75874
C	280	PHE	SER	engineered mutation	UNP O75874
C	415	LEU	-	expression tag	UNP O75874

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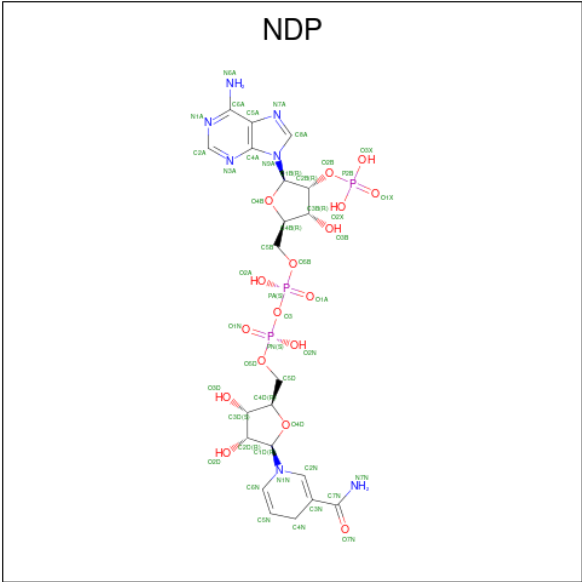
Chain	Residue	Modelled	Actual	Comment	Reference
C	416	GLU	-	expression tag	UNP O75874
C	417	HIS	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



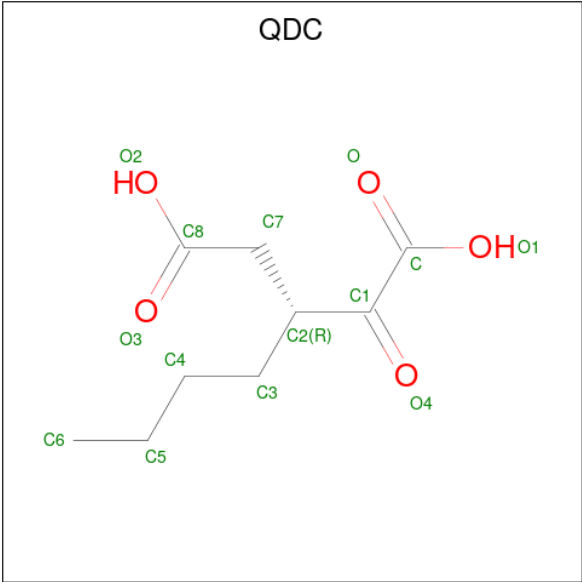
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



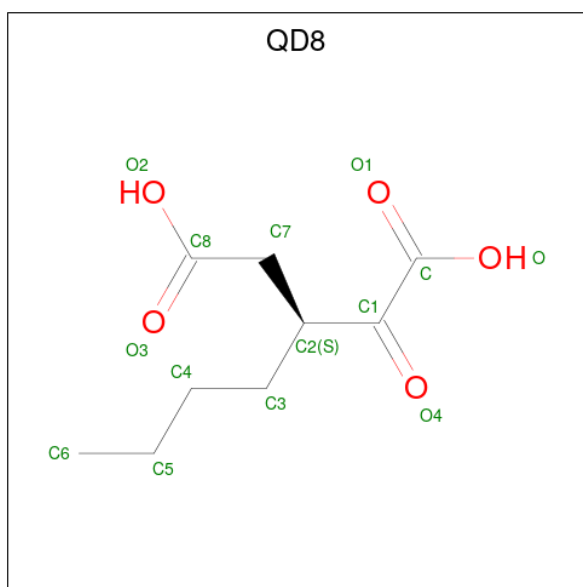
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (R)-3-butyl-2-oxopentanedioic acid (CCD ID: QDC) (formula: C₉H₁₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 14 9 5	0	1
4	B	1	Total C O 14 9 5	0	1
4	C	1	Total C O 14 9 5	0	1

- Molecule 5 is (S)-3-butyl-2-oxopentanedioic acid (CCD ID: QD8) (formula: C₉H₁₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 14 9 5	0	1
5	B	1	Total C O 14 9 5	0	1
5	C	1	Total C O 14 9 5	0	1

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

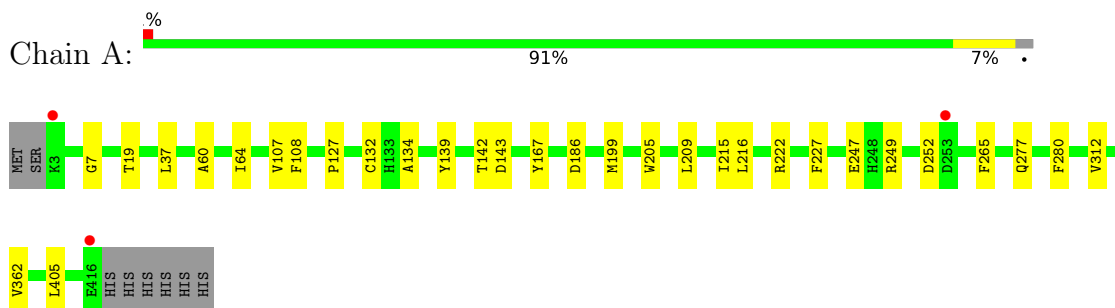
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	52	Total 52	O 52	0	0
7	B	59	Total 59	O 59	0	0
7	C	113	Total 113	O 113	0	0

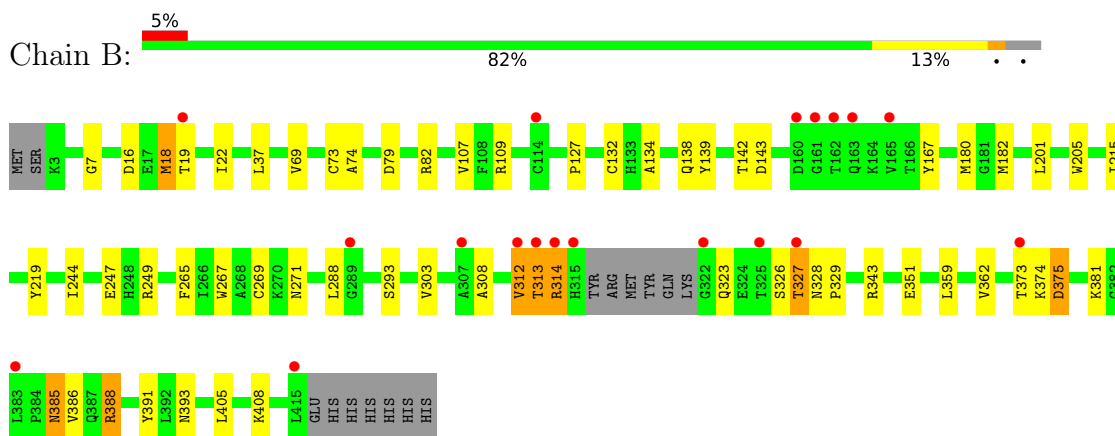
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

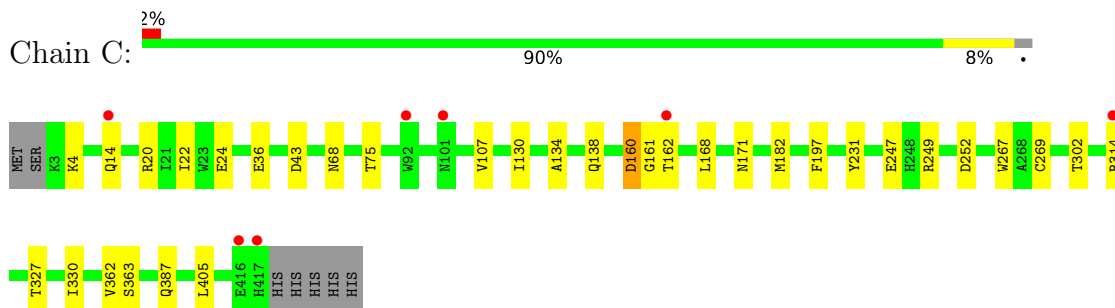
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.54Å 275.78Å 116.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.81 – 2.35 46.81 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.81-2.35) 99.9 (46.81-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.201 , 0.223 0.202 , 0.223	Depositor DCC
R_{free} test set	3301 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10159	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: GOL, QDC, QD8, CA, NDP

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	0.07	0/3292	0.25	0/4457
1	B	0.09	0/3218	0.27	0/4357
1	C	0.09	0/3368	0.27	0/4549
All	All	0.08	0/9878	0.26	0/13363

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3223	0	3090	20	0
1	B	3153	0	3010	42	0
1	C	3298	0	3211	19	0
2	A	12	0	16	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
3	A	48	0	26	0	0
3	B	48	0	26	4	0
3	C	48	0	26	2	0
4	A	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	0	0	0
4	C	14	0	0	0	0
5	A	14	0	0	0	0
5	B	14	0	0	0	0
5	C	14	0	0	0	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
7	A	52	0	0	1	0
7	B	59	0	0	2	0
7	C	113	0	0	0	0
All	All	10159	0	9429	75	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 (75) 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:19:THR:HG21	1:B:74:ALA:HB3	1.69	0.72
1:C:160:ASP:O	1:C:162:THR:N	2.23	0.69
1:B:326:SER:HB2	1:B:393:ASN:HA	1.78	0.65
1:B:381:LYS:O	1:B:385:ASN:ND2	2.32	0.63
1:B:314:ARG:HH11	3:B:801:NDP:H2B	1.65	0.61
1:A:247:GLU:OE1	1:A:249:ARG:NH1	2.33	0.60
1:B:385:ASN:N	1:B:385:ASN:OD1	2.36	0.59
1:C:160:ASP:N	1:C:160:ASP:OD1	2.35	0.58
1:A:107:VAL:HG23	1:A:134:ALA:HB2	1.86	0.58
1:C:138:GLN:HG3	1:C:182:MET:HE1	1.86	0.57
1:C:314:ARG:NH1	3:C:602:NDP:O2X	2.38	0.57
1:B:18:MET:HB3	1:B:312:VAL:HB	1.87	0.55
1:B:69:VAL:HG11	1:B:343:ARG:HD2	1.87	0.55
1:B:293:SER:HB2	1:B:308:ALA:HB2	1.89	0.54
1:C:168:LEU:HD21	1:C:171[B]:ASN:HD21	1.71	0.54
1:C:267:TRP:CD1	1:C:269:CYS:HG	2.25	0.54
1:B:388:ARG:NH1	1:B:391:TYR:O	2.41	0.53
1:C:22:ILE:HD11	1:C:327:THR:HB	1.90	0.53
1:B:267:TRP:CD1	1:B:269:CYS:HG	2.28	0.52
1:B:143:ASP:HB3	1:B:180:MET:HE3	1.91	0.52
1:A:167:TYR:HB3	1:B:142:THR:HG21	1.92	0.51
1:A:127:PRO:HG2	1:A:205:TRP:CH2	2.46	0.51
1:A:362:VAL:HG21	1:A:405:LEU:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HG21	1:B:167:TYR:HB3	1.94	0.49
1:A:186:ASP:OD2	1:A:222:ARG:NH2	2.45	0.49
1:B:138:GLN:HG3	1:B:182:MET:HE1	1.94	0.49
1:C:20:ARG:NH2	1:C:43:ASP:OD1	2.45	0.49
1:C:75:THR:O	3:C:602:NDP:H2N	2.13	0.49
1:C:252:ASP:OD1	1:C:252:ASP:N	2.44	0.49
1:B:313:THR:HG23	3:B:801:NDP:H51N	1.95	0.48
1:A:205:TRP:NE1	7:A:804:HOH:O	2.45	0.48
1:A:216:LEU:HD22	1:B:180:MET:HE1	1.96	0.48
1:B:127:PRO:HG2	1:B:205:TRP:CH2	2.48	0.48
1:B:16:ASP:O	1:B:19:THR:HG22	2.13	0.48
1:B:132[A]:CYS:SG	7:B:931:HOH:O	2.61	0.47
1:B:201:LEU:HD23	1:B:244:ILE:HD11	1.95	0.47
1:B:247:GLU:OE1	1:B:249:ARG:NH2	2.45	0.47
1:A:107:VAL:HB	1:A:132[B]:CYS:HB2	1.96	0.47
1:B:314:ARG:O	1:B:314:ARG:HG2	2.13	0.47
1:A:7:GLY:HA3	1:A:37:LEU:HD23	1.97	0.47
1:B:205:TRP:HB3	1:B:265:PHE:HA	1.96	0.47
1:C:362:VAL:HG21	1:C:405:LEU:HA	1.96	0.47
1:B:7:GLY:HA3	1:B:37:LEU:HD23	1.98	0.46
1:A:139:TYR:CD1	1:B:215:ILE:HG21	2.50	0.46
1:B:107:VAL:HG23	1:B:134:ALA:HB2	1.98	0.46
1:C:107:VAL:HG23	1:C:134:ALA:HB2	1.97	0.46
1:A:215:ILE:HG21	1:B:139:TYR:CD1	2.51	0.45
1:B:388:ARG:HA	1:B:388:ARG:HD2	1.74	0.45
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.99	0.45
1:B:139:TYR:HB2	1:B:271:ASN:ND2	2.32	0.45
1:A:252:ASP:OD1	1:A:252:ASP:N	2.50	0.44
1:C:14[B]:GLN:NE2	1:C:24:GLU:OE2	2.50	0.44
1:C:4:LYS:HB2	1:C:36:GLU:HG3	1.99	0.44
1:C:168:LEU:HD21	1:C:171[B]:ASN:ND2	2.31	0.44
1:C:197:PHE:CZ	1:C:231:TYR:HB2	2.53	0.44
1:C:68:ASN:HA	1:C:302:THR:HG23	1.98	0.44
1:B:362:VAL:HG23	1:B:408:LYS:HD2	2.00	0.44
1:A:209:LEU:HD22	1:A:227:PHE:CG	2.53	0.43
1:B:19:THR:HG23	1:B:73:CYS:SG	2.58	0.43
1:B:314:ARG:NH1	3:B:801:NDP:H2B	2.31	0.43
1:B:18:MET:HG2	1:B:312:VAL:HG21	2.01	0.43
1:B:79:ASP:H	1:B:82:ARG:HB2	1.83	0.43
1:A:60:ALA:O	1:A:64:ILE:HG13	2.18	0.43
1:B:22:ILE:HD13	1:B:329:PRO:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HD13	1:B:405:LEU:HD22	2.01	0.43
1:C:247:GLU:OE1	1:C:249:ARG:NH1	2.44	0.43
1:B:109:ARG:NH1	7:B:905:HOH:O	2.53	0.42
1:B:328:ASN:HB2	1:B:375:ASP:OD2	2.20	0.42
1:A:277:GLN:HA	1:A:280:PHE:HB3	2.01	0.42
1:B:288:LEU:HD23	3:B:801:NDP:O4B	2.20	0.42
1:B:18:MET:SD	1:B:327:THR:HG21	2.60	0.42
1:A:205:TRP:HB3	1:A:265:PHE:HA	2.01	0.41
1:B:374:LYS:HD3	1:B:391:TYR:CZ	2.56	0.41
1:A:143:ASP:HB2	1:B:219:TYR:HB2	2.04	0.40
1:A:108:PHE:CE1	1:A:199:MET:HG3	2.56	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	414/422 (98%)	401 (97%)	12 (3%)	1 (0%)	43	52
1	B	406/422 (96%)	382 (94%)	23 (6%)	1 (0%)	43	52
1	C	418/422 (99%)	400 (96%)	17 (4%)	1 (0%)	43	52
All	All	1238/1266 (98%)	1183 (96%)	52 (4%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	GLY
1	B	312	VAL
1	A	312	VAL

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	328/358 (92%)	327 (100%)	1 (0%)	86	92
1	B	321/358 (90%)	309 (96%)	12 (4%)	30	40
1	C	343/358 (96%)	340 (99%)	3 (1%)	70	82
All	All	992/1074 (92%)	976 (98%)	16 (2%)	55	70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	B	18	MET
1	B	303	VAL
1	B	313	THR
1	B	314	ARG
1	B	323	GLN
1	B	327	THR
1	B	351	GLU
1	B	373	THR
1	B	375	ASP
1	B	385	ASN
1	B	386	VAL
1	B	388	ARG
1	C	130	ILE
1	C	160	ASP
1	C	387	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	228	GLN
1	A	320	GLN
1	B	68	ASN
1	B	101	ASN

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Mol	Chain	Res	Type
1	B	171	ASN
1	B	185	GLN
1	B	228	GLN
1	B	271	ASN
1	C	67	HIS
1	C	170	HIS
1	C	277	GLN
1	C	385	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	NDP	B	801	-	51,52,52	0.29	0	71,80,80	0.38	1 (1%)
5	QD8	C	605[A]	6	13,13,13	0.14	0	15,16,16	0.37	0
2	GOL	A	701	-	5,5,5	0.95	0	5,5,5	1.08	0
2	GOL	C	603	-	5,5,5	0.94	0	5,5,5	1.06	0
3	NDP	A	703	-	51,52,52	0.28	0	71,80,80	0.39	0
2	GOL	A	702	-	5,5,5	0.94	0	5,5,5	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	QDC	C	604[B]	6	13,13,13	1.09	2 (15%)	15,16,16	1.13	2 (13%)
5	QD8	A	705[A]	6	13,13,13	1.26	2 (15%)	15,16,16	1.45	1 (6%)
5	QD8	B	804[A]	6	13,13,13	0.14	0	15,16,16	0.38	0
4	QDC	B	803[B]	6	13,13,13	1.09	2 (15%)	15,16,16	1.17	2 (13%)
2	GOL	C	601	-	5,5,5	0.93	0	5,5,5	1.07	0
4	QDC	A	704[B]	6	13,13,13	0.12	0	15,16,16	0.35	0
3	NDP	C	602	-	51,52,52	0.28	0	71,80,80	0.49	1 (1%)
2	GOL	B	802	-	5,5,5	0.95	0	5,5,5	1.09	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
3	NDP	B	801	-	-	10/34/77/77	0/5/5/5
5	QD8	C	605[A]	6	-	4/15/16/16	-
2	GOL	A	701	-	-	0/4/4/4	-
2	GOL	C	603	-	-	2/4/4/4	-
3	NDP	A	703	-	-	5/34/77/77	0/5/5/5
2	GOL	A	702	-	-	0/4/4/4	-
4	QDC	C	604[B]	6	-	9/15/16/16	-
5	QD8	A	705[A]	6	-	6/15/16/16	-
5	QD8	B	804[A]	6	-	4/15/16/16	-
4	QDC	B	803[B]	6	-	8/15/16/16	-
2	GOL	C	601	-	-	1/4/4/4	-
4	QDC	A	704[B]	6	-	5/15/16/16	-
3	NDP	C	602	-	-	12/34/77/77	0/5/5/5
2	GOL	B	802	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	705[A]	QD8	O1-C	3.50	1.31	1.22
5	A	705[A]	QD8	O-C	-2.85	1.22	1.30
4	B	803[B]	QDC	O3-C8	2.81	1.31	1.22
4	C	604[B]	QDC	O3-C8	2.79	1.31	1.22
4	C	604[B]	QDC	O2-C8	-2.75	1.21	1.30
4	B	803[B]	QDC	O2-C8	-2.72	1.21	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	705[A]	QD8	O1-C-C1	-5.44	115.21	122.15
4	B	803[B]	QDC	O3-C8-C7	-3.03	113.53	122.84
4	C	604[B]	QDC	O3-C8-C7	-2.98	113.70	122.84
4	B	803[B]	QDC	O2-C8-C7	2.87	122.92	114.00
4	C	604[B]	QDC	O2-C8-C7	2.77	122.62	114.00
3	C	602	NDP	P2B-O2B-C2B	2.57	130.28	123.43
3	B	801	NDP	P2B-O2B-C2B	2.04	128.89	123.43

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	802	GOL	O1-C1-C2-C3
2	B	802	GOL	C1-C2-C3-O3
3	B	801	NDP	C5B-O5B-PA-O1A
3	B	801	NDP	C5B-O5B-PA-O2A
3	B	801	NDP	C5B-O5B-PA-O3
3	C	602	NDP	PN-O3-PA-O5B
4	A	704[B]	QDC	O4-C1-C2-C3
4	A	704[B]	QDC	C-C1-C2-C3
4	B	803[B]	QDC	O4-C1-C2-C3
4	B	803[B]	QDC	C-C1-C2-C3
4	B	803[B]	QDC	O-C-C1-O4
4	B	803[B]	QDC	O-C-C1-C2
4	B	803[B]	QDC	C1-C2-C3-C4
4	C	604[B]	QDC	O4-C1-C2-C3
4	C	604[B]	QDC	C-C1-C2-C3
4	C	604[B]	QDC	O1-C-C1-O4
4	C	604[B]	QDC	C1-C2-C3-C4
5	B	804[A]	QD8	O1-C-C1-C2
5	B	804[A]	QD8	O1-C-C1-O4
5	C	605[A]	QD8	O-C-C1-O4
2	C	603	GOL	O1-C1-C2-O2
3	C	602	NDP	O4B-C4B-C5B-O5B
3	C	602	NDP	C3B-C4B-C5B-O5B
4	A	704[B]	QDC	C2-C3-C4-C5
5	B	804[A]	QD8	C7-C2-C3-C4
3	C	602	NDP	C3B-C2B-O2B-P2B
2	C	603	GOL	O1-C1-C2-C3
3	C	602	NDP	C1B-C2B-O2B-P2B
4	B	803[B]	QDC	C7-C2-C3-C4

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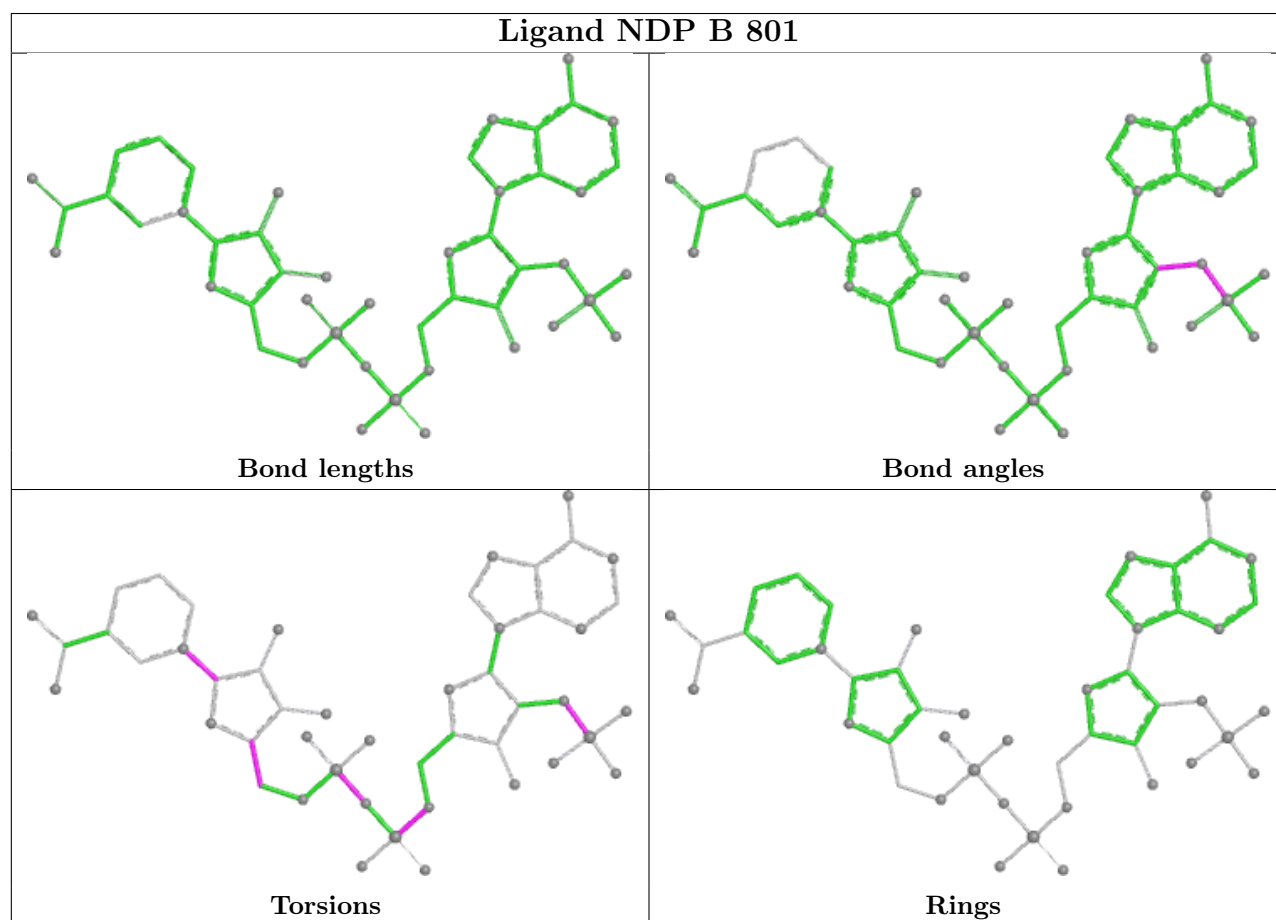
Mol	Chain	Res	Type	Atoms
4	C	604[B]	QDC	C7-C2-C3-C4
3	B	801	NDP	O4D-C4D-C5D-O5D
2	B	802	GOL	O1-C1-C2-O2
3	C	602	NDP	C2B-O2B-P2B-O1X
5	B	804[A]	QD8	C1-C2-C3-C4
5	A	705[A]	QD8	C7-C2-C3-C4
3	C	602	NDP	PA-O3-PN-O1N
3	B	801	NDP	C3D-C4D-C5D-O5D
4	C	604[B]	QDC	O-C-C1-O4
5	A	705[A]	QD8	O1-C-C1-O4
5	C	605[A]	QD8	O1-C-C1-O4
3	B	801	NDP	PA-O3-PN-O5D
4	C	604[B]	QDC	O-C-C1-C2
5	C	605[A]	QD8	O1-C-C1-C2
2	B	802	GOL	O2-C2-C3-O3
3	A	703	NDP	C5D-O5D-PN-O1N
3	A	703	NDP	C5D-O5D-PN-O2N
5	A	705[A]	QD8	C1-C2-C3-C4
3	C	602	NDP	C2D-C1D-N1N-C2N
5	A	705[A]	QD8	C2-C7-C8-O3
3	B	801	NDP	C2B-O2B-P2B-O2X
3	C	602	NDP	O4D-C1D-N1N-C2N
4	A	704[B]	QDC	C2-C7-C8-O2
5	A	705[A]	QD8	C2-C7-C8-O2
3	A	703	NDP	O4D-C1D-N1N-C2N
3	B	801	NDP	O4D-C1D-N1N-C2N
3	C	602	NDP	C2D-C1D-N1N-C6N
4	C	604[B]	QDC	C2-C7-C8-O2
3	C	602	NDP	O4D-C1D-N1N-C6N
5	A	705[A]	QD8	O1-C-C1-C2
5	C	605[A]	QD8	C7-C2-C3-C4
4	A	704[B]	QDC	C2-C7-C8-O3
3	A	703	NDP	C2D-C1D-N1N-C2N
4	B	803[B]	QDC	C2-C7-C8-O3
3	C	602	NDP	PA-O3-PN-O2N
4	B	803[B]	QDC	C2-C7-C8-O2
3	B	801	NDP	C2D-C1D-N1N-C2N
2	C	601	GOL	O1-C1-C2-C3
3	B	801	NDP	C2B-O2B-P2B-O1X
4	C	604[B]	QDC	C2-C7-C8-O3
3	A	703	NDP	PN-O3-PA-O2A

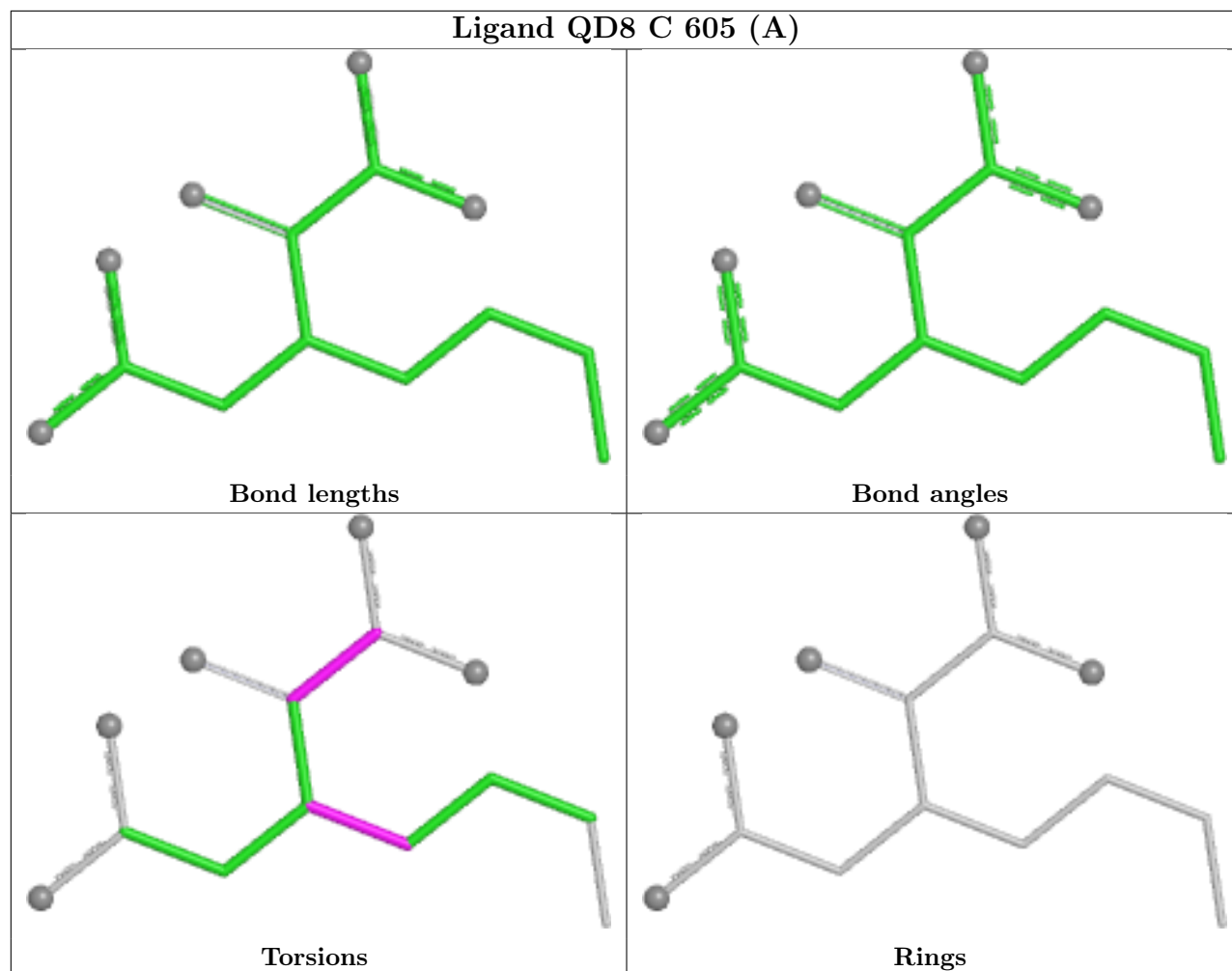
There are no ring outliers.

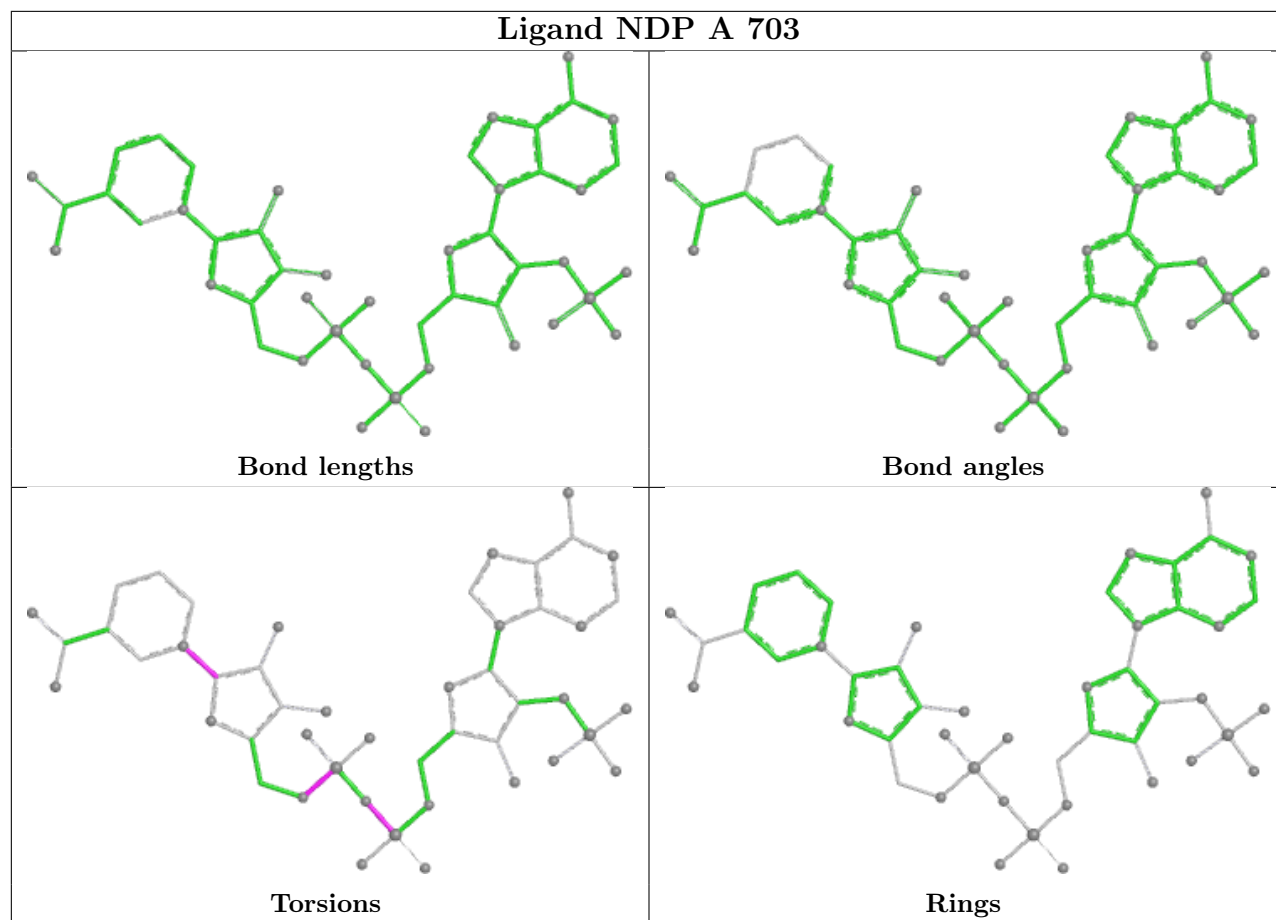
2 monomers are involved in 6 short contacts:

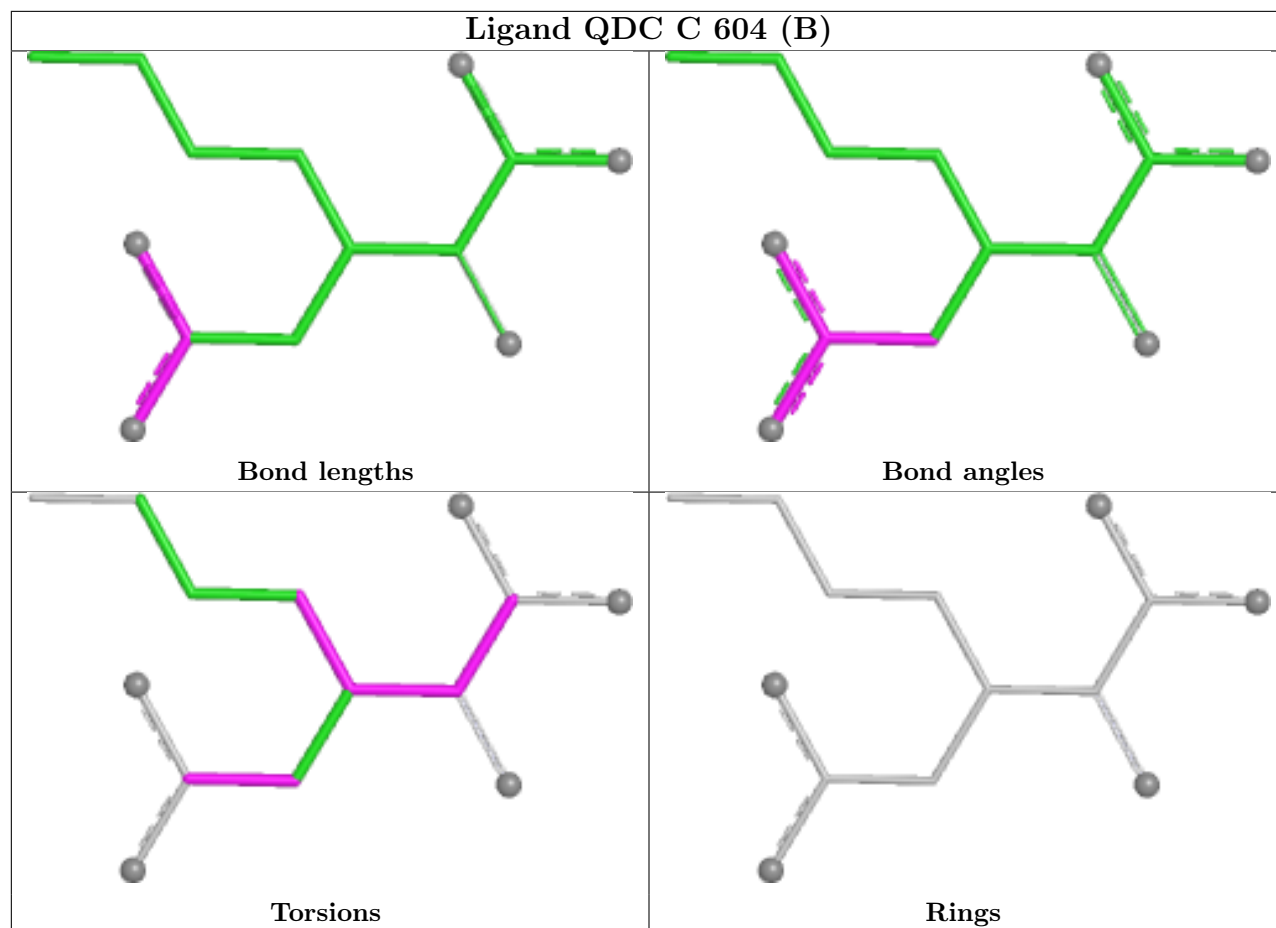
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	NDP	4	0
3	C	602	NDP	2	0

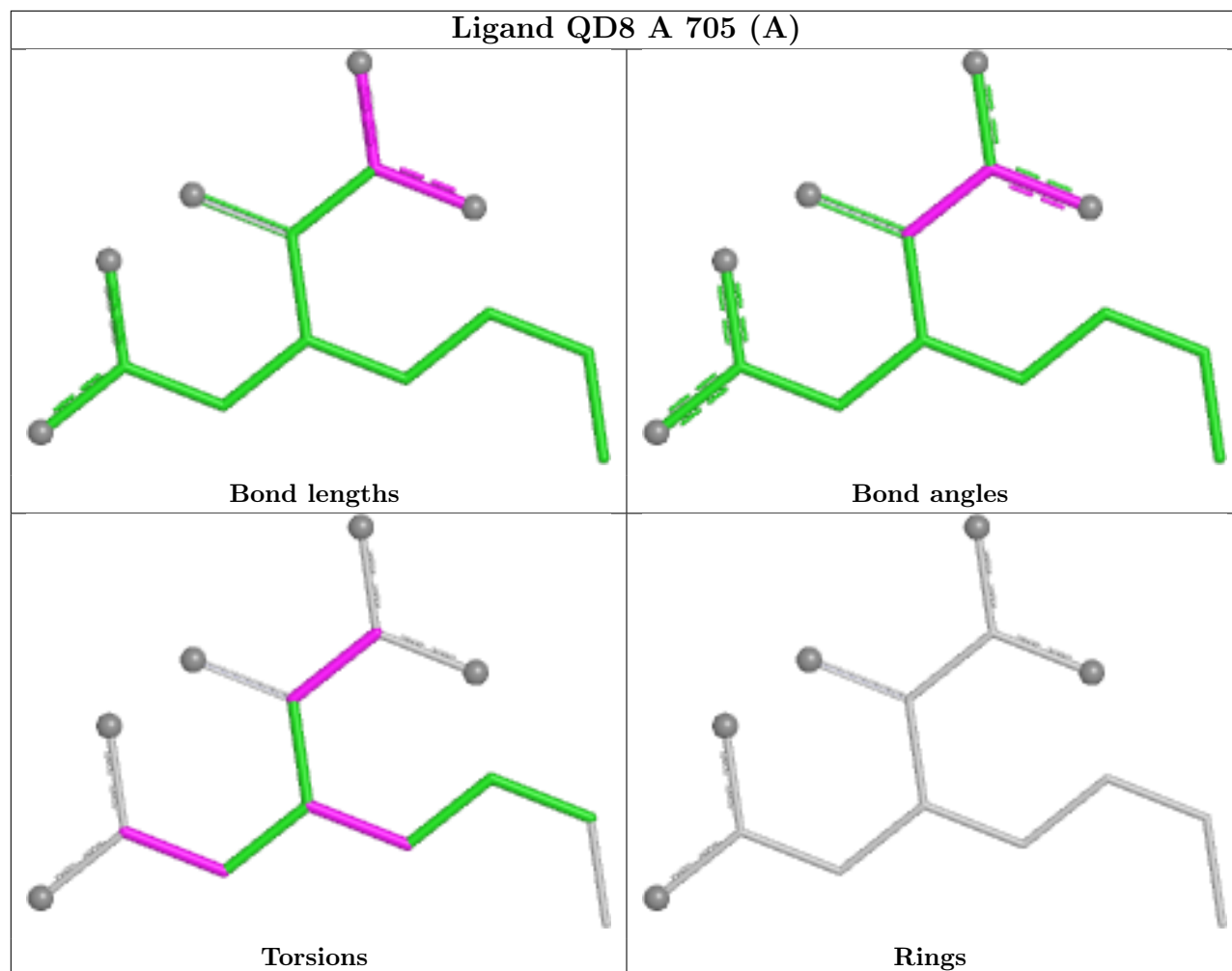
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

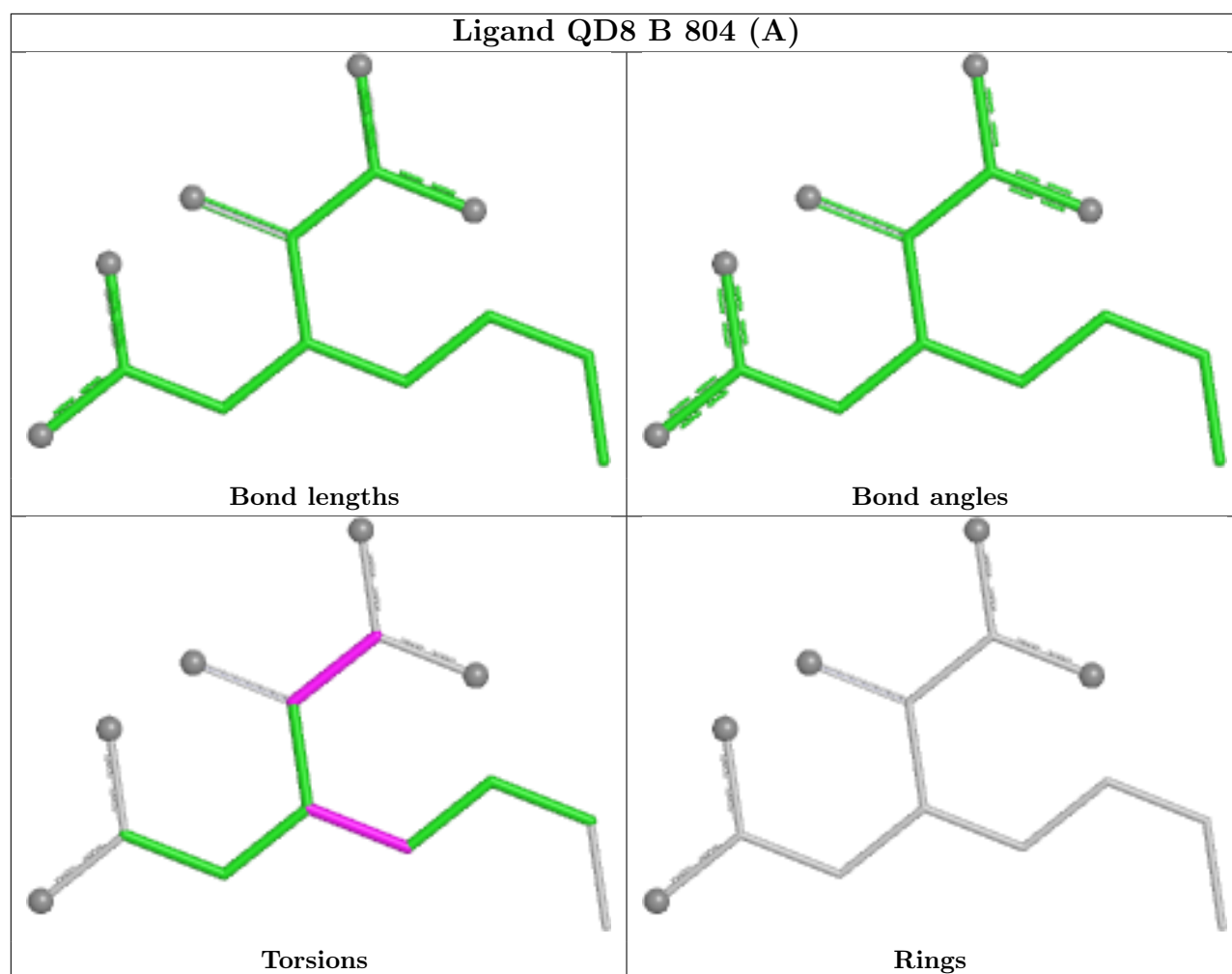


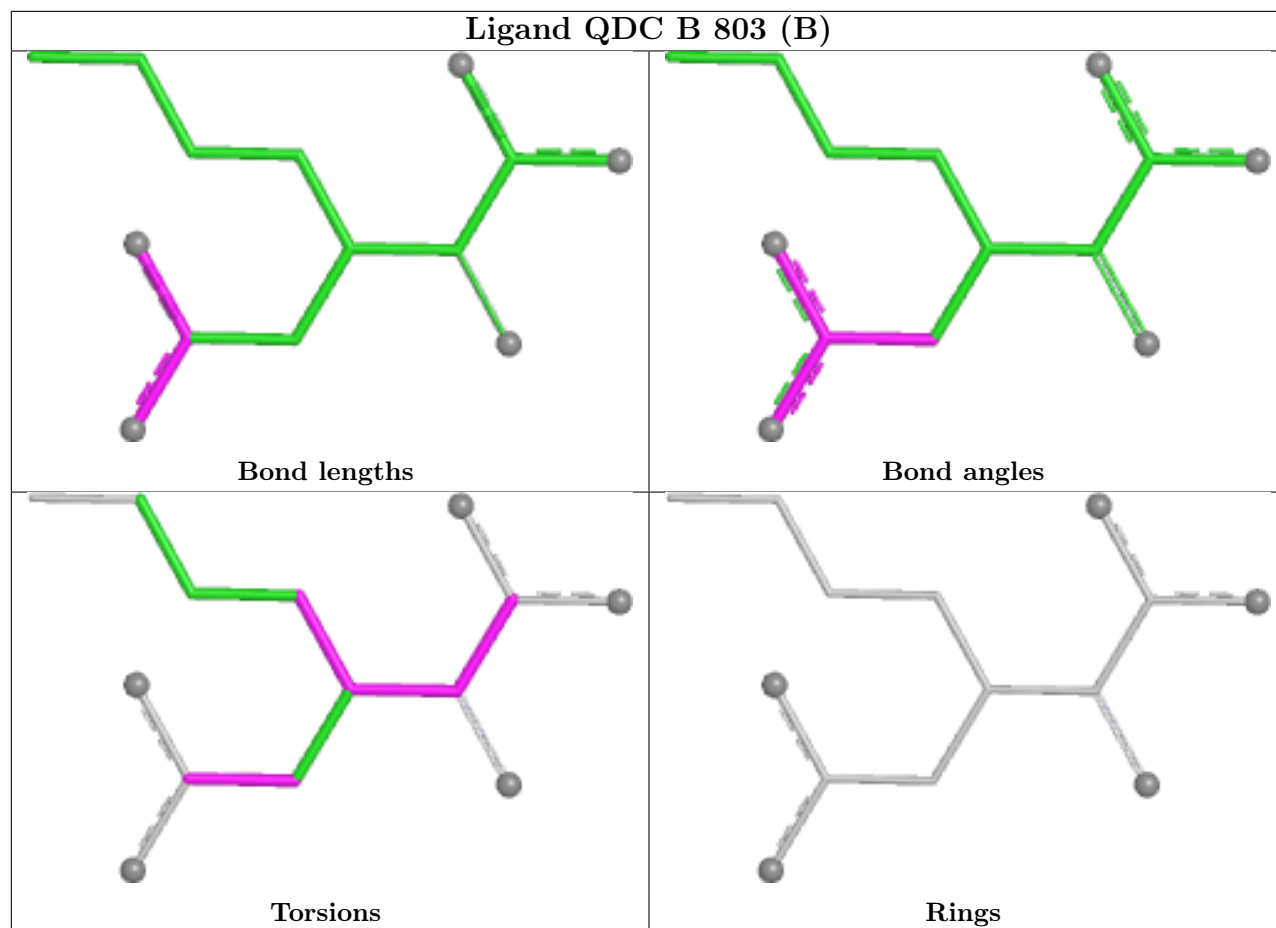


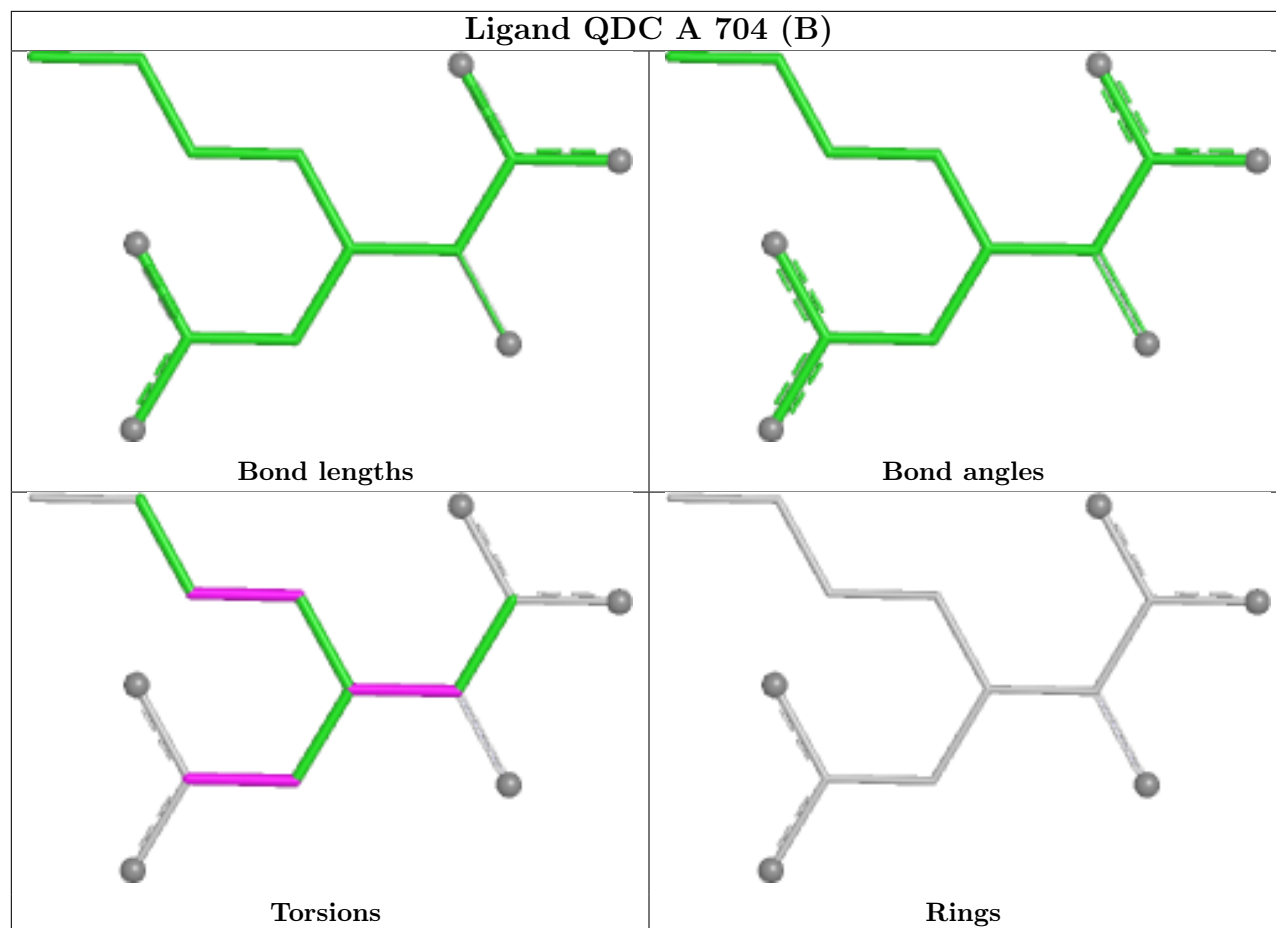


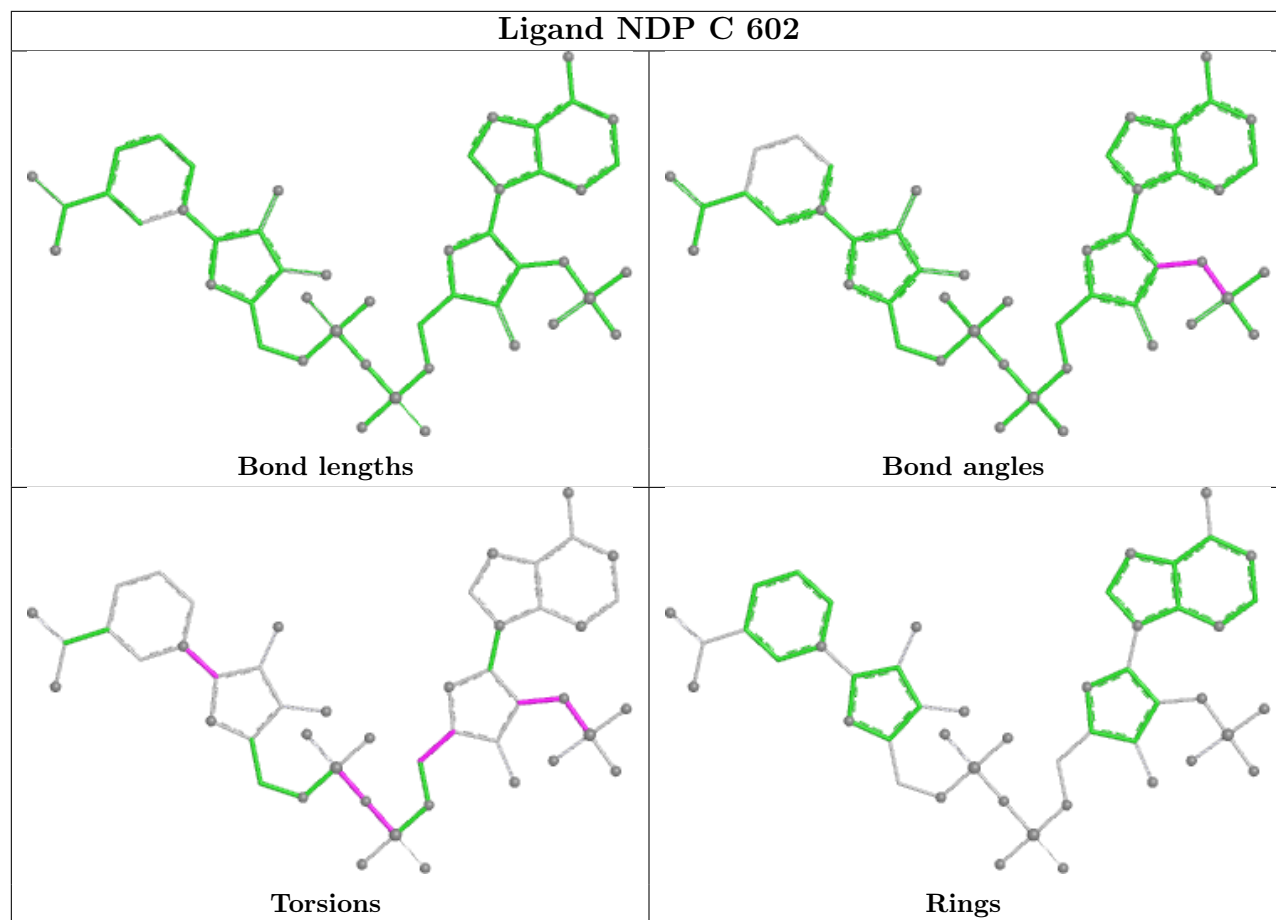












5.7 Other polymers [i](#)

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	414/422 (98%)	0.14	3 (0%) 84 87	29, 68, 93, 123	2 (0%)
1	B	407/422 (96%)	0.34	19 (4%) 36 42	28, 69, 103, 143	3 (0%)
1	C	415/422 (98%)	-0.02	7 (1%) 69 74	25, 57, 83, 136	5 (1%)
All	All	1236/1266 (97%)	0.15	29 (2%) 61 66	25, 65, 94, 143	10 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	HIS	6.8
1	B	313	THR	5.0
1	B	322	GLY	4.9
1	B	312	VAL	4.2
1	A	416	GLU	3.6
1	B	383	LEU	3.6
1	B	314	ARG	3.3
1	B	163	GLN	3.1
1	B	162	THR	3.1
1	B	415	LEU	3.1
1	A	253	ASP	2.9
1	B	307	ALA	2.8
1	B	114	CYS	2.8
1	A	3	LYS	2.8
1	B	160	ASP	2.7
1	B	19	THR	2.6
1	C	101[A]	ASN	2.5
1	B	165	VAL	2.5
1	C	314	ARG	2.5
1	B	161	GLY	2.5
1	B	289	GLY	2.5
1	B	327	THR	2.3
1	C	92	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	325	THR	2.1
1	B	373	THR	2.1
1	C	416	GLU	2.1
1	C	417	HIS	2.1
1	C	14[A]	GLN	2.0
1	C	162	THR	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](#)

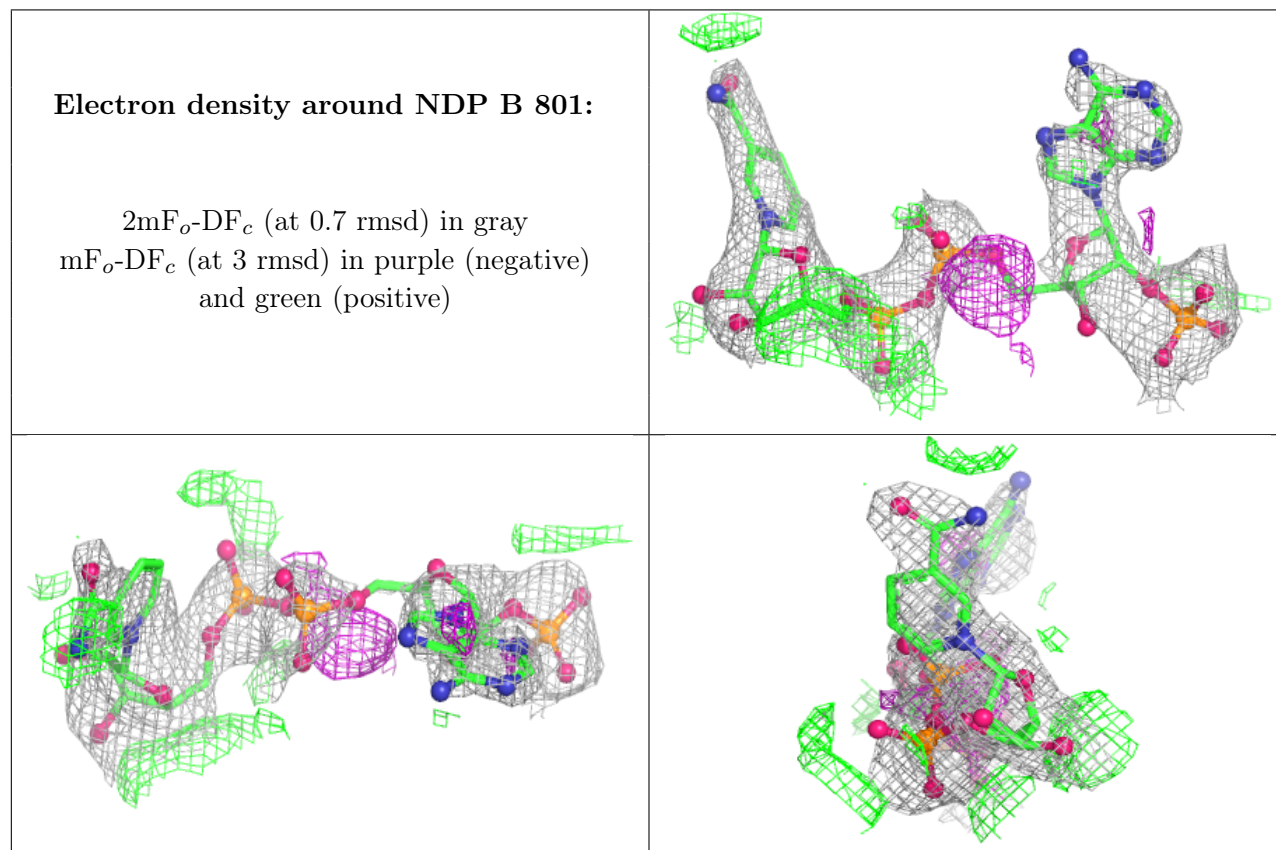
There are no oligosaccharides in this entry.

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.

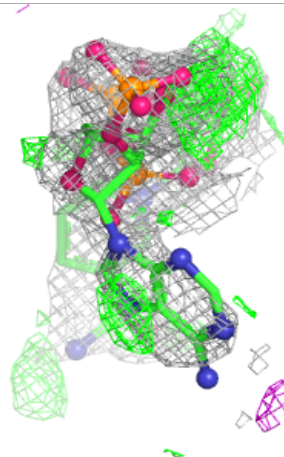
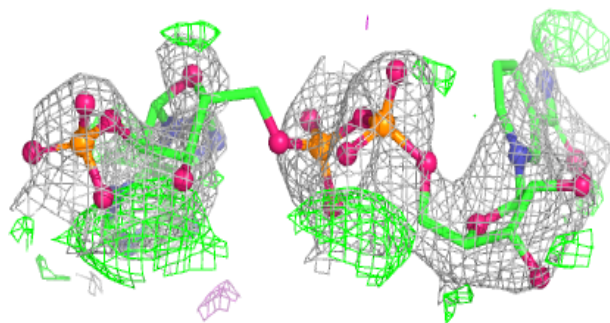
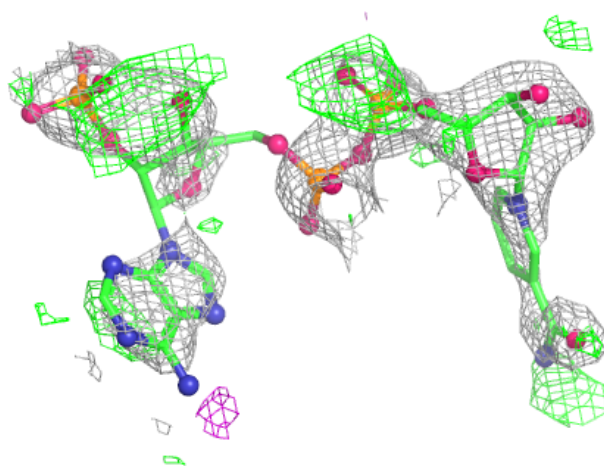
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	802	6/6	0.63	0.23	101,109,112,112	0
2	GOL	A	701	6/6	0.64	0.16	92,93,96,100	0
2	GOL	C	603	6/6	0.66	0.18	73,76,83,86	0
3	NDP	B	801	48/48	0.76	0.17	70,90,100,104	48
2	GOL	C	601	6/6	0.78	0.14	71,86,87,88	0
3	NDP	C	602	48/48	0.79	0.22	54,68,83,87	48
2	GOL	A	702	6/6	0.80	0.14	83,90,91,94	0
4	QDC	B	803[B]	14/14	0.84	0.14	67,70,72,73	14
3	NDP	A	703	48/48	0.85	0.12	62,76,87,95	0
4	QDC	C	604[B]	14/14	0.91	0.12	56,60,61,63	14
5	QD8	C	605[A]	14/14	0.91	0.12	56,60,62,63	14
5	QD8	B	804[A]	14/14	0.93	0.12	67,70,72,73	14
5	QD8	A	705[A]	14/14	0.93	0.13	58,61,65,66	14
4	QDC	A	704[B]	14/14	0.94	0.12	58,61,65,66	14
6	CA	A	706	1/1	0.98	0.04	67,67,67,67	0
6	CA	A	707	1/1	0.99	0.05	57,57,57,57	0
6	CA	C	606	1/1	0.99	0.04	54,54,54,54	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.



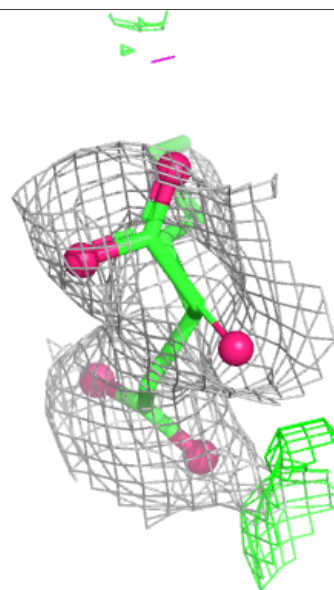
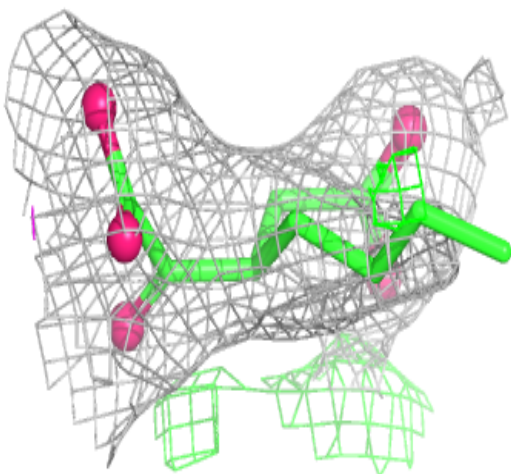
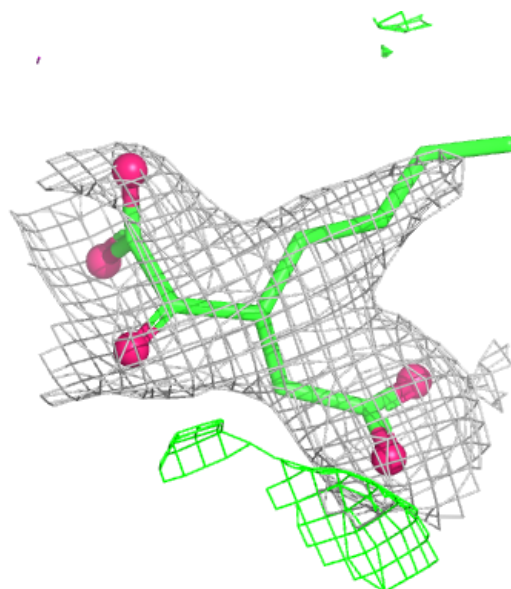
Electron density around NDP C 602:

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



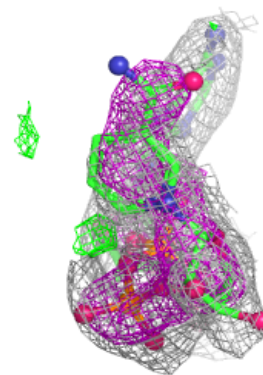
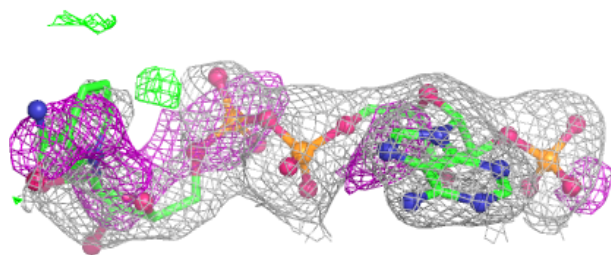
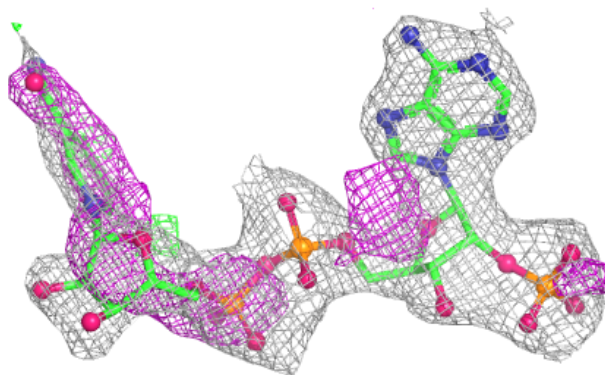
Electron density around QDC B 803 (B):

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

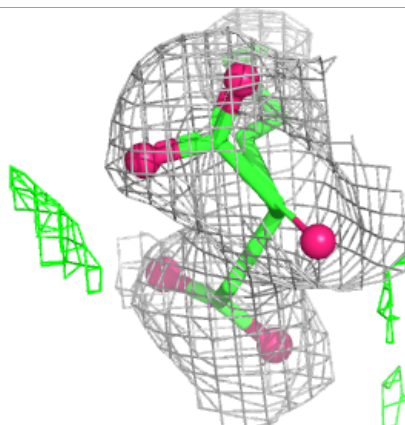
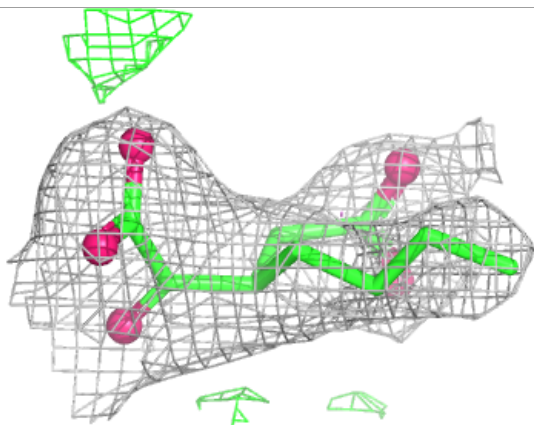


Electron density around NDP A 703:

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

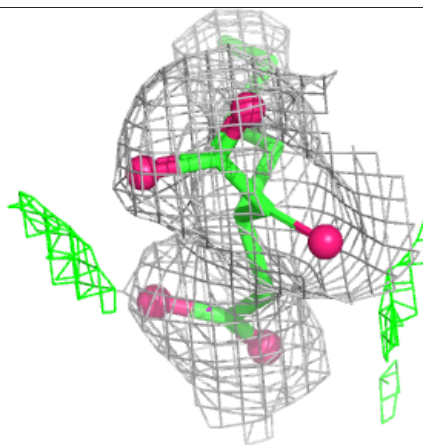
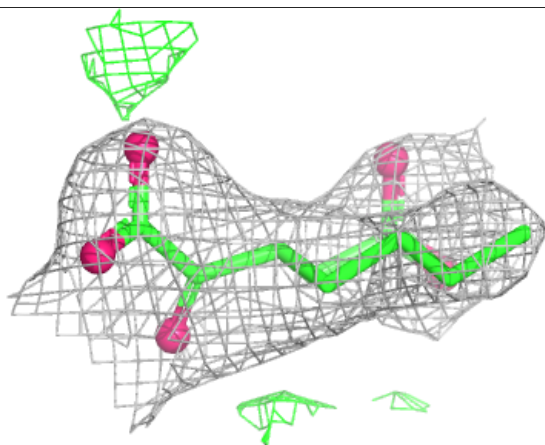
**Electron density around QDC C 604 (B):**

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



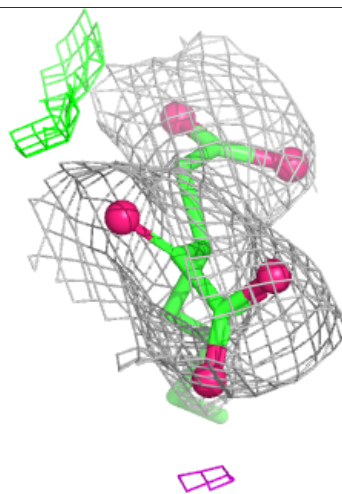
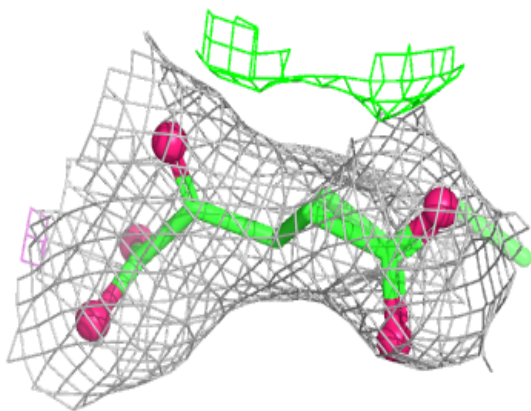
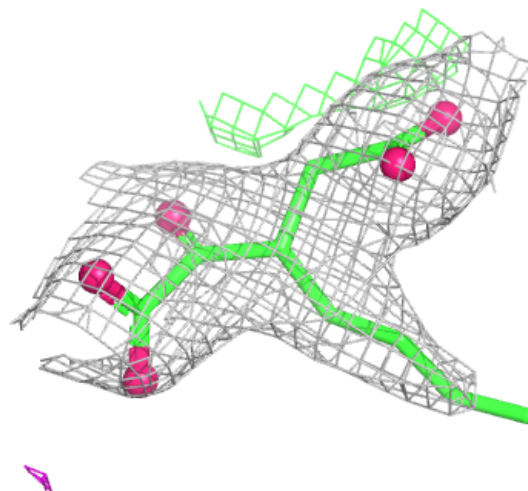
Electron density around QD8 C 605 (A):

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



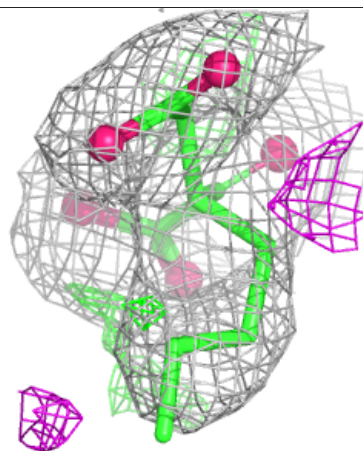
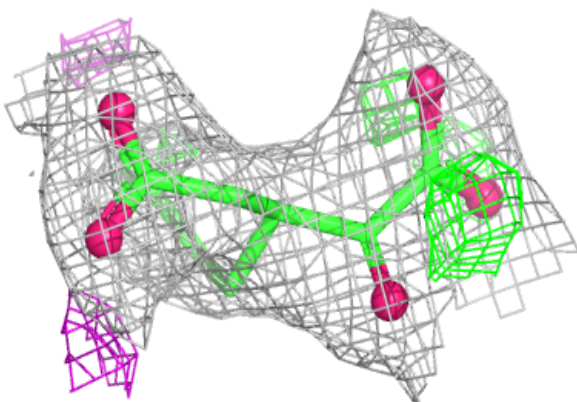
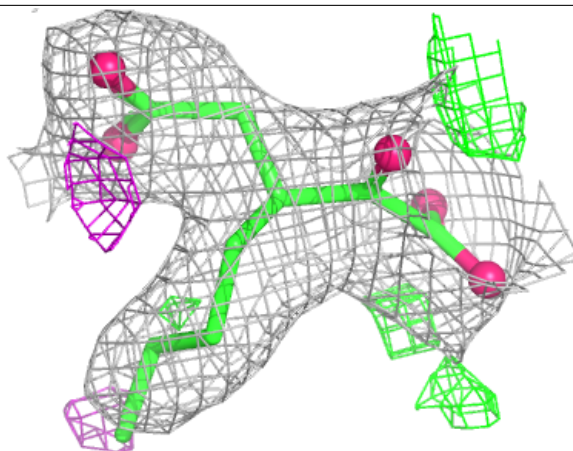
Electron density around QD8 B 804 (A):

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



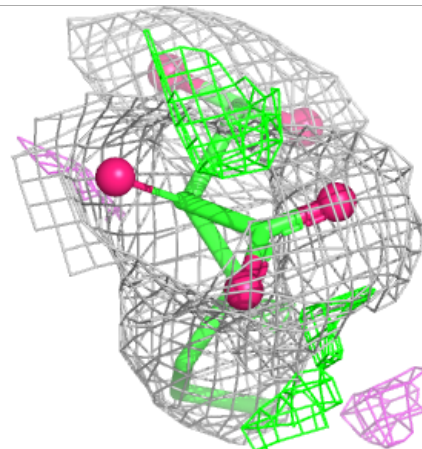
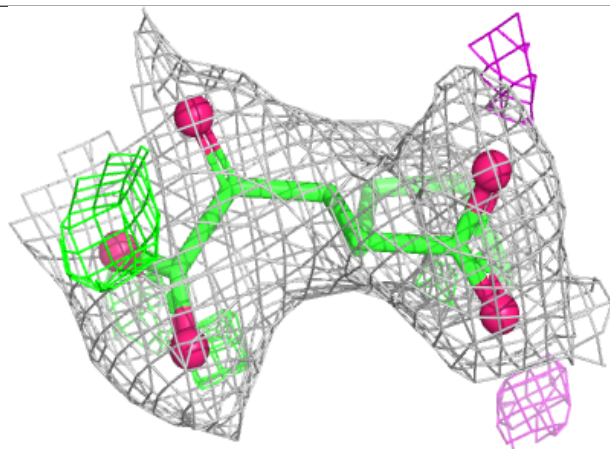
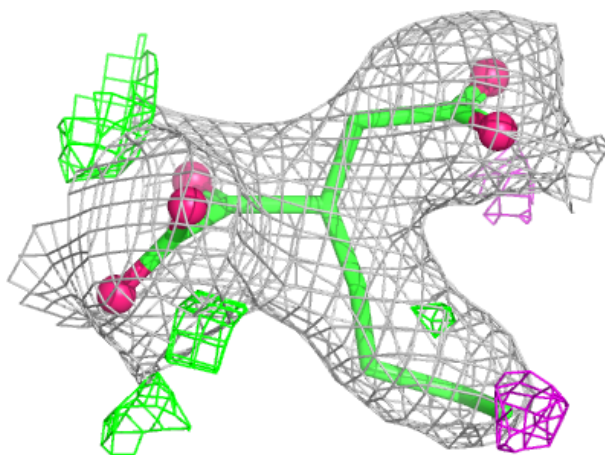
Electron density around QD8 A 705 (A):

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



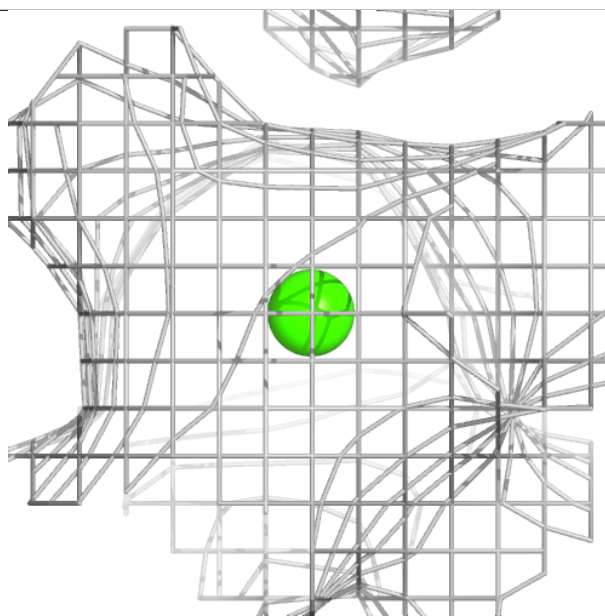
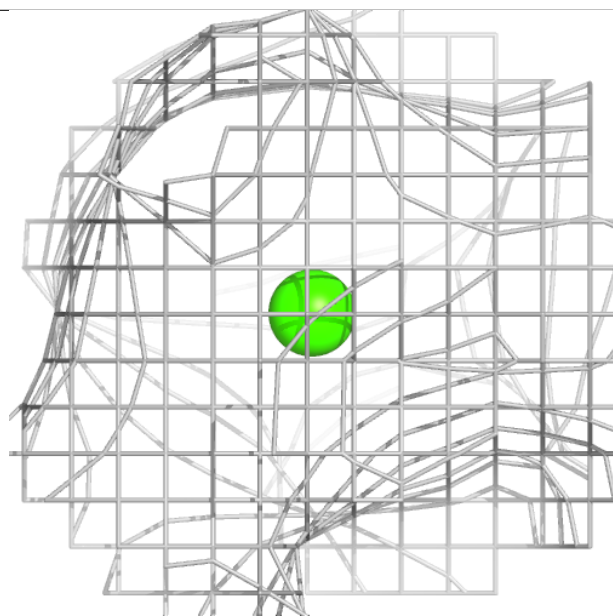
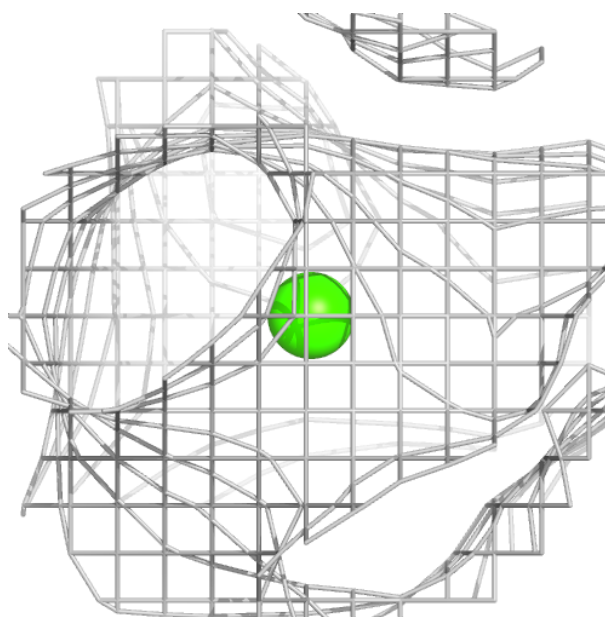
Electron density around QDC A 704 (B):

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



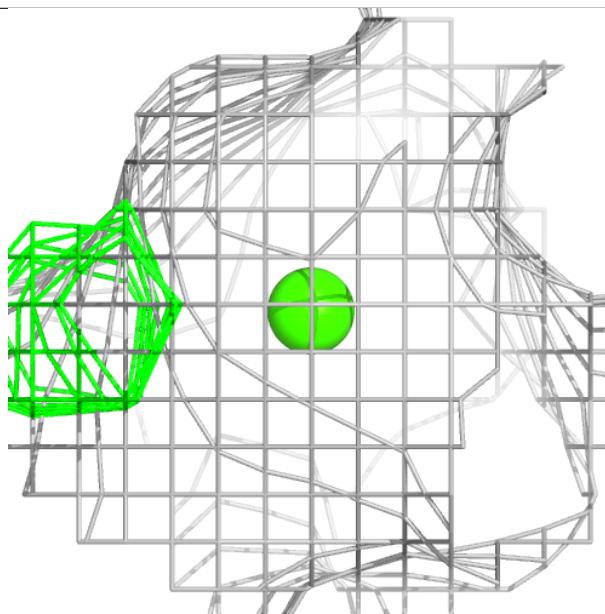
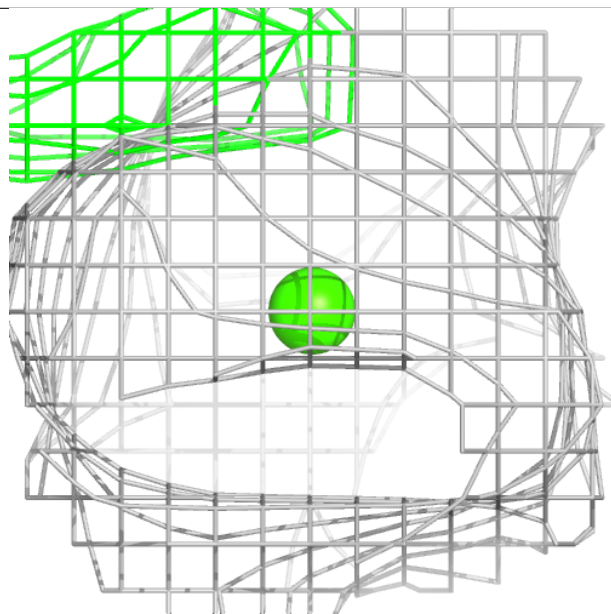
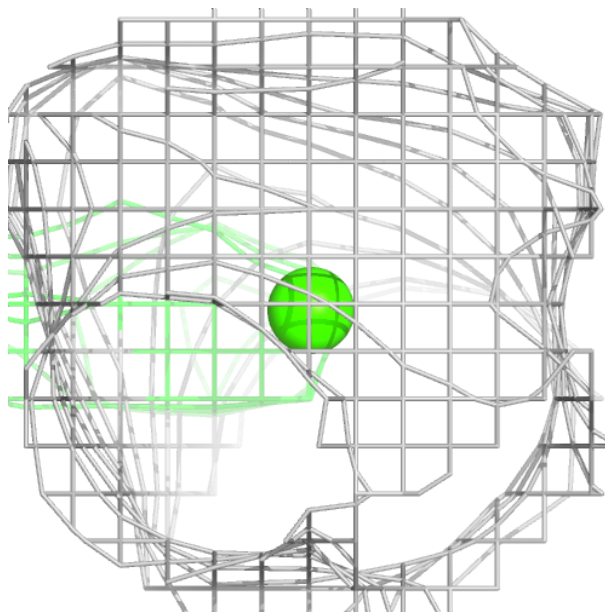
Electron density around CA A 706:

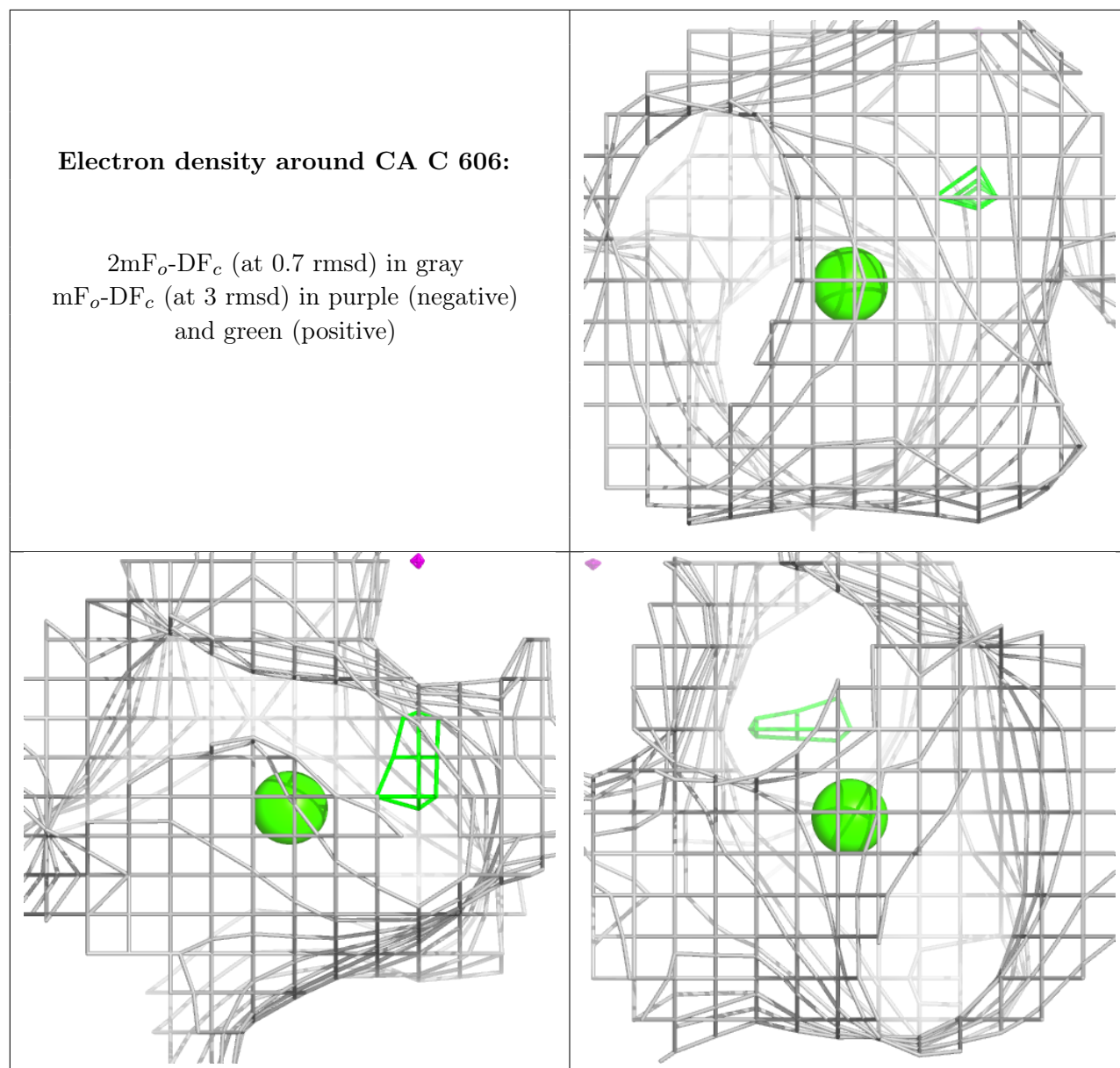
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA A 707:

$2mF_o-DF_c$ (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.