



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 04:06 PM EDT

PDB ID : 9NTN / pdb_00009ntn
Title : Structure of Cap10-CdnD complex containing NDG modification
Authors : Wassarman, D.R.; Pfaff, P.; Paulo, J.A.; Gygi, S.P.; Shokat, K.M.; Kranzusch, P.J.
Deposited on : 2025-03-18
Resolution : 2.43 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 : 2022.3.0, CSD as543be (2022)
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) : 2.43.1

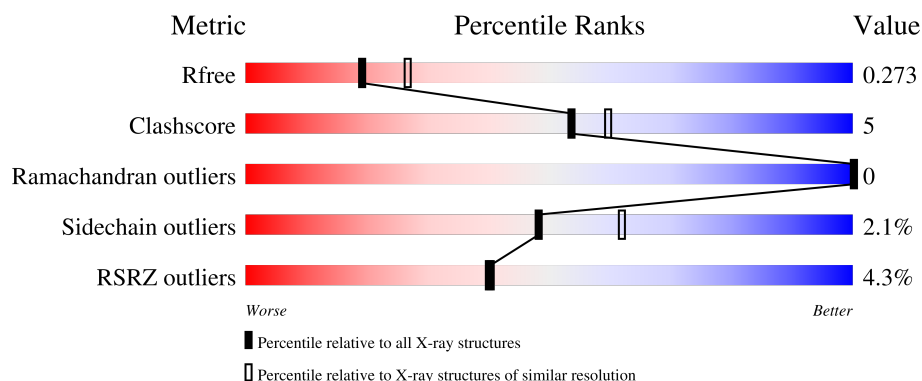
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	332	<div> <div>4%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>
1	B	332	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
2	G	320	<div> <div>2%</div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div>
2	H	320	<div> <div>7%</div> <div>75%</div> <div>15%</div> <div>10%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9942 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.

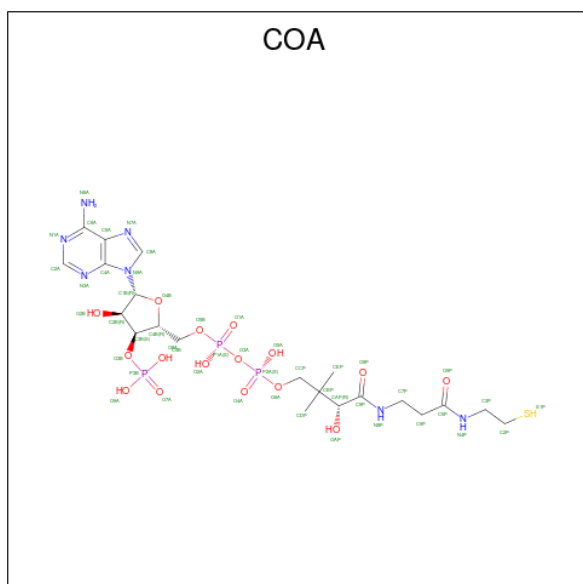
- Molecule 1 is a protein called Cap10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2583	1648	446	474	15			
1	B	325	Total	C	N	O	S	0	0	0
			2576	1643	443	476	14			

- Molecule 2 is a protein called CdnD.

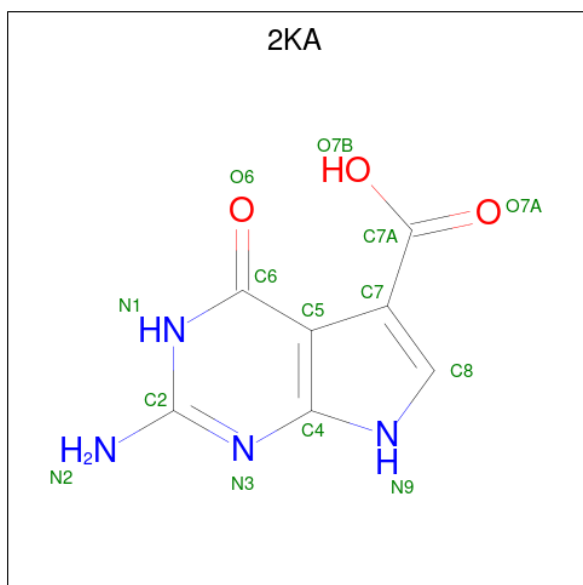
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	305	Total	C	N	O	S	0	0	0
			2302	1436	419	438	9			
2	H	288	Total	C	N	O	S	0	0	0
			2188	1370	398	411	9			

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	0
3	H	1	Total	C	N	O	P	S	
			48	21	7	16	3	1	0

- Molecule 4 is 2-amino-4-oxo-4,7-dihydro-3H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid (CCD ID: 2KA) (formula: C₇H₆N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O		
			13	7	4	2	0	0
4	H	1	Total	C	N	O		
			13	7	4	2	0	0

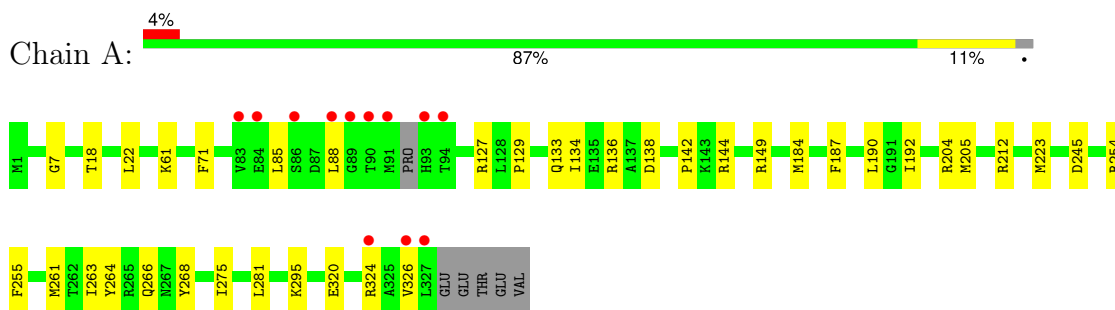
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O		
			62	62	0	0
5	B	61	Total	O		
			61	61	0	0
5	G	40	Total	O		
			40	40	0	0
5	H	8	Total	O		
			8	8	0	0

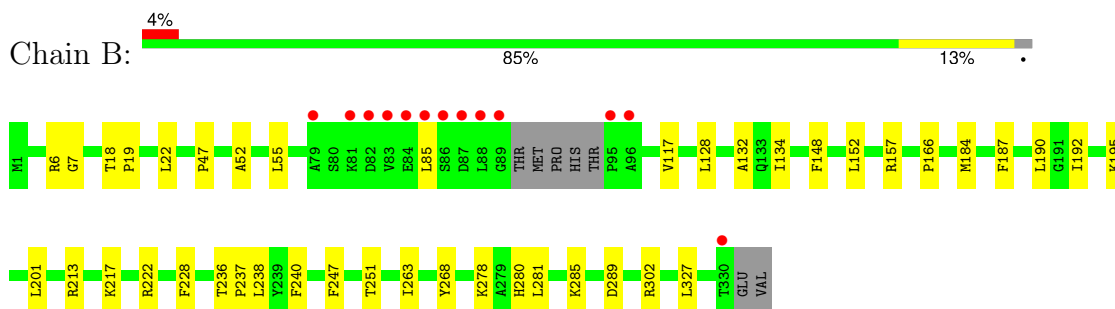
3 Residue-property plots

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.

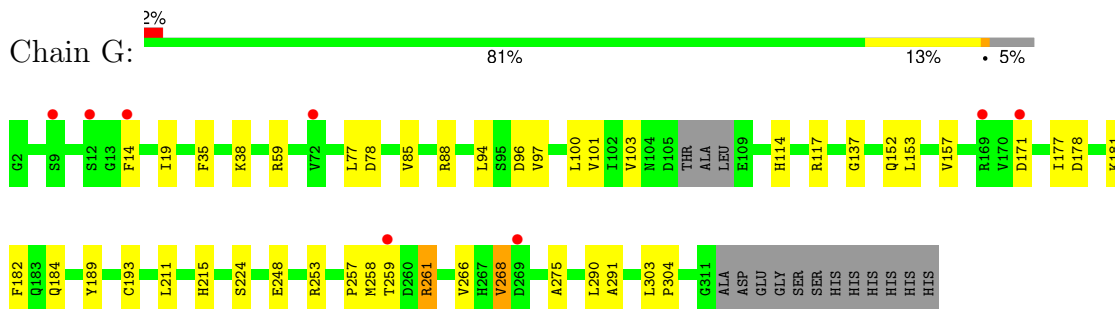
• Molecule 1: Cap10



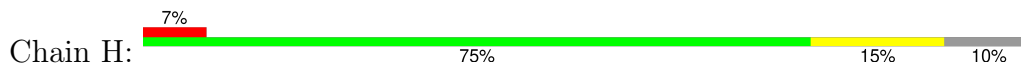
• Molecule 1: Cap10

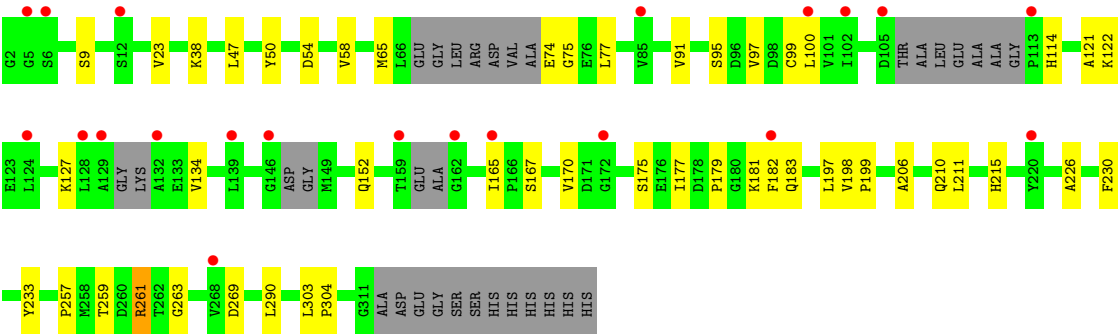


• Molecule 2: CdnD



• Molecule 2: CdnD





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.46Å 82.92Å 231.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.87 – 2.43 33.87 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.2 (33.87-2.43) 99.5 (33.87-2.43)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.235 , 0.278 0.232 , 0.273	Depositor DCC
R_{free} test set	2629 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9942	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 3.85% 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: COA, 2KA

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	0.10	0/2643	0.29	0/3573
1	B	0.15	0/2635	0.33	0/3561
2	G	0.10	0/2340	0.28	0/3156
2	H	0.13	0/2222	0.30	0/2991
All	All	0.12	0/9840	0.30	0/13281

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	2583	0	2568	18	0
1	B	2576	0	2558	25	0
2	G	2302	0	2292	26	0
2	H	2188	0	2185	27	0
3	G	48	0	31	1	0
3	H	48	0	31	4	0
4	G	13	0	5	0	0
4	H	13	0	5	0	0
5	A	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	61	0	0	0	0
5	G	40	0	0	0	0
5	H	8	0	0	0	0
All	All	9942	0	9675	93	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 (93) 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:PRO:HD2	1:B:302:ARG:HG2	1.65	0.76
2:H:257:PRO:HA	2:H:269:ASP:OD2	1.92	0.69
2:G:35:PHE:HA	2:G:38:LYS:HD3	1.81	0.62
2:G:101:VAL:HG21	2:G:153:LEU:HD23	1.82	0.61
1:A:138:ASP:HA	1:A:149:ARG:HH22	1.64	0.61
1:B:157:ARG:HH21	1:B:166:PRO:HG3	1.66	0.61
1:B:278:LYS:HD2	1:B:280:HIS:HE1	1.67	0.60
2:H:211:LEU:HD21	2:H:290:LEU:HD21	1.84	0.60
2:G:177:ILE:HG12	2:G:268:VAL:HG22	1.84	0.59
1:A:142:PRO:HB2	1:A:144:ARG:HG3	1.85	0.58
2:G:211:LEU:HD21	2:G:290:LEU:HD21	1.85	0.58
2:G:14:PHE:HB2	2:G:19:ILE:HD11	1.86	0.56
2:G:38:LYS:HB3	2:G:303:LEU:HD22	1.87	0.55
1:B:157:ARG:NH2	1:B:166:PRO:HG3	2.21	0.55
1:A:264:TYR:CZ	1:A:266:GLN:HB2	2.42	0.54
2:G:77:LEU:HD11	2:G:184:GLN:HG2	1.91	0.53
2:G:177:ILE:HD11	2:G:268:VAL:HG13	1.89	0.52
1:B:117:VAL:HG22	1:B:148:PHE:HB2	1.91	0.52
2:H:38:LYS:HB3	2:H:303:LEU:HD22	1.92	0.52
2:H:77:LEU:HD12	2:H:183:GLN:HB3	1.92	0.51
2:G:59:ARG:NH1	2:G:78:ASP:OD2	2.44	0.51
2:G:253:ARG:NH2	2:G:259:THR:HG22	2.26	0.51
1:B:201:LEU:HD21	1:B:238:LEU:HD13	1.93	0.51
2:H:181:LYS:HZ3	3:H:401:COA:H2B	1.76	0.50
1:B:128:LEU:HB3	1:B:132:ALA:HB3	1.93	0.50
1:A:263:ILE:HD11	1:A:268:TYR:HB2	1.94	0.50
1:A:205:MET:HE2	1:A:326:VAL:HG21	1.94	0.49
2:H:233:TYR:HB3	3:H:401:COA:H21	1.94	0.49
1:A:184:MET:HE2	1:A:190:LEU:HD12	1.93	0.49
2:H:165:ILE:HG12	2:H:179:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LYS:HD2	1:B:280:HIS:CE1	2.48	0.48
2:H:165:ILE:HD11	2:H:177:ILE:HD11	1.95	0.48
2:G:266:VAL:HG23	2:G:268:VAL:HG23	1.95	0.48
2:H:121:ALA:O	2:H:134:VAL:HG11	2.14	0.48
1:A:7:GLY:HA2	1:A:18:THR:HG23	1.96	0.47
1:B:85:LEU:HD23	1:B:195:LYS:HE2	1.95	0.47
1:A:320:GLU:O	1:A:324:ARG:HG2	2.14	0.47
2:H:65:MET:HA	2:H:127:LYS:HG2	1.96	0.47
1:B:19:PRO:HG3	1:B:240:PHE:CE1	2.49	0.47
1:B:7:GLY:HA2	1:B:18:THR:HG23	1.97	0.47
1:A:88:LEU:HD13	1:A:255:PHE:HZ	1.79	0.47
1:B:213:ARG:HH22	1:B:327:LEU:HA	1.80	0.47
2:H:74:GLU:HG2	2:H:75:GLY:H	1.80	0.46
2:H:99:CYS:SG	2:H:100:LEU:N	2.88	0.46
2:H:175:SER:OG	2:H:177:ILE:HG12	2.15	0.46
2:G:189:TYR:O	2:G:193:CYS:N	2.47	0.46
1:B:263:ILE:HD11	1:B:268:TYR:HB2	1.98	0.46
1:B:52:ALA:HA	1:B:55:LEU:HD12	1.96	0.46
1:B:134:ILE:HG23	1:B:187:PHE:HE2	1.81	0.46
1:A:275:ILE:HG22	1:B:201:LEU:HD23	1.97	0.46
1:A:281:LEU:HD23	2:G:19:ILE:HG23	1.97	0.46
2:G:117:ARG:NH1	2:G:137:GLY:O	2.49	0.45
2:H:181:LYS:NZ	3:H:401:COA:H2B	2.30	0.45
2:G:178:ASP:OD2	2:G:181:LYS:HG3	2.16	0.45
2:H:230:PHE:HB3	3:H:401:COA:S1P	2.56	0.45
2:H:261:ARG:HE	2:H:261:ARG:HB3	1.41	0.45
2:G:248:GLU:HG3	2:G:291:ALA:HB1	1.99	0.44
2:G:97:VAL:HA	2:G:152:GLN:HB2	2.00	0.44
2:H:95:SER:HB2	2:H:198:VAL:HG13	1.99	0.44
2:G:114:HIS:NE2	2:G:171:ASP:OD1	2.51	0.44
1:B:236:THR:HG23	1:B:247:PHE:CG	2.52	0.44
2:G:224:SER:OG	2:G:258:MET:HG2	2.17	0.44
2:H:54:ASP:O	2:H:58:VAL:HG23	2.18	0.44
1:B:285:LYS:HE3	1:B:289:ASP:OD2	2.17	0.44
2:G:253:ARG:HH21	2:G:259:THR:HG22	1.83	0.44
1:B:281:LEU:HD22	2:H:23:VAL:HG23	1.99	0.43
2:G:94:LEU:HD12	2:G:182:PHE:CD1	2.54	0.43
2:G:261:ARG:NH1	3:G:401:COA:O1A	2.52	0.43
1:A:134:ILE:HG23	1:A:187:PHE:HE2	1.84	0.43
1:A:22:LEU:HD21	1:A:71:PHE:CG	2.54	0.43
1:B:184:MET:HE2	1:B:190:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:LEU:HD11	2:H:226:ALA:HB1	2.01	0.43
2:H:47:LEU:HD22	2:H:199:PRO:HB3	2.00	0.42
2:H:206:ALA:O	2:H:210:GLN:HG2	2.19	0.42
2:G:88:ARG:HH22	2:G:96:ASP:CG	2.27	0.42
1:A:184:MET:HE3	1:A:223:MET:HE1	2.01	0.42
1:B:22:LEU:HD21	1:B:47:PRO:HB2	2.02	0.42
2:H:97:VAL:HA	2:H:152:GLN:HB2	2.01	0.42
2:G:257:PRO:HD3	2:G:275:ALA:HB2	2.01	0.42
2:G:303:LEU:N	2:G:304:PRO:HD2	2.35	0.41
2:H:50:TYR:CE2	2:H:199:PRO:HG3	2.55	0.41
2:H:259:THR:HB	2:H:263:GLY:O	2.20	0.41
1:B:6:ARG:HG2	1:B:222:ARG:HA	2.02	0.41
2:H:177:ILE:HD12	2:H:182:PHE:CD2	2.55	0.41
1:A:212:ARG:NH2	1:A:245:ASP:OD2	2.53	0.41
1:B:152:LEU:HD13	1:B:228:PHE:CD1	2.56	0.41
2:G:103:VAL:O	2:G:157:VAL:HA	2.21	0.41
1:A:85:LEU:HD11	1:A:204:ARG:CZ	2.51	0.41
1:B:217:LYS:HB3	1:B:217:LYS:HE3	1.79	0.41
2:H:303:LEU:N	2:H:304:PRO:HD2	2.35	0.41
1:A:129:PRO:O	1:A:133:GLN:HG3	2.21	0.40
1:A:295:LYS:HD3	1:A:295:LYS:HA	1.83	0.40
1:B:236:THR:HB	1:B:237:PRO:HD3	2.04	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	322/332 (97%)	313 (97%)	9 (3%)	0	100	100
1	B	321/332 (97%)	312 (97%)	9 (3%)	0	100	100
2	G	301/320 (94%)	293 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	276/320 (86%)	265 (96%)	11 (4%)	0	100	100
All	All	1220/1304 (94%)	1183 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	275/281 (98%)	269 (98%)	6 (2%)	47	60
1	B	274/281 (98%)	272 (99%)	2 (1%)	81	89
2	G	233/245 (95%)	228 (98%)	5 (2%)	48	62
2	H	224/245 (91%)	216 (96%)	8 (4%)	30	41
All	All	1006/1052 (96%)	985 (98%)	21 (2%)	48	62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	127	ARG
1	A	136	ARG
1	A	192	ILE
1	A	254	ARG
1	A	261	MET
1	B	192	ILE
1	B	251	THR
2	G	85	VAL
2	G	100	LEU
2	G	215	HIS
2	G	261	ARG
2	G	268	VAL
2	H	9	SER
2	H	91	VAL
2	H	114	HIS

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Mol	Chain	Res	Type
2	H	122	LYS
2	H	167	SER
2	H	170	VAL
2	H	215	HIS
2	H	261	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	314	HIS
2	G	232	ASN
2	G	276	HIS
2	G	305	GLN
2	H	52	ASN
2	H	276	HIS

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2KA	G	402	2	12,14,15	3.05	8 (66%)	10,20,22	2.10	3 (30%)
3	COA	G	401	2	43,50,50	0.66	1 (2%)	56,75,75	1.04	3 (5%)
3	COA	H	401	2	43,50,50	0.60	0	56,75,75	1.16	3 (5%)
4	2KA	H	402	2	12,14,15	3.05	8 (66%)	10,20,22	2.09	2 (20%)

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	2KA	G	402	2	-	0/1/2/4	0/2/2/2
3	COA	G	401	2	-	11/44/64/64	0/3/3/3
3	COA	H	401	2	-	18/44/64/64	0/3/3/3
4	2KA	H	402	2	-	0/1/2/4	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	402	2KA	C2-N3	5.47	1.46	1.33
4	H	402	2KA	C2-N3	5.44	1.46	1.33
4	G	402	2KA	C2-N2	4.89	1.45	1.34
4	H	402	2KA	C2-N2	4.88	1.45	1.34
4	G	402	2KA	C6-N1	3.77	1.43	1.37
4	H	402	2KA	C6-N1	3.76	1.43	1.37
4	G	402	2KA	C5-C6	3.21	1.53	1.47
4	H	402	2KA	C5-C6	3.19	1.53	1.47
4	H	402	2KA	C2-N1	2.96	1.44	1.37
4	G	402	2KA	C2-N1	2.92	1.44	1.37
4	G	402	2KA	C7-C7A	2.78	1.53	1.47
4	H	402	2KA	C7-C7A	2.78	1.53	1.47
4	H	402	2KA	C5-C4	-2.58	1.38	1.42
4	G	402	2KA	C5-C4	-2.56	1.38	1.42
4	H	402	2KA	C4-N3	2.33	1.49	1.38
4	G	402	2KA	C4-N3	2.33	1.49	1.38
3	G	401	COA	C1B-N9A	-2.07	1.44	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	COA	P3B-O3B-C3B	-6.65	105.69	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	COA	P3B-O3B-C3B	-5.71	108.17	123.43
4	H	402	2KA	C5-C6-N1	4.56	120.15	115.05
4	G	402	2KA	C5-C6-N1	4.51	120.09	115.05
4	H	402	2KA	C2-N1-C6	-2.88	119.83	125.11
4	G	402	2KA	C2-N1-C6	-2.82	119.95	125.11
3	H	401	COA	C5A-C6A-N6A	2.37	123.93	120.31
3	G	401	COA	C5A-C6A-N6A	2.34	123.88	120.31
3	H	401	COA	O6A-CCP-CBP	-2.09	107.19	110.55
4	G	402	2KA	O7A-C7A-C7	-2.08	119.17	124.41
3	G	401	COA	C3B-C2B-C1B	2.05	104.40	99.89

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	401	COA	CDP-CBP-CCP-O6A
3	G	401	COA	CEP-CBP-CCP-O6A
3	G	401	COA	CAP-CBP-CCP-O6A
3	G	401	COA	CAP-C9P-N8P-C7P
3	G	401	COA	C6P-C5P-N4P-C3P
3	G	401	COA	O5P-C5P-N4P-C3P
3	H	401	COA	CCP-O6A-P2A-O3A
3	H	401	COA	CCP-O6A-P2A-O4A
3	H	401	COA	CCP-O6A-P2A-O5A
3	H	401	COA	OAP-CAP-CBP-CCP
3	H	401	COA	C9P-CAP-CBP-CCP
3	H	401	COA	OAP-CAP-CBP-CDP
3	H	401	COA	C9P-CAP-CBP-CDP
3	H	401	COA	OAP-CAP-CBP-CEP
3	H	401	COA	C9P-CAP-CBP-CEP
3	H	401	COA	CAP-C9P-N8P-C7P
3	H	401	COA	O9P-C9P-N8P-C7P
3	H	401	COA	C6P-C5P-N4P-C3P
3	H	401	COA	O5P-C5P-N4P-C3P
3	G	401	COA	O9P-C9P-N8P-C7P
3	H	401	COA	O4B-C4B-C5B-O5B
3	H	401	COA	C5P-C6P-C7P-N8P
3	H	401	COA	C3B-C4B-C5B-O5B
3	G	401	COA	CBP-CCP-O6A-P2A
3	G	401	COA	C3B-O3B-P3B-O8A
3	H	401	COA	C3B-O3B-P3B-O7A
3	H	401	COA	N8P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
3	G	401	COA	S1P-C2P-C3P-N4P
3	G	401	COA	P2A-O3A-P1A-O2A

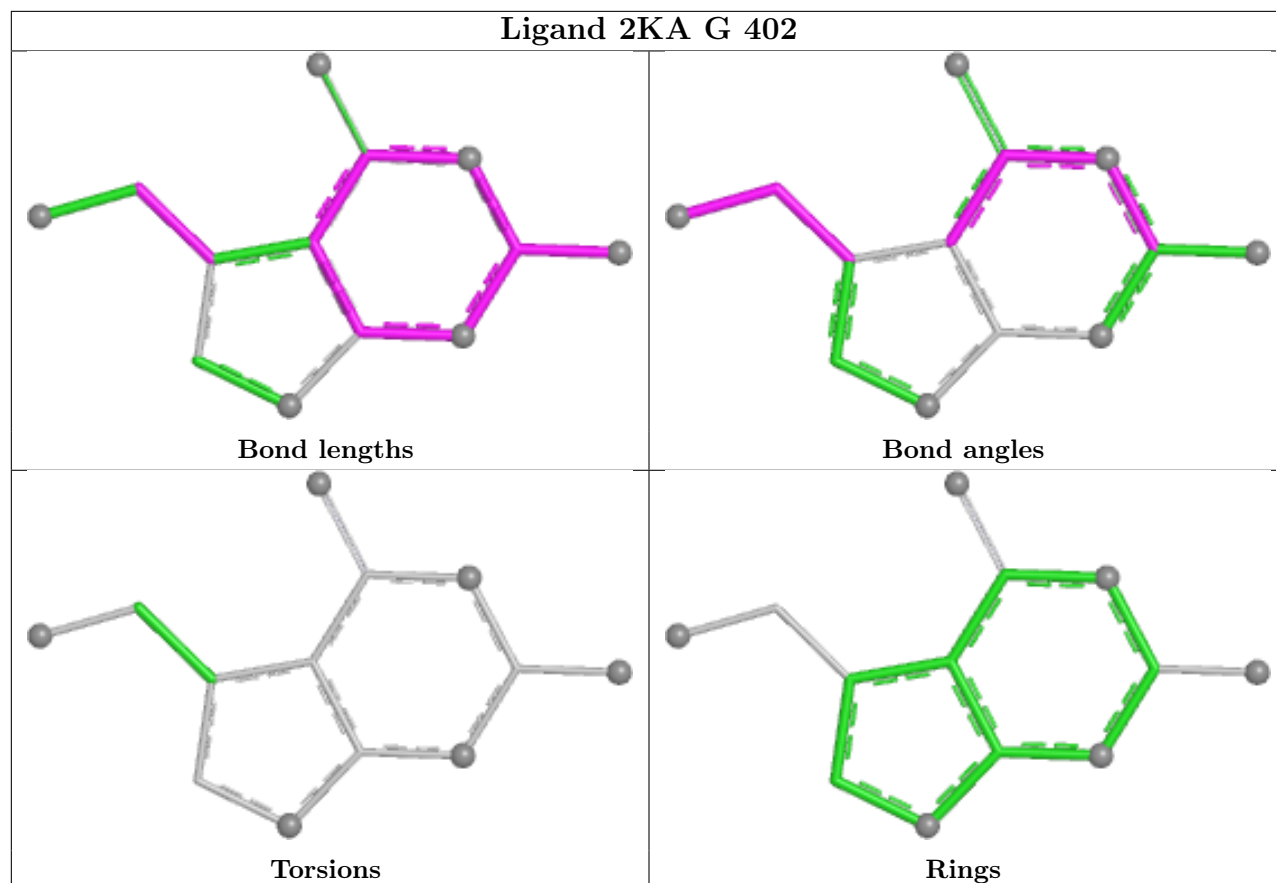
There are no ring outliers.

2 monomers are involved in 5 short contacts:

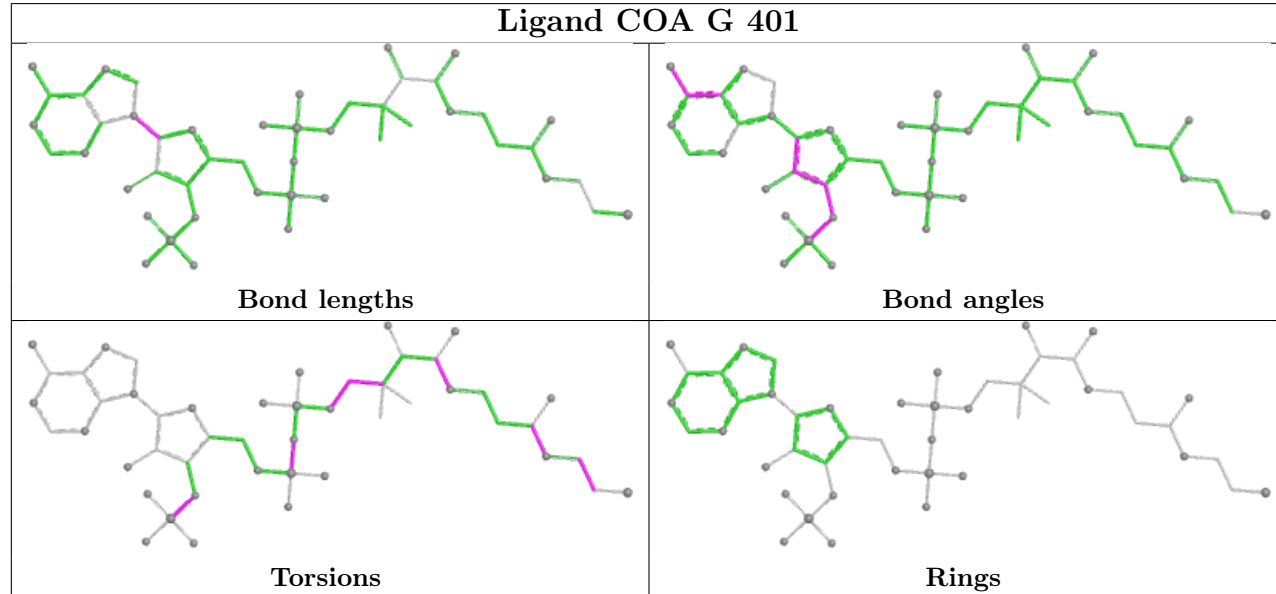
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	COA	1	0
3	H	401	COA	4	0

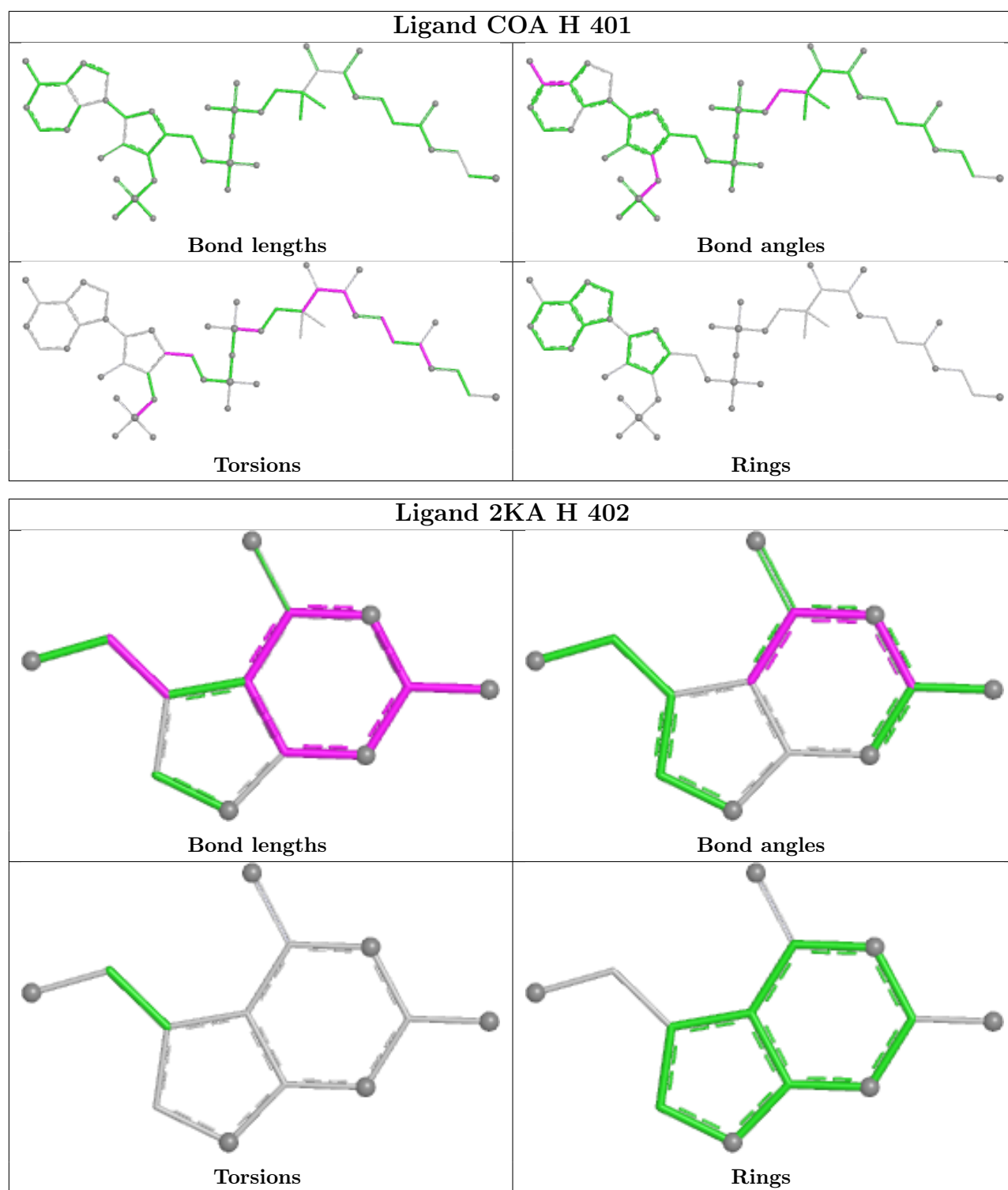
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 2KA G 402



Ligand COA G 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	326/332 (98%)	-0.02	12 (3%) 45 45	35, 52, 76, 94	0
1	B	325/332 (97%)	0.07	13 (4%) 43 43	38, 58, 82, 111	0
2	G	305/320 (95%)	0.22	8 (2%) 57 58	38, 64, 92, 138	0
2	H	288/320 (90%)	0.73	21 (7%) 22 23	49, 90, 141, 162	0
All	All	1244/1304 (95%)	0.24	54 (4%) 40 40	35, 62, 116, 162	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	5.6
1	B	86	SER	5.1
1	B	88	LEU	4.8
2	H	124	LEU	4.3
1	A	326	VAL	3.8
1	B	84	GLU	3.5
1	B	83	VAL	3.5
2	H	146	GLY	3.4
1	A	93	HIS	3.4
2	H	159	THR	3.3
1	A	84	GLU	3.1
1	B	96	ALA	3.1
1	A	91	MET	3.1
1	B	85	LEU	3.0
1	B	87	ASP	3.0
2	H	128	LEU	2.7
2	H	172	GLY	2.7
2	H	12	SER	2.7
2	H	132	ALA	2.7
1	A	94	THR	2.6
1	B	79	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	83	VAL	2.6
2	H	139	LEU	2.5
2	H	129	ALA	2.5
1	A	90	THR	2.5
2	H	182	PHE	2.5
1	B	95	PRO	2.5
1	A	89	GLY	2.5
2	H	113	PRO	2.5
2	H	6	SER	2.4
1	A	327	LEU	2.4
2	H	268	VAL	2.4
2	H	100	LEU	2.3
2	H	105	ASP	2.3
2	H	102	ILE	2.3
1	B	82	ASP	2.3
2	H	220	TYR	2.3
2	G	169	ARG	2.3
2	G	171	ASP	2.2
1	B	330	THR	2.2
2	H	85	VAL	2.2
1	B	81	LYS	2.2
2	H	5	GLY	2.2
1	B	89	GLY	2.1
2	G	14	PHE	2.1
2	H	165	ILE	2.1
2	G	259	THR	2.1
2	G	72	VAL	2.1
2	G	9	SER	2.1
2	G	269	ASP	2.0
2	H	162	GLY	2.0
1	A	86	SER	2.0
2	G	12	SER	2.0
1	A	324	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

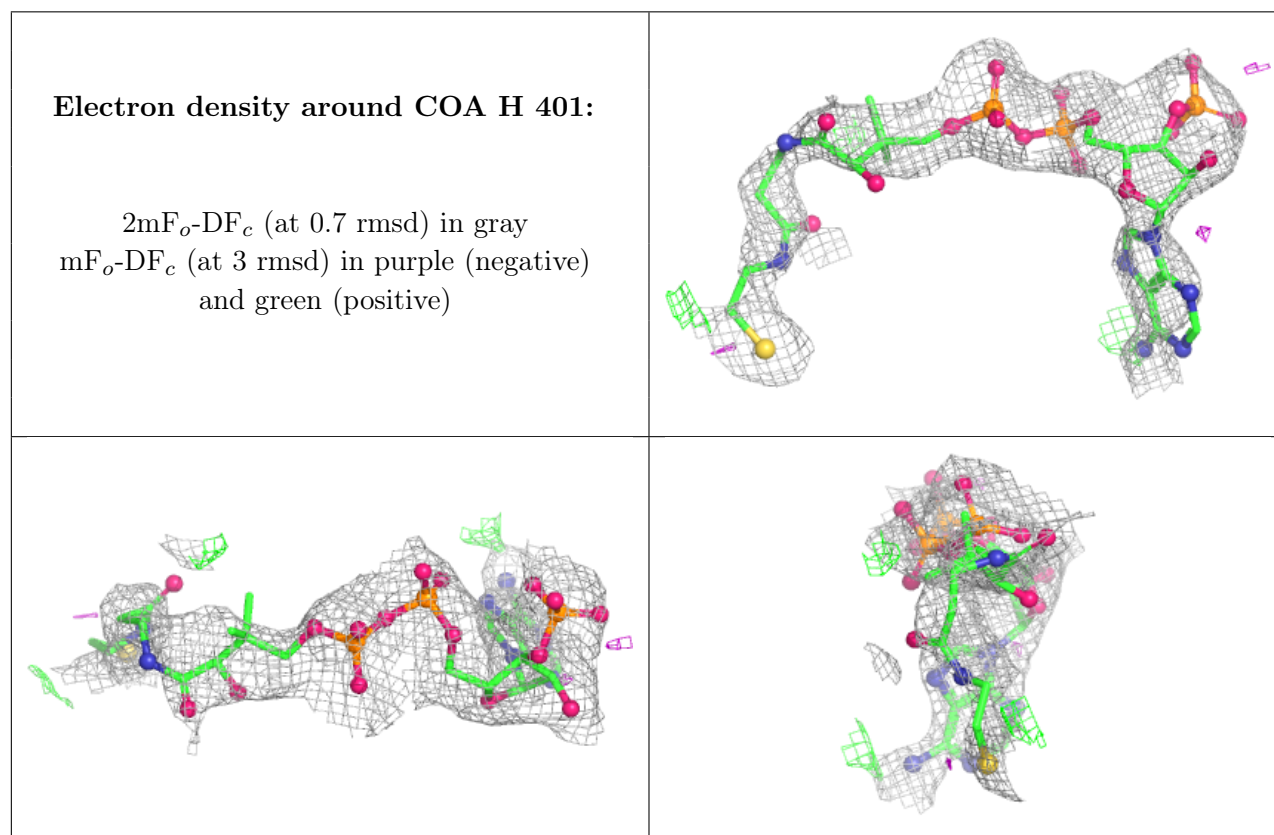
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

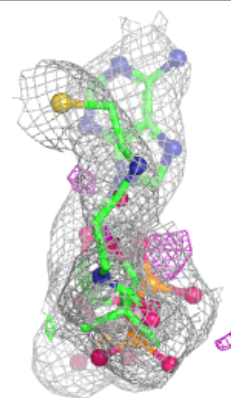
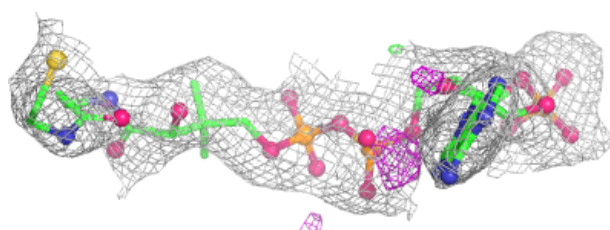
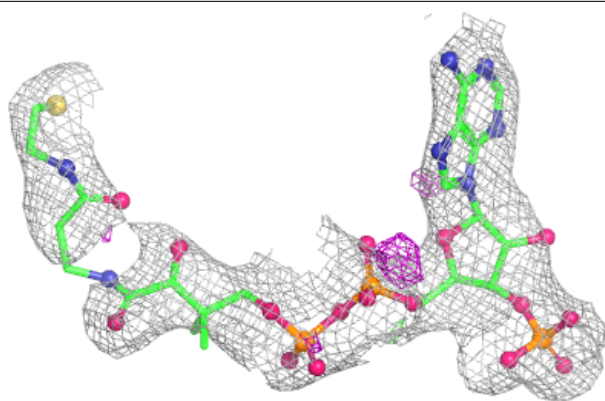
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	H	401	48/48	0.61	0.15	100,122,149,157	0
3	COA	G	401	48/48	0.75	0.12	59,97,118,145	0
4	2KA	G	402	13/14	0.88	0.13	55,61,68,69	0
4	2KA	H	402	13/14	0.90	0.13	44,51,60,62	0

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.

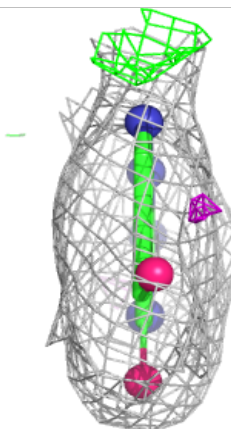
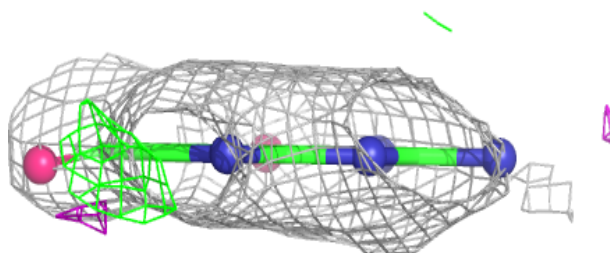
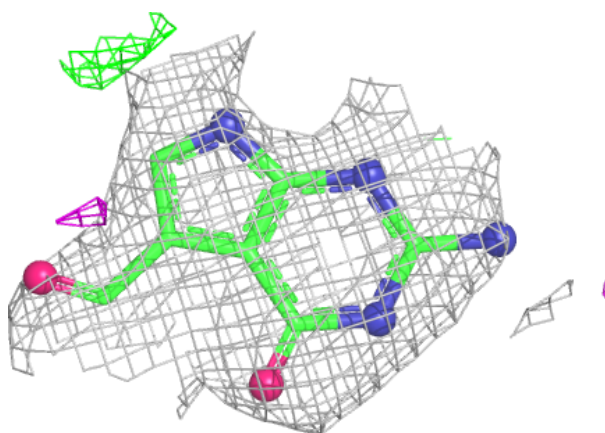


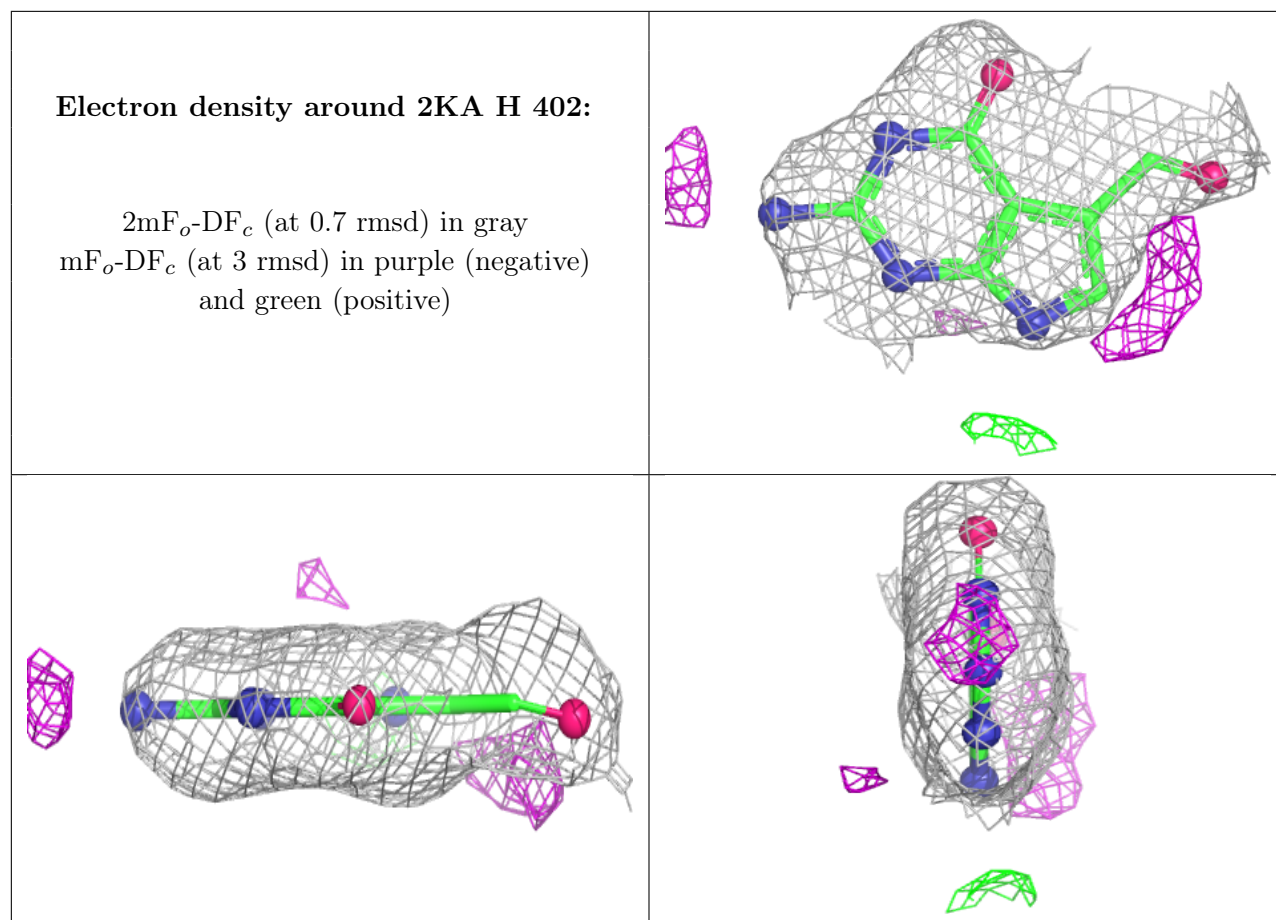
Electron density around COA G 401:

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

**Electron density around 2KA G 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.