



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 08:14 AM EST

PDB ID : 8W0L
Title : Crystal structure of Acetyl-CoA synthetase 2 from *Candida albicans* in complex with a propyne AMP ester inhibitor and CoA
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-02-13
Resolution : 2.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

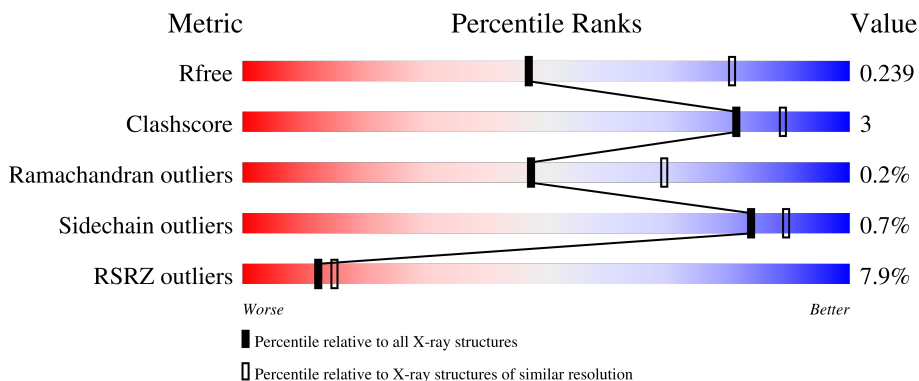
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	686	 2% 90% 7%
1	B	686	 11% 81% 6% 12%
1	C	686	 8% 79% 6% 15%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COA	C	702	-	-	-	X
6	SO4	A	714	-	-	-	X
6	SO4	B	706	-	-	-	X
6	SO4	C	703	-	-	-	X
6	SO4	C	704	-	-	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 14724 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 Acetyl-coenzyme A synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	Total 5153	C 3286	N 876	O 977	S 14	0	0	0
1	B	604	Total 4695	C 3004	N 796	O 882	S 13	0	0	0
1	C	582	Total 4527	C 2897	N 762	O 855	S 13	0	0	0

There are 51 discrepancies between the modelled and reference sequences:

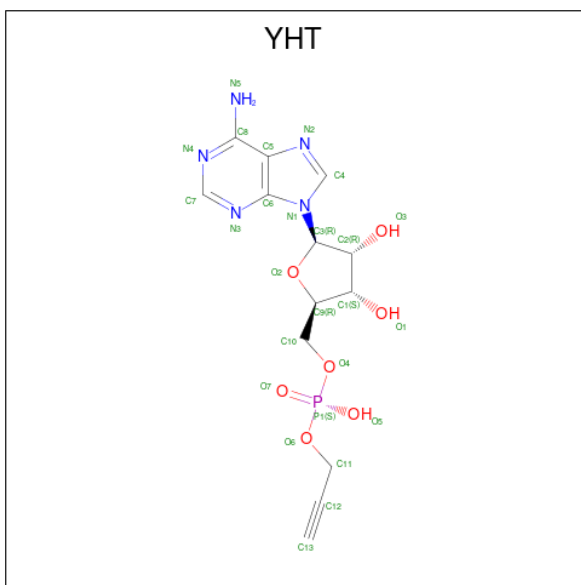
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8N3JN3
A	2	HIS	-	expression tag	UNP Q8N3JN3
A	3	HIS	-	expression tag	UNP Q8N3JN3
A	4	HIS	-	expression tag	UNP Q8N3JN3
A	5	HIS	-	expression tag	UNP Q8N3JN3
A	6	HIS	-	expression tag	UNP Q8N3JN3
A	7	HIS	-	expression tag	UNP Q8N3JN3
A	8	HIS	-	expression tag	UNP Q8N3JN3
A	9	HIS	-	expression tag	UNP Q8N3JN3
A	10	GLU	-	expression tag	UNP Q8N3JN3
A	11	ASN	-	expression tag	UNP Q8N3JN3
A	12	LEU	-	expression tag	UNP Q8N3JN3
A	13	TYR	-	expression tag	UNP Q8N3JN3
A	14	PHE	-	expression tag	UNP Q8N3JN3
A	15	GLN	-	expression tag	UNP Q8N3JN3
A	16	GLY	-	expression tag	UNP Q8N3JN3
A	403	ALA	VAL	engineered mutation	UNP Q8N3JN3
B	1	MET	-	initiating methionine	UNP Q8N3JN3
B	2	HIS	-	expression tag	UNP Q8N3JN3
B	3	HIS	-	expression tag	UNP Q8N3JN3
B	4	HIS	-	expression tag	UNP Q8N3JN3
B	5	HIS	-	expression tag	UNP Q8N3JN3
B	6	HIS	-	expression tag	UNP Q8N3JN3

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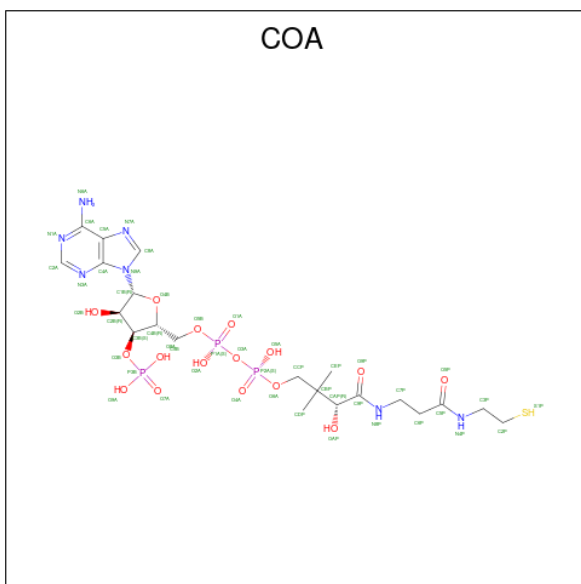
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8N3N3
B	8	HIS	-	expression tag	UNP Q8N3N3
B	9	HIS	-	expression tag	UNP Q8N3N3
B	10	GLU	-	expression tag	UNP Q8N3N3
B	11	ASN	-	expression tag	UNP Q8N3N3
B	12	LEU	-	expression tag	UNP Q8N3N3
B	13	TYR	-	expression tag	UNP Q8N3N3
B	14	PHE	-	expression tag	UNP Q8N3N3
B	15	GLN	-	expression tag	UNP Q8N3N3
B	16	GLY	-	expression tag	UNP Q8N3N3
B	403	ALA	VAL	engineered mutation	UNP Q8N3N3
C	1	MET	-	initiating methionine	UNP Q8N3N3
C	2	HIS	-	expression tag	UNP Q8N3N3
C	3	HIS	-	expression tag	UNP Q8N3N3
C	4	HIS	-	expression tag	UNP Q8N3N3
C	5	HIS	-	expression tag	UNP Q8N3N3
C	6	HIS	-	expression tag	UNP Q8N3N3
C	7	HIS	-	expression tag	UNP Q8N3N3
C	8	HIS	-	expression tag	UNP Q8N3N3
C	9	HIS	-	expression tag	UNP Q8N3N3
C	10	GLU	-	expression tag	UNP Q8N3N3
C	11	ASN	-	expression tag	UNP Q8N3N3
C	12	LEU	-	expression tag	UNP Q8N3N3
C	13	TYR	-	expression tag	UNP Q8N3N3
C	14	PHE	-	expression tag	UNP Q8N3N3
C	15	GLN	-	expression tag	UNP Q8N3N3
C	16	GLY	-	expression tag	UNP Q8N3N3
C	403	ALA	VAL	engineered mutation	UNP Q8N3N3

- Molecule 2 is 5'-O-{(S)-hydroxy[(prop-2-yn-1-yl)oxy]phosphoryl}adenosine (three-letter code: YHT) (formula: C₁₃H₁₆N₅O₇P) (labeled as "Ligand of Interest" by depositor).



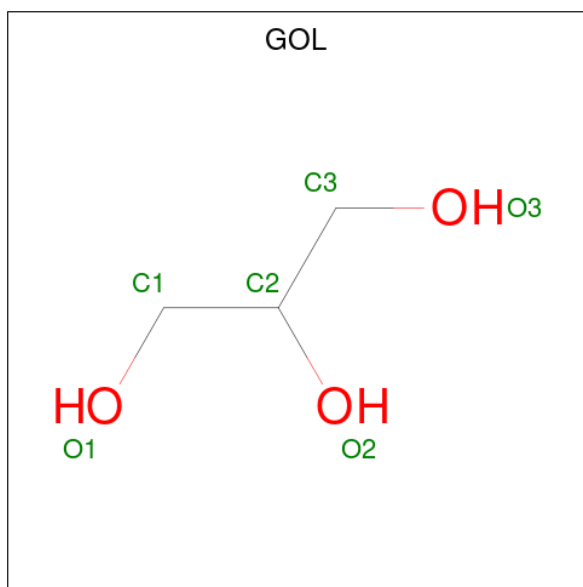
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P		0	0
			31	10	5	13	3			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



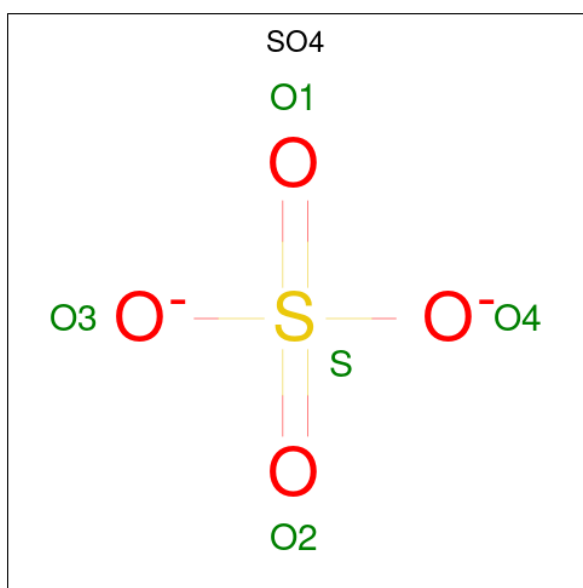
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			6	3 3		
4	A	1	Total	C O	0	0
			6	3 3		
4	A	1	Total	C O	0	0
			6	3 3		
4	B	1	Total	C O	0	0
			6	3 3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Cl	0	0
			2	2		

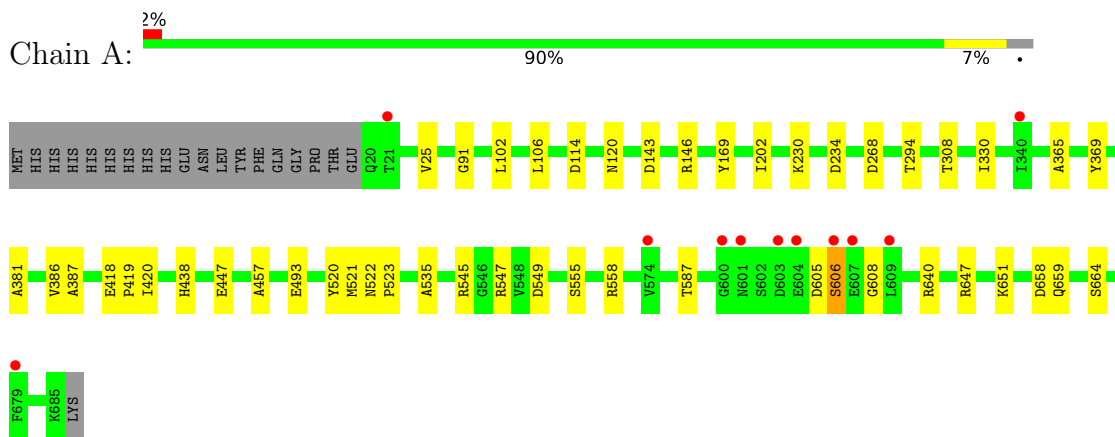
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	39	Total	O	0	0
			39	39		
8	B	27	Total	O	0	0
			27	27		

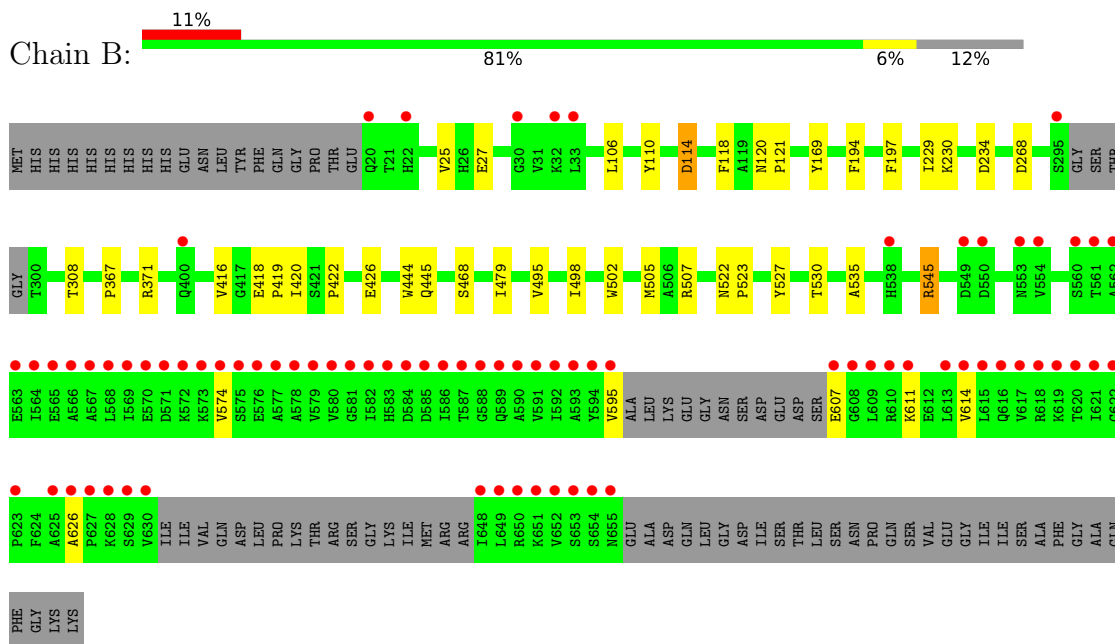
3 Residue-property plots i

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: Acetyl-coenzyme A synthetase 2

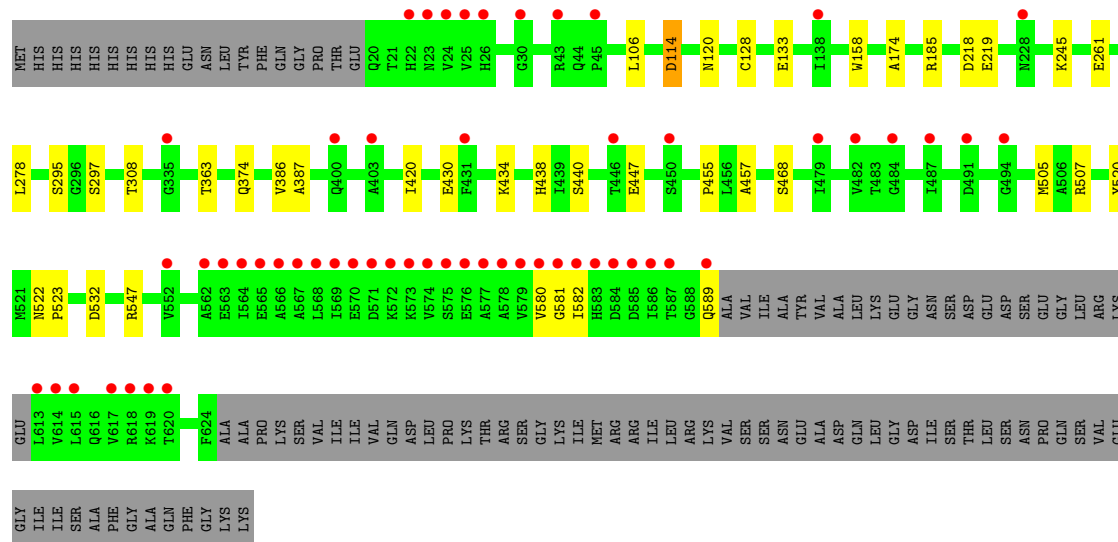


- Molecule 1: Acetyl-coenzyme A synthetase 2



- Molecule 1: Acetyl-coenzyme A synthetase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.18Å 139.18Å 543.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.62 – 2.75 48.62 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.62-2.75) 100.0 (48.62-2.75)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (dev_5233: ???)	Depositor
R, R_{free}	0.203 , 0.239 0.205 , 0.239	Depositor DCC
R_{free} test set	4109 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtrriage
Anisotropy	0.622	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14724	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: CL, PGE, GOL, YHT, COA, SO4

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	0.45	0/5283	0.58	0/7186
1	B	0.40	0/4818	0.55	0/6557
1	C	0.34	0/4650	0.52	0/6333
All	All	0.40	0/14751	0.55	0/20076

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	5153	0	5027	28	0
1	B	4695	0	4560	29	0
1	C	4527	0	4383	19	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
3	A	48	0	32	0	0
3	C	31	0	11	0	0
4	A	18	0	24	2	0
4	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	10	0	14	0	0
5	B	10	0	14	0	0
6	A	40	0	0	0	0
6	B	25	0	0	0	0
6	C	15	0	0	0	0
7	B	2	0	0	0	0
8	A	39	0	0	0	0
8	B	27	0	0	0	0
All	All	14724	0	14073	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 3.

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:479:ILE:O	1:B:495:VAL:HG22	1.82	0.79
1:B:574:VAL:HG13	1:B:595:VAL:HG23	1.76	0.67
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.78	0.66
1:A:106:LEU:HD11	1:A:308:THR:HG22	1.76	0.66
1:C:114:ASP:OD1	1:C:185:ARG:NH2	2.29	0.65
1:A:91:GLY:H	4:A:704:GOL:H2	1.62	0.64
1:B:479:ILE:HB	1:B:495:VAL:CG2	2.27	0.64
1:B:479:ILE:HB	1:B:495:VAL:HG23	1.79	0.64
1:A:493:GLU:OE1	1:A:545:ARG:NH1	2.32	0.63
1:C:106:LEU:HD11	1:C:308:THR:HG22	1.80	0.62
1:C:185:ARG:NH1	1:C:278:LEU:O	2.37	0.58
1:A:268:ASP:OD1	1:A:268:ASP:N	2.36	0.57
1:B:498:ILE:HD12	1:B:502:TRP:CH2	2.40	0.56
1:A:658:ASP:O	1:A:659:GLN:HB2	2.06	0.56
1:B:106:LEU:C	1:B:106:LEU:HD12	2.27	0.55
1:A:386:VAL:HG22	1:A:387:ALA:N	2.22	0.55
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.44	0.52
1:A:106:LEU:HD12	1:A:106:LEU:C	2.29	0.52
1:A:547:ARG:NH2	1:A:549:ASP:OD2	2.40	0.52
1:B:110:TYR:CD1	1:B:114:ASP:HB2	2.45	0.51
1:B:420:ILE:O	1:B:420:ILE:HG23	2.11	0.50
1:B:479:ILE:HD11	1:B:527:TYR:CD2	2.47	0.50
1:B:445:GLN:NE2	1:B:530:THR:O	2.42	0.50
1:B:106:LEU:HD11	1:B:308:THR:HG22	1.94	0.49
1:C:580:VAL:HG22	1:C:581:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ARG:NH2	1:A:664:SER:O	2.46	0.48
1:A:365:ALA:HB2	1:A:369:TYR:CE1	2.49	0.47
1:A:605:ASP:O	1:A:608:GLY:N	2.47	0.47
1:B:614:VAL:HG13	1:B:626:ALA:HB1	1.95	0.47
4:A:704:GOL:H12	1:B:121:PRO:HB3	1.97	0.47
1:C:218:ASP:OD1	1:C:219:GLU:N	2.46	0.47
1:A:447:GLU:HG2	1:A:520:TYR:CZ	2.50	0.47
1:C:420:ILE:O	1:C:420:ILE:HG23	2.15	0.47
1:B:574:VAL:HG13	1:B:595:VAL:CG2	2.42	0.47
1:B:422:PRO:O	1:B:426:GLU:HG2	2.14	0.46
1:A:330:ILE:HB	1:A:381:ALA:HA	1.97	0.46
1:A:106:LEU:HD11	1:A:308:THR:CG2	2.45	0.46
1:B:230:LYS:HE2	1:B:234:ASP:OD1	2.16	0.45
1:C:505:MET:O	1:C:507:ARG:NH1	2.49	0.45
1:A:605:ASP:O	1:A:606:SER:C	2.55	0.45
1:B:367:PRO:HD2	1:B:371:ARG:HD3	1.98	0.45
1:B:522:ASN:N	1:B:523:PRO:CD	2.80	0.45
1:B:607:GLU:O	1:B:611:LYS:HG2	2.17	0.45
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.50	0.44
1:C:158:TRP:CG	1:C:245:LYS:HD2	2.53	0.44
1:B:169:TYR:CE2	1:B:229:ILE:HG23	2.52	0.44
1:B:268:ASP:N	1:B:268:ASP:OD1	2.49	0.44
1:C:438:HIS:CD2	1:C:457:ALA:HA	2.53	0.44
1:A:522:ASN:N	1:A:523:PRO:CD	2.80	0.44
1:A:25:VAL:HG22	1:A:535:ALA:HB1	2.00	0.43
1:A:647:ARG:O	1:A:651:LYS:HG2	2.18	0.43
1:A:294:THR:HG21	1:A:558:ARG:CZ	2.48	0.43
1:A:555:SER:OG	1:A:587:THR:HG22	2.18	0.43
1:B:194:PHE:HB3	1:B:197:PHE:CD2	2.53	0.43
1:C:430:GLU:O	1:C:434:LYS:HA	2.19	0.43
1:C:133:GLU:OE1	1:C:374:GLN:NE2	2.52	0.42
1:C:532:ASP:OD1	1:C:547:ARG:HD2	2.19	0.42
1:C:582:ILE:O	1:C:589:GLN:NE2	2.52	0.42
1:A:420:ILE:O	1:A:420:ILE:HG23	2.20	0.42
1:A:230:LYS:HE2	1:A:234:ASP:OD1	2.20	0.42
1:A:418:GLU:HB2	1:A:419:PRO:HD2	2.01	0.42
1:B:169:TYR:CD2	1:B:229:ILE:HG23	2.54	0.42
1:B:418:GLU:HB2	1:B:419:PRO:HD2	2.02	0.42
1:B:505:MET:O	1:B:507:ARG:NH1	2.53	0.42
1:A:521:MET:HE2	1:A:521:MET:HA	2.00	0.42
1:B:416:VAL:HG23	1:B:444:TRP:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:ASN:N	1:C:523:PRO:CD	2.83	0.41
1:A:438:HIS:CD2	1:A:457:ALA:HA	2.55	0.41
1:C:106:LEU:C	1:C:106:LEU:HD12	2.41	0.41
1:C:386:VAL:HG22	1:C:387:ALA:N	2.35	0.41
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.55	0.41
1:C:440:SER:HA	1:C:455:PRO:HG2	2.02	0.41
1:B:27:GLU:CD	1:B:545:ARG:HH11	2.24	0.40
1:C:128:CYS:SG	1:C:174:ALA:HB2	2.61	0.40
1:C:447:GLU:HG2	1:C:520:TYR:CZ	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	664/686 (97%)	644 (97%)	19 (3%)	1 (0%)	47 69
1	B	596/686 (87%)	583 (98%)	12 (2%)	1 (0%)	47 69
1	C	578/686 (84%)	561 (97%)	16 (3%)	1 (0%)	47 69
All	All	1838/2058 (89%)	1788 (97%)	47 (3%)	3 (0%)	47 69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	606	SER
1	C	468	SER
1	B	468	SER

5.3.2 Protein sidechains [i](#)

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	542/568 (95%)	540 (100%)	2 (0%)	91	93
1	B	492/568 (87%)	489 (99%)	3 (1%)	86	90
1	C	476/568 (84%)	470 (99%)	6 (1%)	69	81
All	All	1510/1704 (89%)	1499 (99%)	11 (1%)	84	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASP
1	A	120	ASN
1	B	114	ASP
1	B	120	ASN
1	B	545	ARG
1	C	114	ASP
1	C	120	ASN
1	C	261	GLU
1	C	295	SER
1	C	297	SER
1	C	363	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	589	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	COA	C	702	-	28,33,50	0.75	0	35,52,75	0.83	2 (5%)
6	SO4	B	709	-	4,4,4	0.79	0	6,6,6	0.68	0
6	SO4	C	705	-	4,4,4	0.60	0	6,6,6	0.17	0
6	SO4	A	710	-	4,4,4	0.68	0	6,6,6	0.36	0
6	SO4	A	712	-	4,4,4	0.82	0	6,6,6	0.43	0
6	SO4	A	714	-	4,4,4	0.64	0	6,6,6	0.47	0
6	SO4	A	707	-	4,4,4	0.69	0	6,6,6	0.32	0
5	PGE	A	706	-	9,9,9	0.34	0	8,8,8	0.61	0
4	GOL	A	704	-	5,5,5	0.33	0	5,5,5	0.67	0
2	YHT	B	701	-	25,28,28	0.67	0	26,41,41	0.75	1 (3%)
6	SO4	C	703	-	4,4,4	0.64	0	6,6,6	0.14	0
6	SO4	A	708	-	4,4,4	0.75	0	6,6,6	0.52	0
6	SO4	B	706	-	4,4,4	0.69	0	6,6,6	0.48	0
6	SO4	A	711	-	4,4,4	0.73	0	6,6,6	0.56	0
6	SO4	B	710	-	4,4,4	0.67	0	6,6,6	0.37	0
2	YHT	A	701	-	25,28,28	0.67	0	26,41,41	0.86	0
4	GOL	A	705	-	5,5,5	0.33	0	5,5,5	0.25	0
6	SO4	A	713	-	4,4,4	0.62	0	6,6,6	0.12	0
6	SO4	B	707	-	4,4,4	0.71	0	6,6,6	0.27	0
6	SO4	A	709	-	4,4,4	0.70	0	6,6,6	0.50	0
4	GOL	A	703	-	5,5,5	0.35	0	5,5,5	0.27	0
2	YHT	C	701	-	25,28,28	0.65	0	26,41,41	0.70	1 (3%)
3	COA	A	702	-	41,50,50	0.58	0	52,75,75	0.69	1 (1%)
5	PGE	B	703	-	9,9,9	0.33	0	8,8,8	0.48	0
6	SO4	B	708	-	4,4,4	0.67	0	6,6,6	0.18	0
6	SO4	C	704	-	4,4,4	0.67	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	702	-	5,5,5	0.21	0	5,5,5	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
3	COA	A	702	-	-	11/44/64/64	0/3/3/3
3	COA	C	702	-	-	2/17/37/64	0/3/3/3
5	PGE	A	706	-	-	3/7/7/7	-
4	GOL	A	704	-	-	1/4/4/4	-
5	PGE	B	703	-	-	2/7/7/7	-
2	YHT	B	701	-	-	1/11/31/31	0/3/3/3
4	GOL	B	702	-	-	2/4/4/4	-
2	YHT	A	701	-	-	3/11/31/31	0/3/3/3
4	GOL	A	705	-	-	4/4/4/4	-
4	GOL	A	703	-	-	4/4/4/4	-
2	YHT	C	701	-	-	1/11/31/31	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	COA	C5A-C6A-N6A	2.30	123.85	120.35
3	A	702	COA	C5A-C6A-N6A	2.29	123.83	120.35
2	B	701	YHT	C5-C8-N5	2.26	123.79	120.35
2	C	701	YHT	C5-C8-N5	2.14	123.60	120.35
3	C	702	COA	O5A-P2A-O4A	2.10	118.91	110.68

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	YHT	C11-O6-P1-O7
2	C	701	YHT	O6-C11-C12-C13
3	A	702	COA	C3B-O3B-P3B-O8A
3	A	702	COA	CDP-CBP-CCP-O6A
3	A	702	COA	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
3	A	702	COA	CAP-C9P-N8P-C7P
3	C	702	COA	C3B-O3B-P3B-O7A
4	A	703	GOL	O1-C1-C2-O2
4	A	703	GOL	O1-C1-C2-C3
4	A	705	GOL	C1-C2-C3-O3
4	B	702	GOL	O1-C1-C2-C3
3	A	702	COA	O9P-C9P-N8P-C7P
5	A	706	PGE	O3-C5-C6-O4
5	A	706	PGE	O2-C3-C4-O3
5	B	703	PGE	O3-C5-C6-O4
3	A	702	COA	CEP-CBP-CCP-O6A
4	A	705	GOL	O1-C1-C2-C3
4	A	705	GOL	O2-C2-C3-O3
4	B	702	GOL	O1-C1-C2-O2
3	A	702	COA	C5P-C6P-C7P-N8P
3	C	702	COA	C3B-O3B-P3B-O8A
4	A	703	GOL	O2-C2-C3-O3
4	A	704	GOL	O2-C2-C3-O3
4	A	703	GOL	C1-C2-C3-O3
5	A	706	PGE	C4-C3-O2-C2
5	B	703	PGE	O2-C3-C4-O3
4	A	705	GOL	O1-C1-C2-O2
2	A	701	YHT	O4-C10-C9-C1
3	A	702	COA	P2A-O3A-P1A-O1A
2	A	701	YHT	C11-O6-P1-O4
3	A	702	COA	O5P-C5P-C6P-C7P
3	A	702	COA	OAP-CAP-CBP-CDP
3	A	702	COA	CCP-O6A-P2A-O4A
2	B	701	YHT	O4-C10-C9-C1

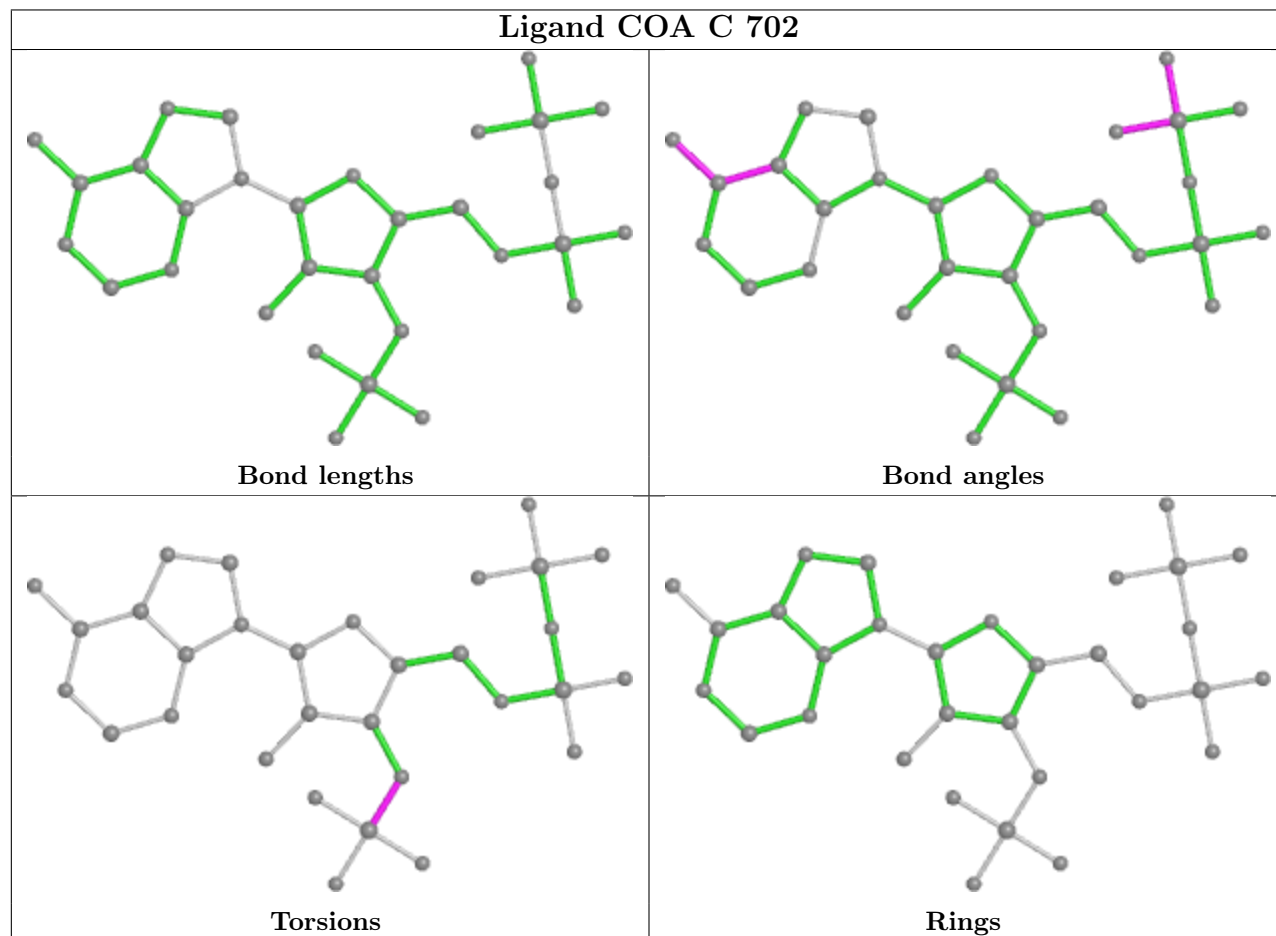
There are no ring outliers.

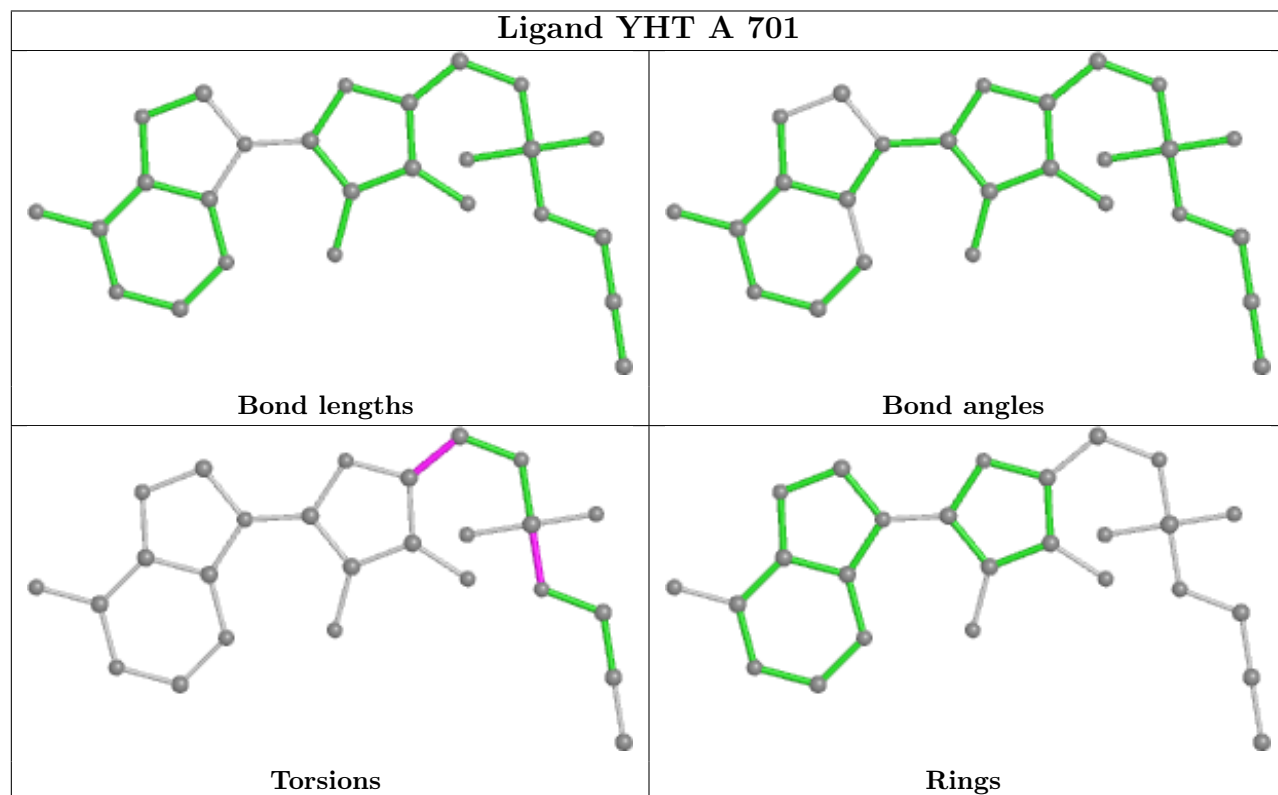
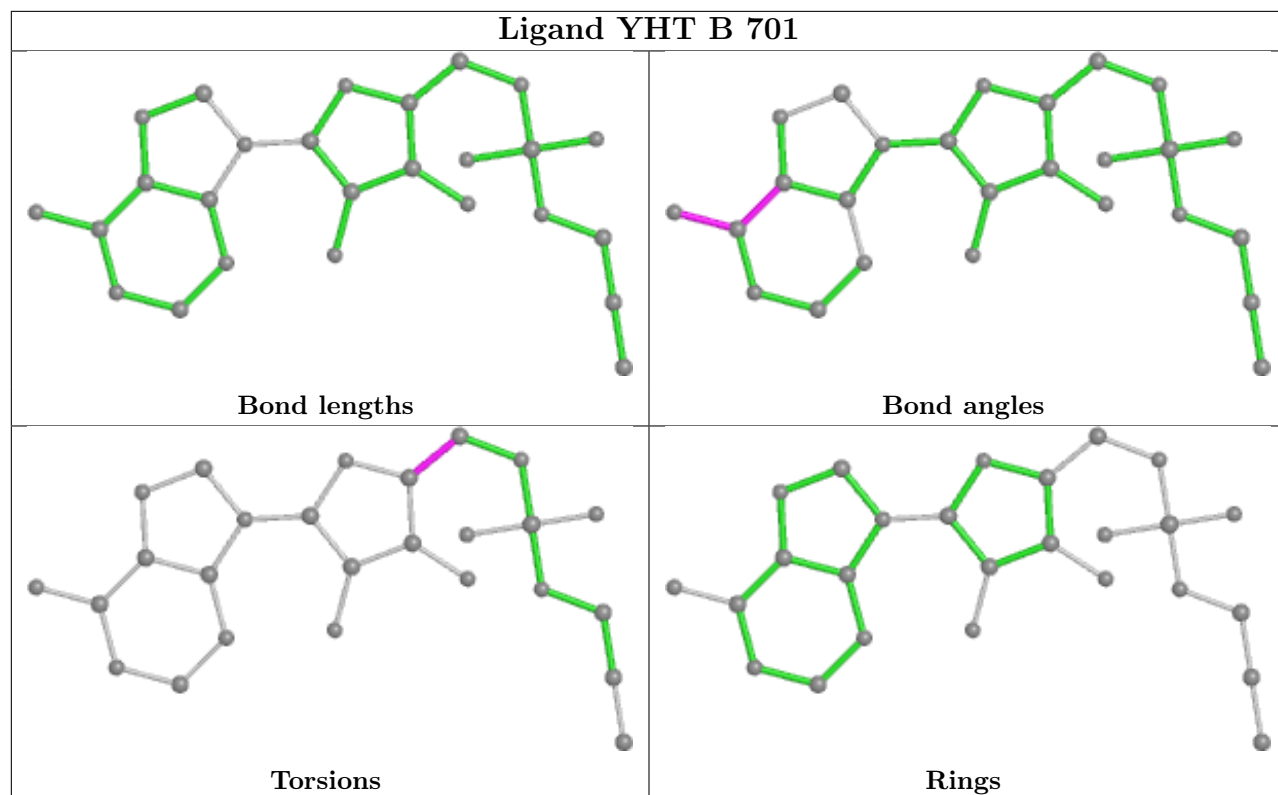
1 monomer is involved in 2 short contacts:

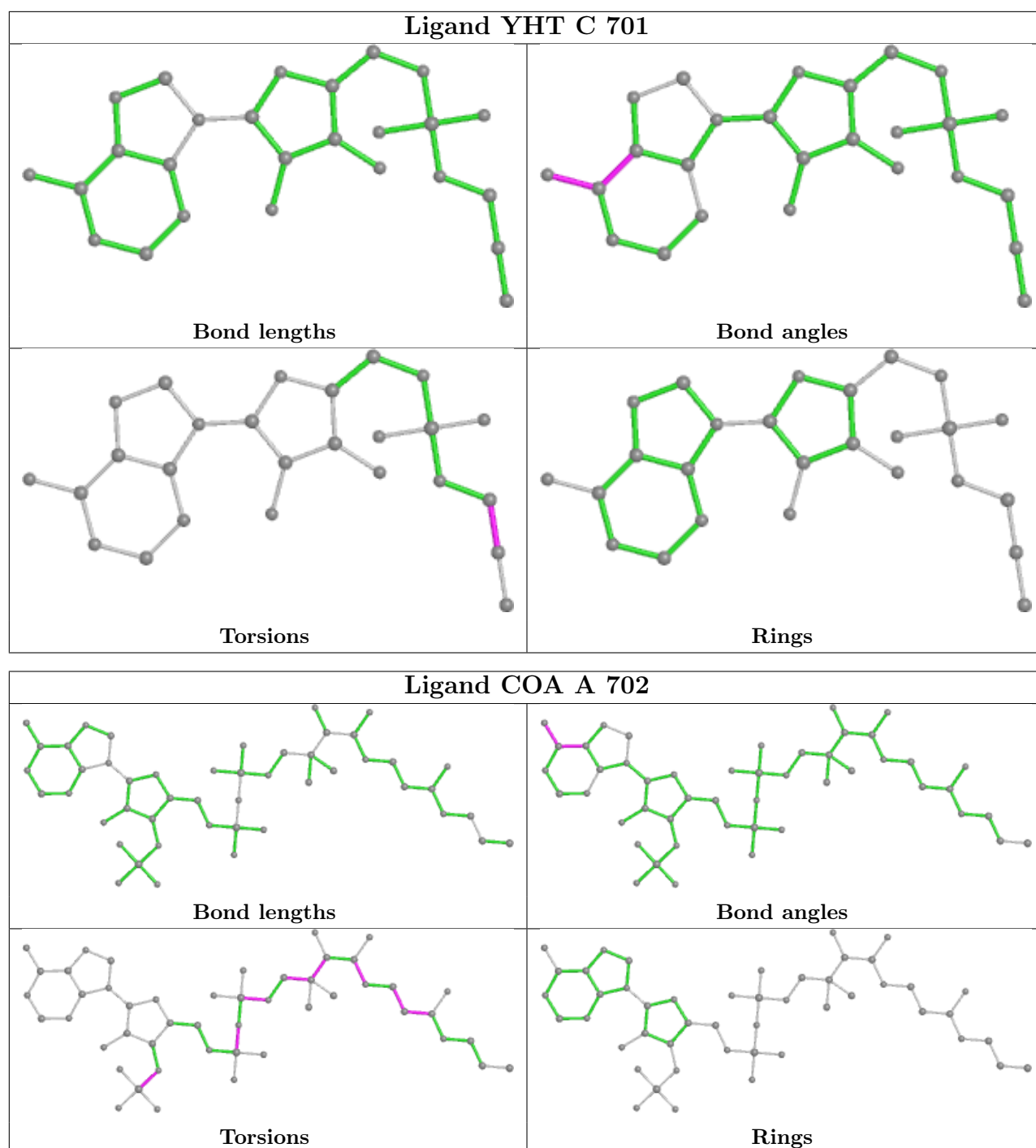
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	704	GOL	2	0

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	666/686 (97%)	0.08	11 (1%) 70 78	49, 68, 99, 195	0
1	B	604/686 (88%)	0.47	78 (12%) 3 4	51, 72, 146, 199	0
1	C	582/686 (84%)	0.52	57 (9%) 7 8	65, 100, 151, 186	0
All	All	1852/2058 (89%)	0.34	146 (7%) 12 15	49, 77, 143, 199	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	579	VAL	9.3
1	C	577	ALA	9.0
1	B	653	SER	8.5
1	B	654	SER	7.3
1	B	652	VAL	7.1
1	B	592	ILE	7.0
1	B	630	VAL	6.7
1	B	574	VAL	6.6
1	B	567	ALA	6.6
1	B	629	SER	6.6
1	C	620	THR	6.5
1	C	575	SER	6.5
1	B	569	ILE	6.4
1	B	588	GLY	6.4
1	C	576	GLU	6.3
1	B	586	ILE	6.2
1	B	566	ALA	6.0
1	A	604	GLU	6.0
1	B	617	VAL	6.0
1	B	564	ILE	5.8
1	C	564	ILE	5.8
1	B	651	LYS	5.8
1	B	595	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	568	LEU	5.6
1	B	575	SER	5.6
1	B	655	ASN	5.5
1	C	580	VAL	5.4
1	C	569	ILE	5.4
1	B	584	ASP	5.4
1	C	24	VAL	5.2
1	C	578	ALA	5.1
1	B	610	ARG	5.1
1	B	550	ASP	5.0
1	B	580	VAL	4.9
1	B	587	THR	4.9
1	B	613	LEU	4.7
1	B	562	ALA	4.7
1	B	583	HIS	4.7
1	B	615	LEU	4.5
1	B	571	ASP	4.5
1	B	572	LYS	4.5
1	B	628	LYS	4.5
1	B	578	ALA	4.5
1	C	574	VAL	4.5
1	B	619	LYS	4.4
1	C	566	ALA	4.4
1	B	576	GLU	4.4
1	B	593	ALA	4.3
1	B	648	ILE	4.2
1	B	627	PRO	4.2
1	B	650	ARG	4.2
1	B	573	LYS	4.2
1	B	616	GLN	4.2
1	B	621	ILE	4.2
1	B	565	GLU	4.1
1	B	568	LEU	4.1
1	B	649	LEU	4.1
1	C	613	LEU	4.1
1	B	582	ILE	4.0
1	B	594	TYR	3.9
1	B	620	THR	3.9
1	B	579	VAL	3.9
1	C	582	ILE	3.9
1	B	577	ALA	3.8
1	C	570	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	614	VAL	3.7
1	C	565	GLU	3.7
1	C	562	ALA	3.7
1	B	585	ASP	3.7
1	C	563	GLU	3.7
1	B	553	ASN	3.7
1	B	591	VAL	3.7
1	C	572	LYS	3.7
1	B	622	GLY	3.6
1	C	583	HIS	3.6
1	C	552	VAL	3.6
1	C	25	VAL	3.6
1	C	571	ASP	3.4
1	A	606	SER	3.4
1	C	585	ASP	3.4
1	B	618	ARG	3.3
1	C	573	LYS	3.3
1	B	611	LYS	3.2
1	B	22	HIS	3.1
1	B	570	GLU	3.1
1	A	609	LEU	3.0
1	C	581	GLY	3.0
1	B	623	PRO	3.0
1	C	431	PHE	2.9
1	C	138	ILE	2.9
1	B	538	HIS	2.9
1	C	618	ARG	2.9
1	C	494	GLY	2.9
1	C	617	VAL	2.8
1	B	561	THR	2.8
1	C	479	ILE	2.8
1	C	587	THR	2.8
1	B	607	GLU	2.8
1	A	679	PHE	2.8
1	B	563	GLU	2.7
1	C	30	GLY	2.7
1	C	589	GLN	2.7
1	B	625	ALA	2.7
1	B	581	GLY	2.6
1	A	601	ASN	2.6
1	B	20	GLN	2.6
1	C	450	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	30	GLY	2.5
1	B	560	SER	2.5
1	B	590	ALA	2.5
1	B	400	GLN	2.5
1	C	43	ARG	2.5
1	B	609	LEU	2.5
1	B	554	VAL	2.4
1	B	589	GLN	2.4
1	C	584	ASP	2.4
1	B	608	GLY	2.4
1	C	619	LYS	2.4
1	B	295	SER	2.3
1	C	482	VAL	2.3
1	C	614	VAL	2.3
1	C	491	ASP	2.3
1	C	446	THR	2.3
1	C	586	ILE	2.3
1	A	600	GLY	2.3
1	B	626	ALA	2.3
1	C	26	HIS	2.2
1	A	340	ILE	2.2
1	A	574	VAL	2.2
1	C	615	LEU	2.2
1	C	400	GLN	2.2
1	C	23	ASN	2.2
1	C	403	ALA	2.1
1	A	603	ASP	2.1
1	B	32	LYS	2.1
1	C	567	ALA	2.1
1	A	607	GLU	2.1
1	C	45	PRO	2.1
1	C	487	ILE	2.1
1	A	21	THR	2.1
1	B	549	ASP	2.1
1	B	33	LEU	2.0
1	C	335	GLY	2.0
1	C	484	GLY	2.0
1	C	22	HIS	2.0
1	C	228	ASN	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 monosaccharides 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.

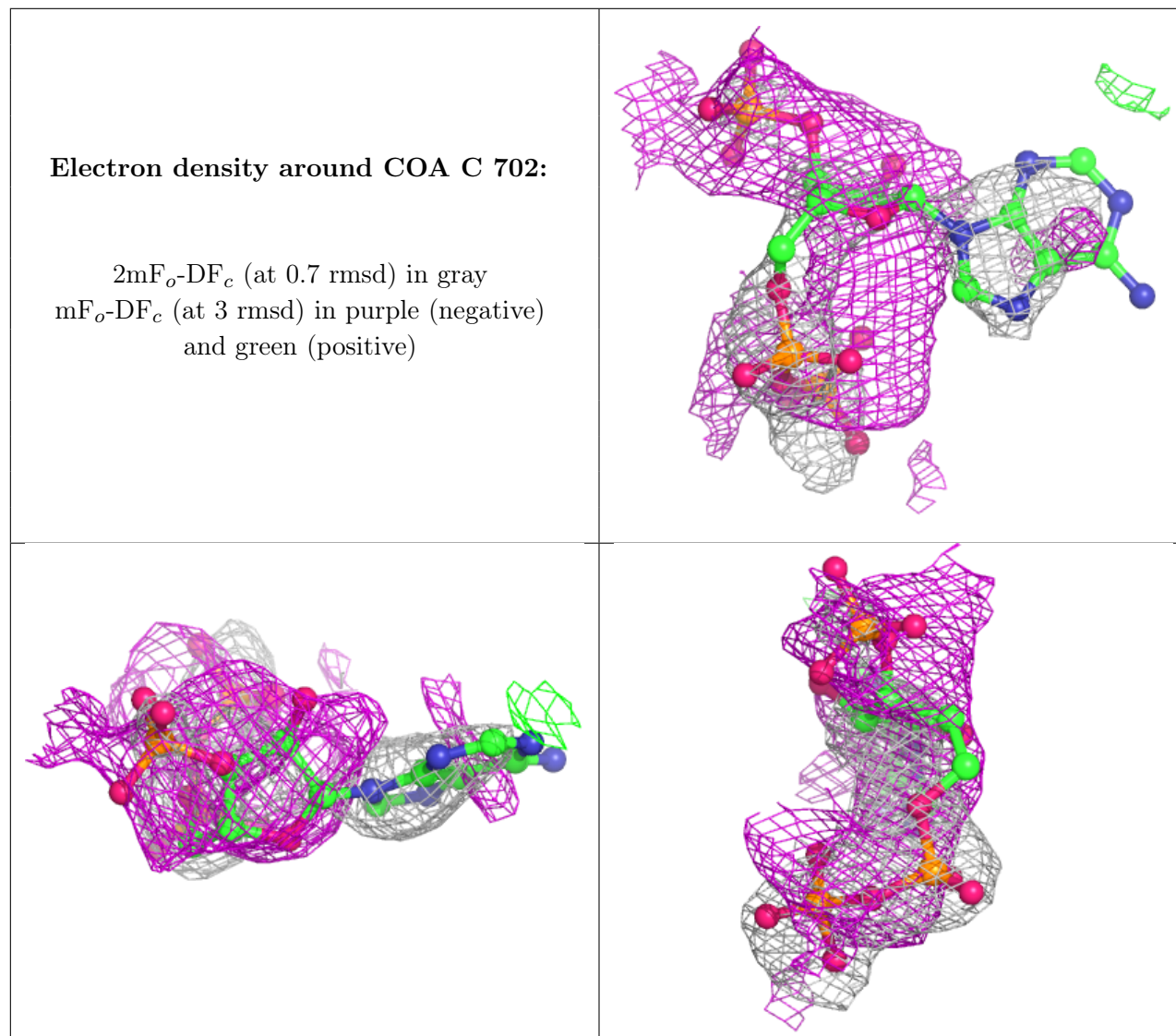
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	C	702	31/48	0.67	0.48	134,159,166,170	0
5	PGE	A	706	10/10	0.73	0.37	73,85,93,95	0
6	SO4	C	703	5/5	0.76	0.47	141,146,152,156	0
6	SO4	A	714	5/5	0.78	0.42	104,107,119,128	0
6	SO4	B	706	5/5	0.79	0.47	108,108,132,134	0
6	SO4	C	704	5/5	0.79	0.60	110,115,117,129	0
6	SO4	B	707	5/5	0.81	0.34	91,104,126,132	0
6	SO4	B	710	5/5	0.82	0.40	117,125,136,140	0
6	SO4	B	708	5/5	0.84	0.48	113,116,135,140	0
6	SO4	B	709	5/5	0.85	0.16	72,84,101,120	0
6	SO4	A	712	5/5	0.85	0.39	88,90,110,116	0
4	GOL	A	705	6/6	0.86	0.33	71,86,92,94	0
4	GOL	B	702	6/6	0.86	0.47	83,87,94,96	0
3	COA	A	702	48/48	0.86	0.30	79,95,110,118	0
7	CL	B	704	1/1	0.86	0.20	121,121,121,121	0
4	GOL	A	704	6/6	0.88	0.19	66,74,76,79	0
4	GOL	A	703	6/6	0.89	0.57	74,76,82,83	0
5	PGE	B	703	10/10	0.89	0.26	83,92,97,98	0
6	SO4	A	709	5/5	0.90	0.17	80,87,105,110	0
6	SO4	A	711	5/5	0.91	0.20	78,84,94,103	0
7	CL	B	705	1/1	0.91	0.31	103,103,103,103	0
6	SO4	A	708	5/5	0.93	0.20	70,76,89,90	0
2	YHT	C	701	26/26	0.94	0.25	92,106,108,110	0
6	SO4	A	707	5/5	0.94	0.15	86,90,99,102	0
6	SO4	A	710	5/5	0.94	0.19	81,85,94,98	0
6	SO4	C	705	5/5	0.95	0.28	103,112,116,122	0
2	YHT	B	701	26/26	0.95	0.22	61,69,72,75	0

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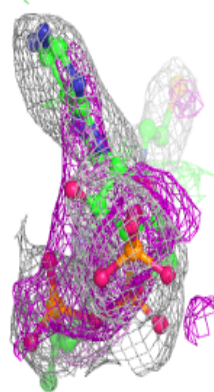
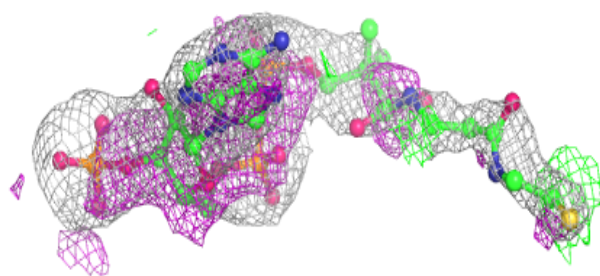
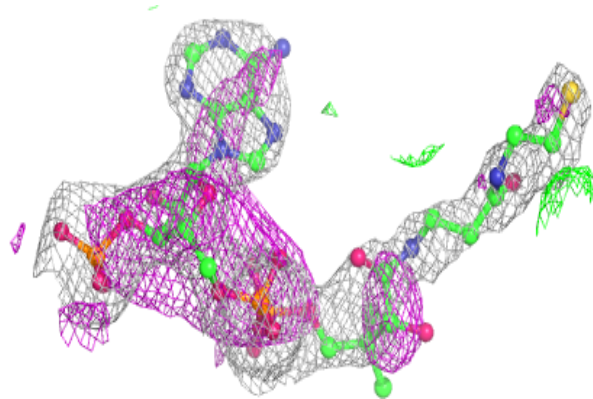
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	SO4	A	713	5/5	0.95	0.13	121,121,128,132	0
2	YHT	A	701	26/26	0.97	0.23	54,58,66,68	0

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.

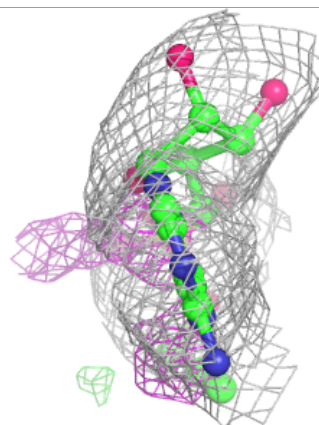
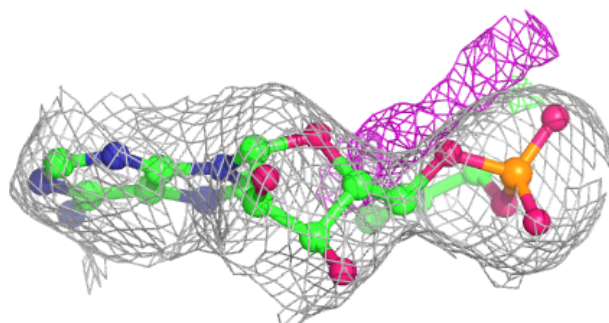
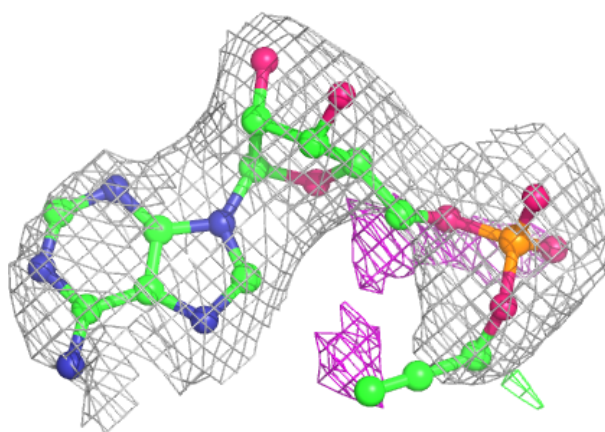


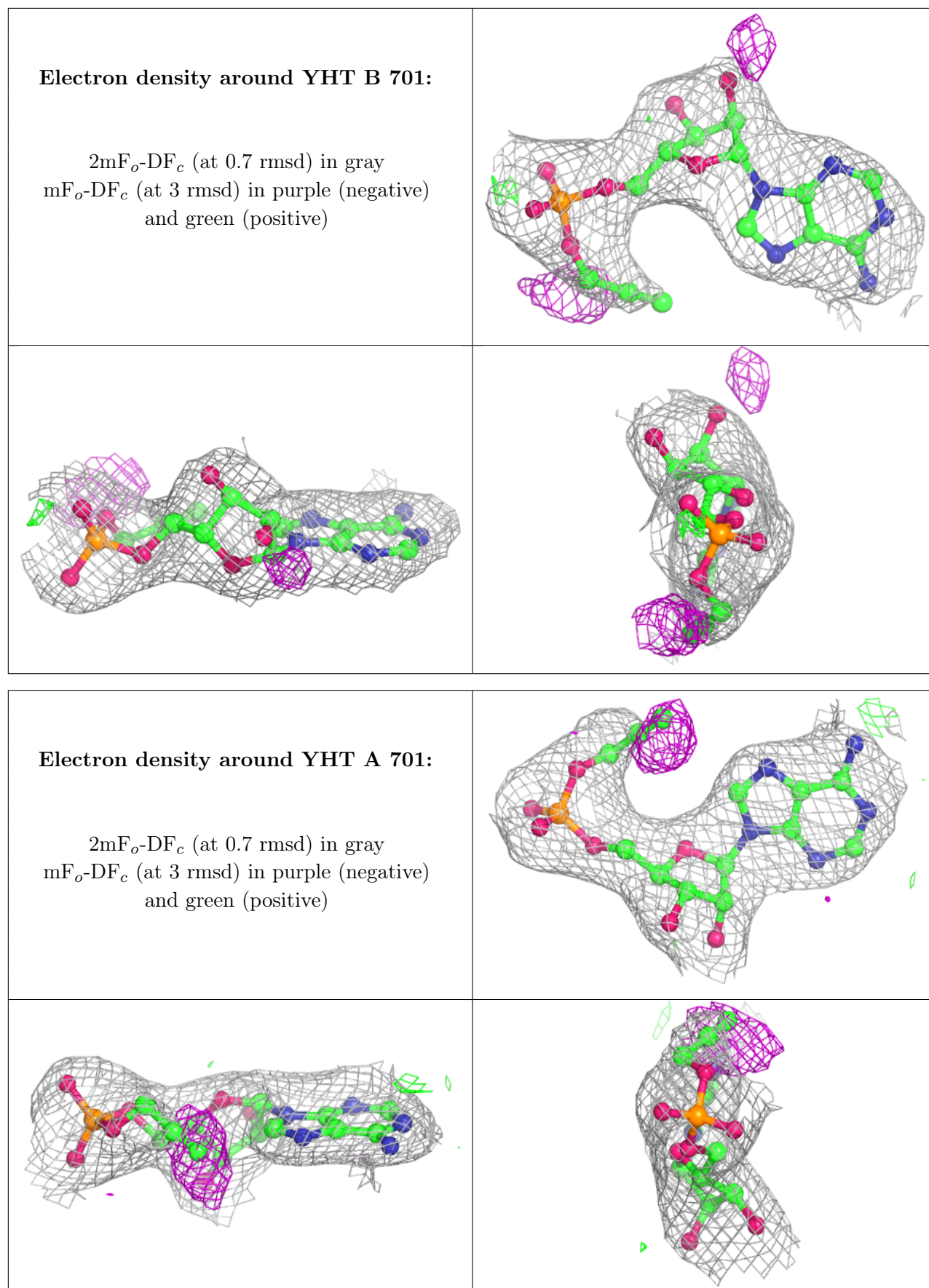
Electron density around COA A 702:

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

**Electron density around YHT C 701:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.