



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:57 AM UTC

PDB ID : 3F5O / pdb_00003f5o
Title : Crystal Structure of hTHEM2(undecan-2-one-CoA) complex
Authors : Xu, H.; Gong, W.
Deposited on : 2008-11-04
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

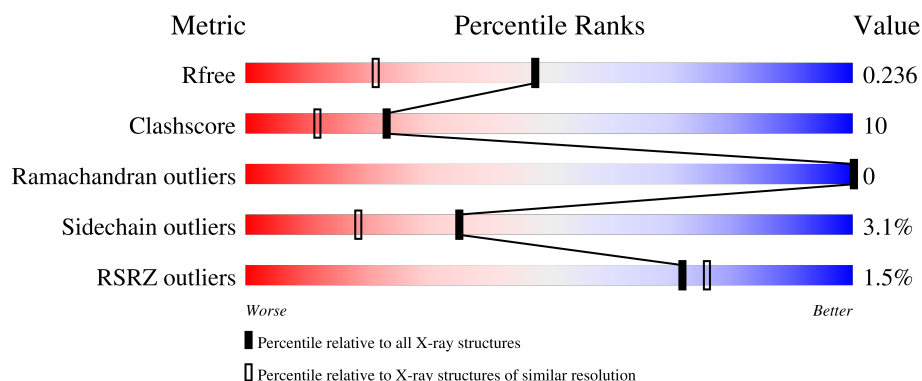
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	148	% 83% 10% 7%
1	B	148	3% 76% 14% • 8%
1	C	148	% 72% 19% • 7%
1	D	148	% 78% 14% 7%
1	E	148	% 74% 16% • • 7%

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Mol	Chain	Length	Quality of chain
1	F	148	
1	G	148	
1	H	148	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	COA	A	150	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9600 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 Thioesterase superfamily member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	3	0
			1039	651	180	198	10			
1	B	136	Total	C	N	O	S	0	4	0
			1025	643	182	192	8			
1	C	137	Total	C	N	O	S	0	4	0
			1036	650	182	195	9			
1	D	137	Total	C	N	O	S	0	5	0
			1025	643	177	195	10			
1	E	138	Total	C	N	O	S	0	1	0
			1021	639	178	196	8			
1	F	138	Total	C	N	O	S	0	1	0
			1024	639	181	196	8			
1	G	136	Total	C	N	O	S	0	3	0
			1017	642	177	189	9			
1	H	138	Total	C	N	O	S	0	5	0
			1036	651	181	194	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	LEU	-	expression tag	UNP Q9NPJ3
A	142	GLU	-	expression tag	UNP Q9NPJ3
A	143	HIS	-	expression tag	UNP Q9NPJ3
A	144	HIS	-	expression tag	UNP Q9NPJ3
A	145	HIS	-	expression tag	UNP Q9NPJ3
A	146	HIS	-	expression tag	UNP Q9NPJ3
A	147	HIS	-	expression tag	UNP Q9NPJ3
A	148	HIS	-	expression tag	UNP Q9NPJ3
B	141	LEU	-	expression tag	UNP Q9NPJ3
B	142	GLU	-	expression tag	UNP Q9NPJ3
B	143	HIS	-	expression tag	UNP Q9NPJ3
B	144	HIS	-	expression tag	UNP Q9NPJ3
B	145	HIS	-	expression tag	UNP Q9NPJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NPJ3
B	147	HIS	-	expression tag	UNP Q9NPJ3
B	148	HIS	-	expression tag	UNP Q9NPJ3
C	141	LEU	-	expression tag	UNP Q9NPJ3
C	142	GLU	-	expression tag	UNP Q9NPJ3
C	143	HIS	-	expression tag	UNP Q9NPJ3
C	144	HIS	-	expression tag	UNP Q9NPJ3
C	145	HIS	-	expression tag	UNP Q9NPJ3
C	146	HIS	-	expression tag	UNP Q9NPJ3
C	147	HIS	-	expression tag	UNP Q9NPJ3
C	148	HIS	-	expression tag	UNP Q9NPJ3
D	141	LEU	-	expression tag	UNP Q9NPJ3
D	142	GLU	-	expression tag	UNP Q9NPJ3
D	143	HIS	-	expression tag	UNP Q9NPJ3
D	144	HIS	-	expression tag	UNP Q9NPJ3
D	145	HIS	-	expression tag	UNP Q9NPJ3
D	146	HIS	-	expression tag	UNP Q9NPJ3
D	147	HIS	-	expression tag	UNP Q9NPJ3
D	148	HIS	-	expression tag	UNP Q9NPJ3
E	141	LEU	-	expression tag	UNP Q9NPJ3
E	142	GLU	-	expression tag	UNP Q9NPJ3
E	143	HIS	-	expression tag	UNP Q9NPJ3
E	144	HIS	-	expression tag	UNP Q9NPJ3
E	145	HIS	-	expression tag	UNP Q9NPJ3
E	146	HIS	-	expression tag	UNP Q9NPJ3
E	147	HIS	-	expression tag	UNP Q9NPJ3
E	148	HIS	-	expression tag	UNP Q9NPJ3
F	141	LEU	-	expression tag	UNP Q9NPJ3
F	142	GLU	-	expression tag	UNP Q9NPJ3
F	143	HIS	-	expression tag	UNP Q9NPJ3
F	144	HIS	-	expression tag	UNP Q9NPJ3
F	145	HIS	-	expression tag	UNP Q9NPJ3
F	146	HIS	-	expression tag	UNP Q9NPJ3
F	147	HIS	-	expression tag	UNP Q9NPJ3
F	148	HIS	-	expression tag	UNP Q9NPJ3
G	141	LEU	-	expression tag	UNP Q9NPJ3
G	142	GLU	-	expression tag	UNP Q9NPJ3
G	143	HIS	-	expression tag	UNP Q9NPJ3
G	144	HIS	-	expression tag	UNP Q9NPJ3
G	145	HIS	-	expression tag	UNP Q9NPJ3
G	146	HIS	-	expression tag	UNP Q9NPJ3
G	147	HIS	-	expression tag	UNP Q9NPJ3

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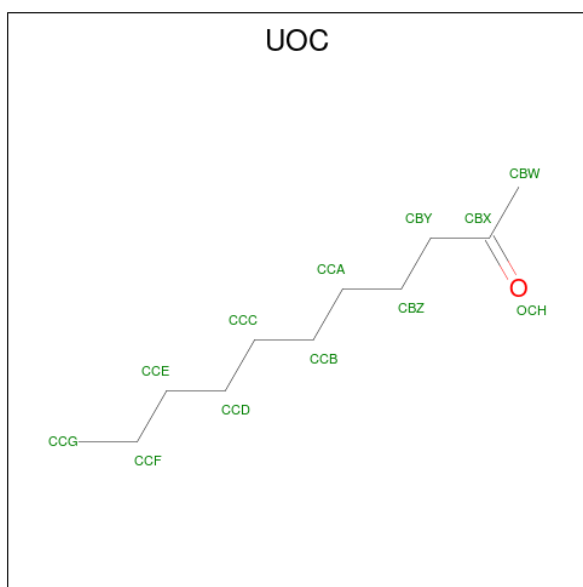
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Chain	Residue	Modelled	Actual	Comment	Reference
G	148	HIS	-	expression tag	UNP Q9NPJ3
H	141	LEU	-	expression tag	UNP Q9NPJ3
H	142	GLU	-	expression tag	UNP Q9NPJ3
H	143	HIS	-	expression tag	UNP Q9NPJ3
H	144	HIS	-	expression tag	UNP Q9NPJ3
H	145	HIS	-	expression tag	UNP Q9NPJ3
H	146	HIS	-	expression tag	UNP Q9NPJ3
H	147	HIS	-	expression tag	UNP Q9NPJ3
H	148	HIS	-	expression tag	UNP Q9NPJ3

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

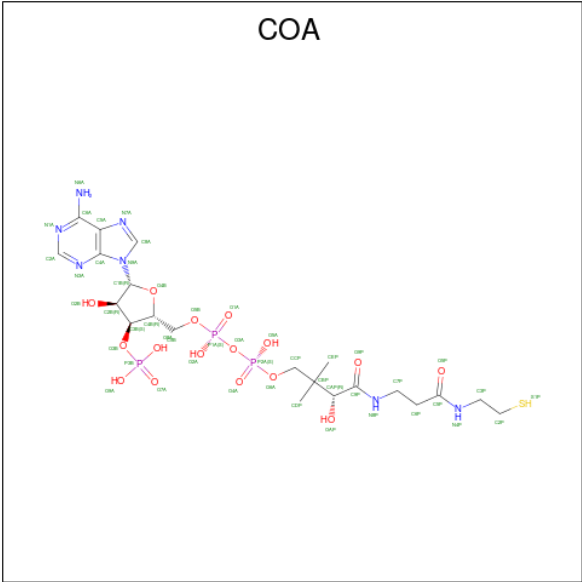
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0

- Molecule 3 is undecan-2-one (CCD ID: UOC) (formula: C₁₁H₂₂O).



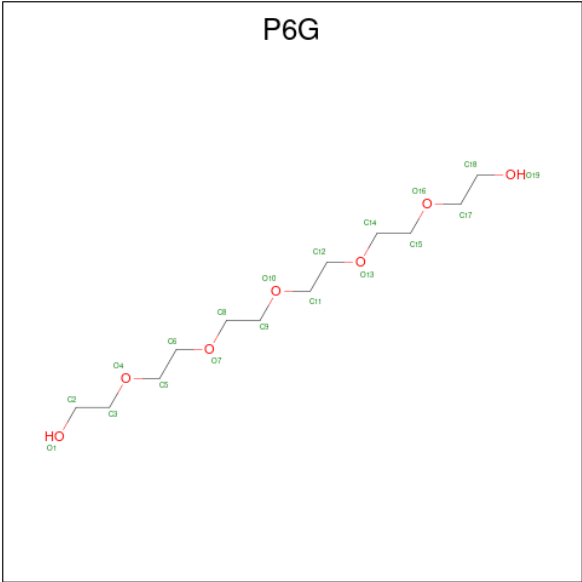
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	11	1		
3	B	1	Total	C	O	0	0
			12	11	1		
3	C	1	Total	C	O	0	0
			12	11	1		
3	D	1	Total	C	O	0	0
			12	11	1		
3	E	1	Total	C	O	0	0
			12	11	1		
3	F	1	Total	C	O	0	0
			12	11	1		
3	G	1	Total	C	O	0	0
			12	11	1		
3	H	1	Total	C	O	0	0
			12	11	1		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			38	16	2	16	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			38	16	2	16	3	1		

- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			15	10	5		
5	C	1	Total	C	O	0	0
			15	10	5		
5	E	1	Total	C	O	0	0
			15	10	5		
5	G	1	Total	C	O	0	0
			15	10	5		

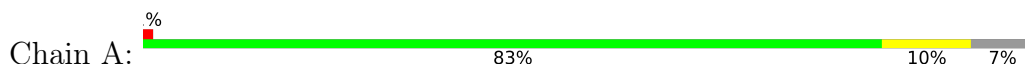
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	111	Total	O	0	0
			111	111		
6	B	95	Total	O	0	0
			95	95		
6	C	127	Total	O	0	0
			127	127		
6	D	92	Total	O	0	0
			92	92		
6	E	118	Total	O	0	0
			118	118		
6	F	107	Total	O	0	0
			107	107		
6	G	102	Total	O	0	0
			102	102		
6	H	98	Total	O	0	0
			98	98		

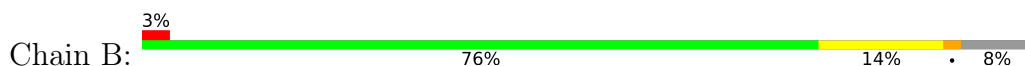
3 Residue-property plots [i](#)

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.

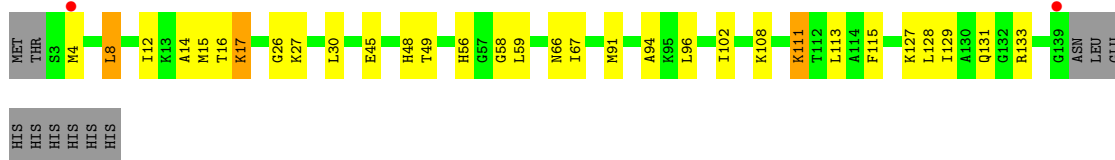
- Molecule 1: Thioesterase superfamily member 2



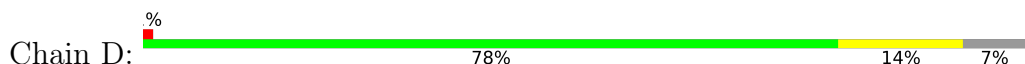
- Molecule 1: Thioesterase superfamily member 2



- Molecule 1: Thioesterase superfamily member 2



- Molecule 1: Thioesterase superfamily member 2



- Molecule 1: Thioesterase superfamily member 2



HIS
HIS
HIS

- Molecule 1: Thioesterase superfamily member 2

Chain F: 3% 79% 13% 7%

MET T2 S3 M4 T5 Q6 V11 I12 K13 K17 L25 P35 I52 H56 G57 G58 N66 C74 P93 V101 G110 Y121 K127 Q131 G132 R133 H137 L138 G139 ASN LEU GLU HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Thioesterase superfamily member 2

Chain G: 80% 12% 8%

MET THR SER M4 L8 M15 T16 L25 Q26 P35 H48 H56 G57 G58 L59 N66 I67 C74 A79 A94 I129 A130 Q131 G132 R133 V139 ASN LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Thioesterase superfamily member 2

Chain H: 3% 77% 15% 7%

MET T2 I12 K13 A14 V38 I39 C40 H56 G57 G58 A61 N66 I67 S68 I69 M70 A71 L72 M86 N87 I88 M91 L96 H105 A114 F115 T116 S117 Q131 G132 R133 H134 G139 ASN LEU GLU HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.03Å 110.63Å 119.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.73 – 1.70 20.73 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.73-1.70) 99.0 (20.73-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.237 0.197 , 0.236	Depositor DCC
R_{free} test set	6645 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.9	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	0.97	EDS
Total number of atoms	9600	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3689e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, UOC, CL, P6G

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	0.76	0/1055	0.84	0/1422
1	B	0.79	0/1048	0.88	0/1415
1	C	0.76	0/1059	0.85	0/1427
1	D	0.78	1/1050 (0.1%)	0.86	0/1419
1	E	0.83	0/1034	0.94	4/1397 (0.3%)
1	F	0.81	1/1037 (0.1%)	0.97	3/1401 (0.2%)
1	G	0.77	0/1037	0.84	2/1399 (0.1%)
1	H	0.70	0/1062	0.91	3/1434 (0.2%)
All	All	0.78	2/8382 (0.0%)	0.89	12/11314 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	13	LYS	C-O	-5.47	1.17	1.24
1	D	129	ILE	CA-C	5.10	1.59	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	116	THR	OG1-CB-CG2	6.93	123.17	109.30
1	F	121	THR	OG1-CB-CG2	6.72	122.75	109.30
1	E	116	THR	N-CA-CB	-6.72	99.04	111.53
1	H	116	THR	N-CA-CB	-6.59	99.26	111.52
1	F	121	THR	N-CA-CB	-6.00	100.37	111.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1039	0	1090	22	0
1	B	1025	0	1074	20	0
1	C	1036	0	1092	29	0
1	D	1025	0	1068	25	0
1	E	1021	0	1062	34	0
1	F	1024	0	1073	16	0
1	G	1017	0	1058	15	0
1	H	1036	0	1087	34	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	20	6	0
3	B	12	0	21	0	0
3	C	12	0	21	1	0
3	D	12	0	21	1	0
3	E	12	0	21	2	0
3	F	12	0	21	0	0
3	G	12	0	21	1	0
3	H	12	0	21	2	0
4	A	38	0	26	6	0
4	B	48	0	31	1	0
4	C	48	0	31	0	0
4	D	48	0	31	0	0
4	E	48	0	31	1	0
4	F	48	0	31	3	0
4	G	48	0	31	5	0
4	H	38	0	26	3	0
5	B	15	0	16	0	0
5	C	15	0	16	0	0
5	E	15	0	16	1	0
5	G	15	0	16	1	0
6	A	111	0	0	1	0
6	B	95	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	127	0	0	0	0
6	D	92	0	0	1	0
6	E	118	0	0	5	0
6	F	107	0	0	1	0
6	G	102	0	0	1	0
6	H	98	0	0	1	0
All	All	9600	0	9073	183	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 10.

The worst 5 of 183 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86[B]:MET:HE1	1:A:88:ILE:HD11	1.38	1.04
1:C:56:HIS:HD2	1:C:58:GLY:H	1.08	0.99
1:D:56:HIS:HD2	1:D:58:GLY:H	1.08	0.97
1:C:27:LYS:HE3	1:C:45:GLU:HG3	1.45	0.97
1:A:133:ARG:HE	1:D:131:GLN:HE21	1.10	0.96

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	139/148 (94%)	136 (98%)	3 (2%)	0	100	100
1	B	138/148 (93%)	134 (97%)	4 (3%)	0	100	100
1	C	139/148 (94%)	137 (99%)	2 (1%)	0	100	100
1	D	140/148 (95%)	139 (99%)	1 (1%)	0	100	100
1	E	137/148 (93%)	133 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	137/148 (93%)	135 (98%)	2 (2%)	0	100	100
1	G	136/148 (92%)	134 (98%)	2 (2%)	0	100	100
1	H	141/148 (95%)	140 (99%)	1 (1%)	0	100	100
All	All	1107/1184 (94%)	1088 (98%)	19 (2%)	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	114/123 (93%)	113 (99%)	1 (1%)	70	62
1	B	111/123 (90%)	105 (95%)	6 (5%)	20	6
1	C	115/123 (94%)	109 (95%)	6 (5%)	21	7
1	D	112/123 (91%)	111 (99%)	1 (1%)	70	62
1	E	111/123 (90%)	104 (94%)	7 (6%)	16	5
1	F	113/123 (92%)	110 (97%)	3 (3%)	39	23
1	G	108/123 (88%)	107 (99%)	1 (1%)	70	62
1	H	114/123 (93%)	111 (97%)	3 (3%)	40	23
All	All	898/984 (91%)	870 (97%)	28 (3%)	35	18

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	SER
1	H	116	THR
1	E	66	ASN
1	G	8	LEU
1	E	16	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	56	HIS
1	E	131	GLN
1	H	56	HIS
1	E	105	HIS
1	F	56	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	COA	C	150	3	47,50,50	2.33	12 (25%)	69,75,75	1.90	18 (26%)
4	COA	F	150	3	47,50,50	2.36	11 (23%)	69,75,75	1.76	14 (20%)
3	UOC	G	149	4	11,11,11	0.57	0	11,11,11	1.05	1 (9%)
3	UOC	B	149	4	11,11,11	0.53	0	11,11,11	0.84	0
3	UOC	E	149	4	11,11,11	0.41	0	11,11,11	0.62	0
5	P6G	E	1001	-	14,14,18	0.78	0	13,13,17	0.56	0
5	P6G	C	1001	-	14,14,18	0.63	0	13,13,17	0.61	0
4	COA	A	150	3	35,38,50	3.52	12 (34%)	49,56,75	1.75	12 (24%)
3	UOC	C	149	4	11,11,11	0.61	0	11,11,11	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UOC	D	149	4	11,11,11	0.64	0	11,11,11	0.93	0
3	UOC	H	149	4	11,11,11	0.65	0	11,11,11	0.71	0
3	UOC	A	149	4	11,11,11	0.77	0	11,11,11	1.07	1 (9%)
4	COA	B	150	3	47,50,50	1.82	12 (25%)	69,75,75	1.85	14 (20%)
3	UOC	F	149	4	11,11,11	0.51	0	11,11,11	1.26	1 (9%)
5	P6G	B	1001	-	14,14,18	0.71	0	13,13,17	0.40	0
5	P6G	G	1001	-	14,14,18	0.65	0	13,13,17	0.74	0
4	COA	G	150	3	47,50,50	1.92	10 (21%)	69,75,75	1.82	15 (21%)
4	COA	H	150	3	35,38,50	2.00	9 (25%)	49,56,75	1.60	8 (16%)
4	COA	D	150	3	47,50,50	2.59	15 (31%)	69,75,75	2.10	18 (26%)
4	COA	E	150	3	47,50,50	2.56	16 (34%)	69,75,75	1.85	15 (21%)

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	COA	C	150	3	-	4/48/64/64	0/3/3/3
4	COA	F	150	3	-	3/48/64/64	0/3/3/3
3	UOC	G	149	4	-	4/9/9/9	-
3	UOC	B	149	4	-	6/9/9/9	-
3	UOC	E	149	4	-	4/9/9/9	-
5	P6G	E	1001	-	-	7/12/12/16	-
5	P6G	C	1001	-	-	7/12/12/16	-
4	COA	A	150	3	1/1/10/13	19/44/57/64	0/1/1/3
3	UOC	C	149	4	-	2/9/9/9	-
3	UOC	D	149	4	-	3/9/9/9	-
3	UOC	H	149	4	-	7/9/9/9	-
3	UOC	A	149	4	-	7/9/9/9	-
4	COA	B	150	3	-	6/48/64/64	0/3/3/3
3	UOC	F	149	4	-	3/9/9/9	-
5	P6G	B	1001	-	-	7/12/12/16	-
5	P6G	G	1001	-	-	8/12/12/16	-
4	COA	G	150	3	-	1/48/64/64	0/3/3/3
4	COA	H	150	3	-	5/44/57/64	0/1/1/3
4	COA	D	150	3	-	3/48/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	COA	E	150	3	-	2/48/64/64	0/3/3/3

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	150	COA	P2A-O3A	-13.08	1.45	1.59
4	A	150	COA	P1A-O3A	-12.68	1.45	1.59
4	E	150	COA	P2A-O3A	-10.13	1.48	1.59
4	C	150	COA	P2A-O3A	-9.86	1.48	1.59
4	F	150	COA	P2A-O3A	-9.58	1.49	1.59

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	150	COA	O4B-C1B-N9A	10.22	127.72	108.09
4	E	150	COA	O4B-C1B-N9A	-7.20	94.26	108.09
4	F	150	COA	C5A-C4A-N3A	-6.31	118.02	126.72
4	E	150	COA	C5A-C4A-N3A	-5.93	118.56	126.72
4	B	150	COA	O4B-C1B-N9A	5.64	118.91	108.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	150	COA	CAP

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	150	COA	C2B-C3B-O3B-P3B
4	A	150	COA	O4B-C4B-C5B-O5B
4	A	150	COA	CCP-O6A-P2A-O3A
4	A	150	COA	CCP-O6A-P2A-O4A
4	A	150	COA	CDP-CBP-CCP-O6A

There are no ring outliers.

14 monomers are involved in 33 short contacts:

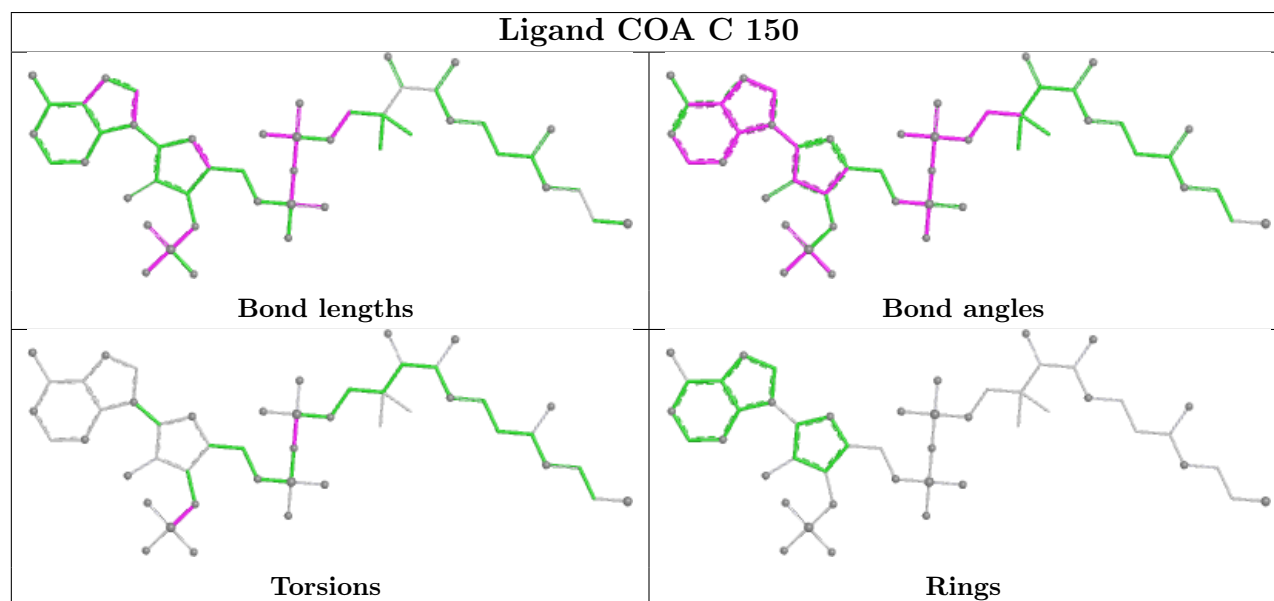
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	150	COA	3	0
3	G	149	UOC	1	0
3	E	149	UOC	2	0

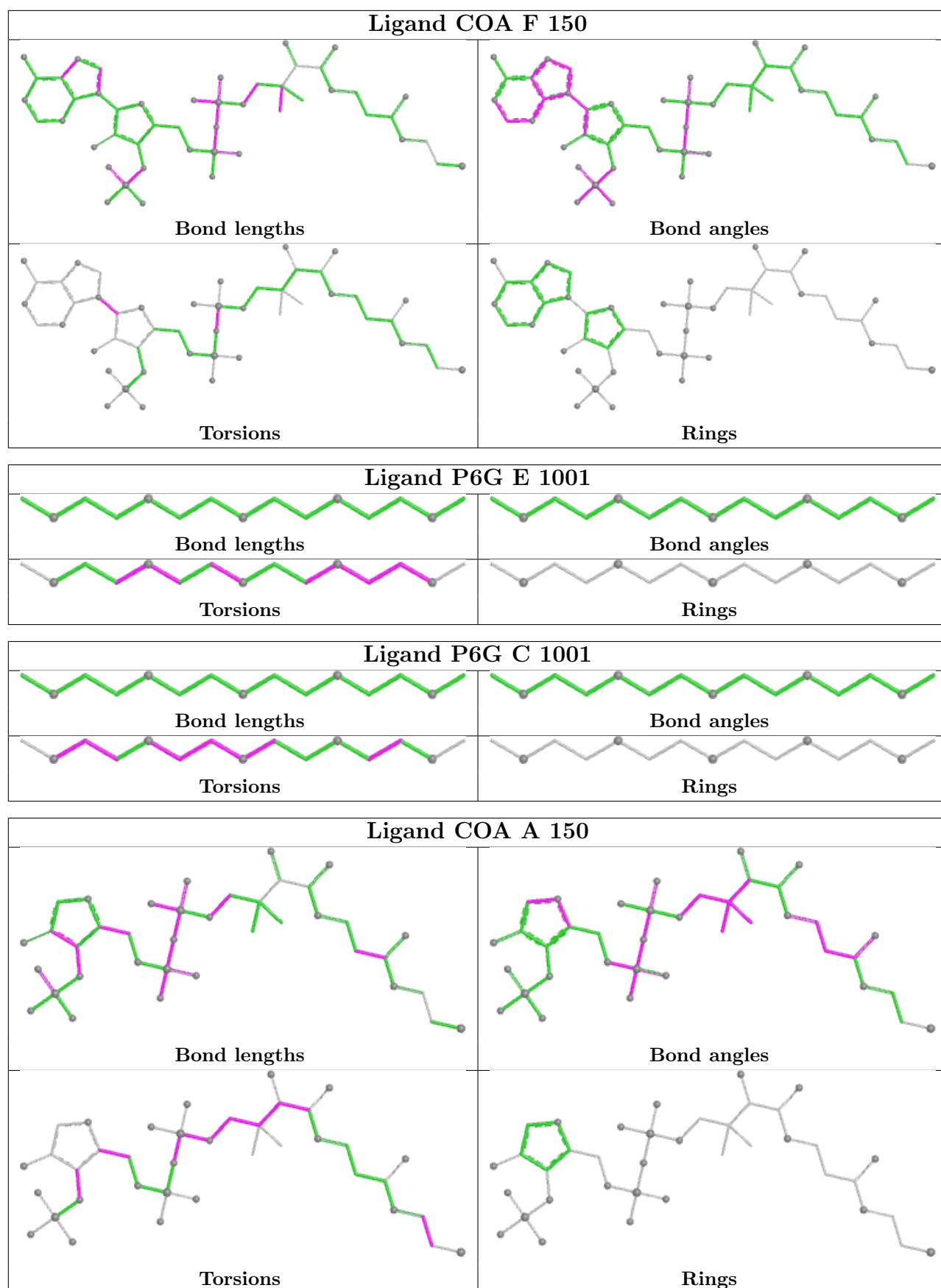
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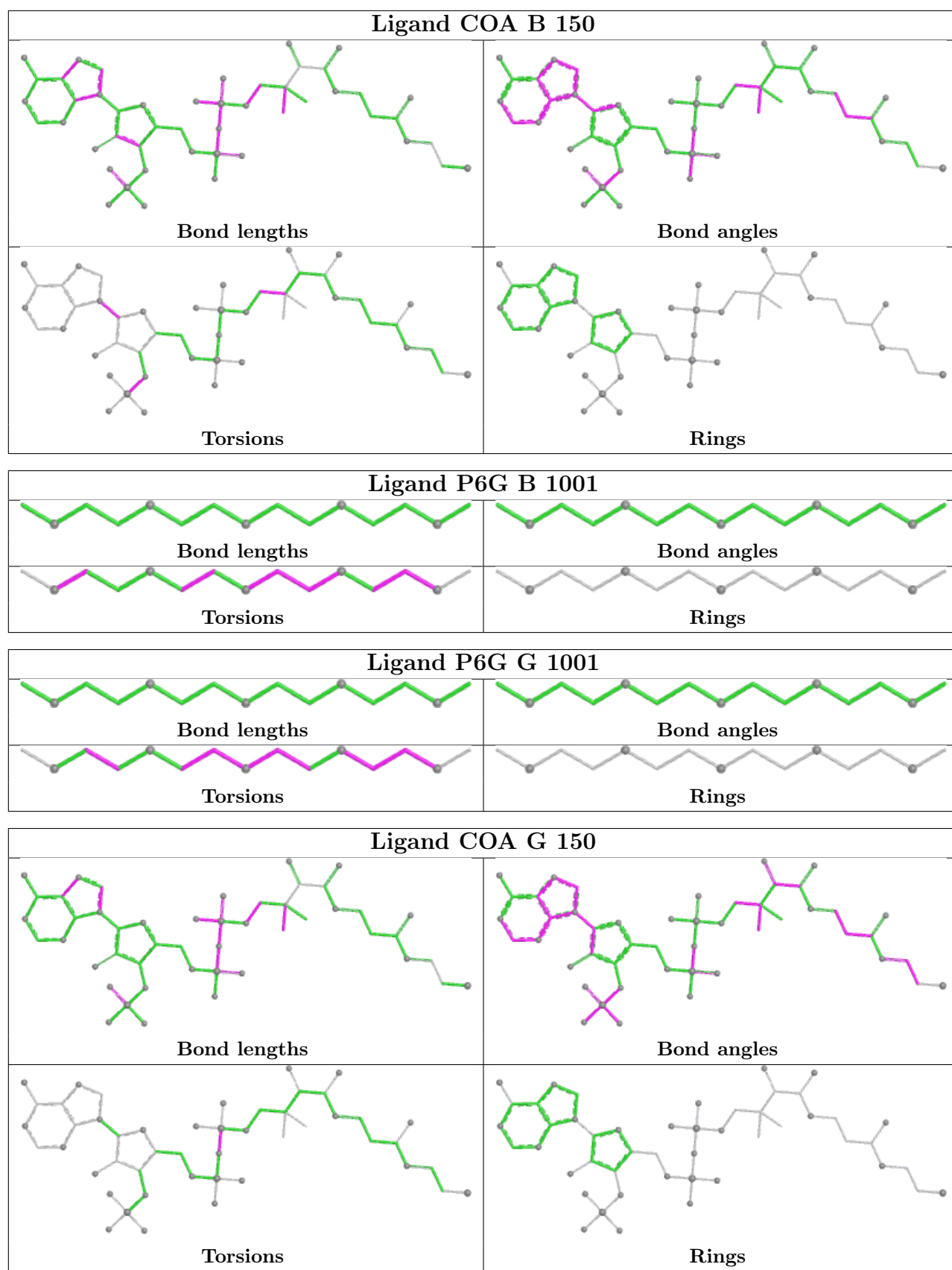
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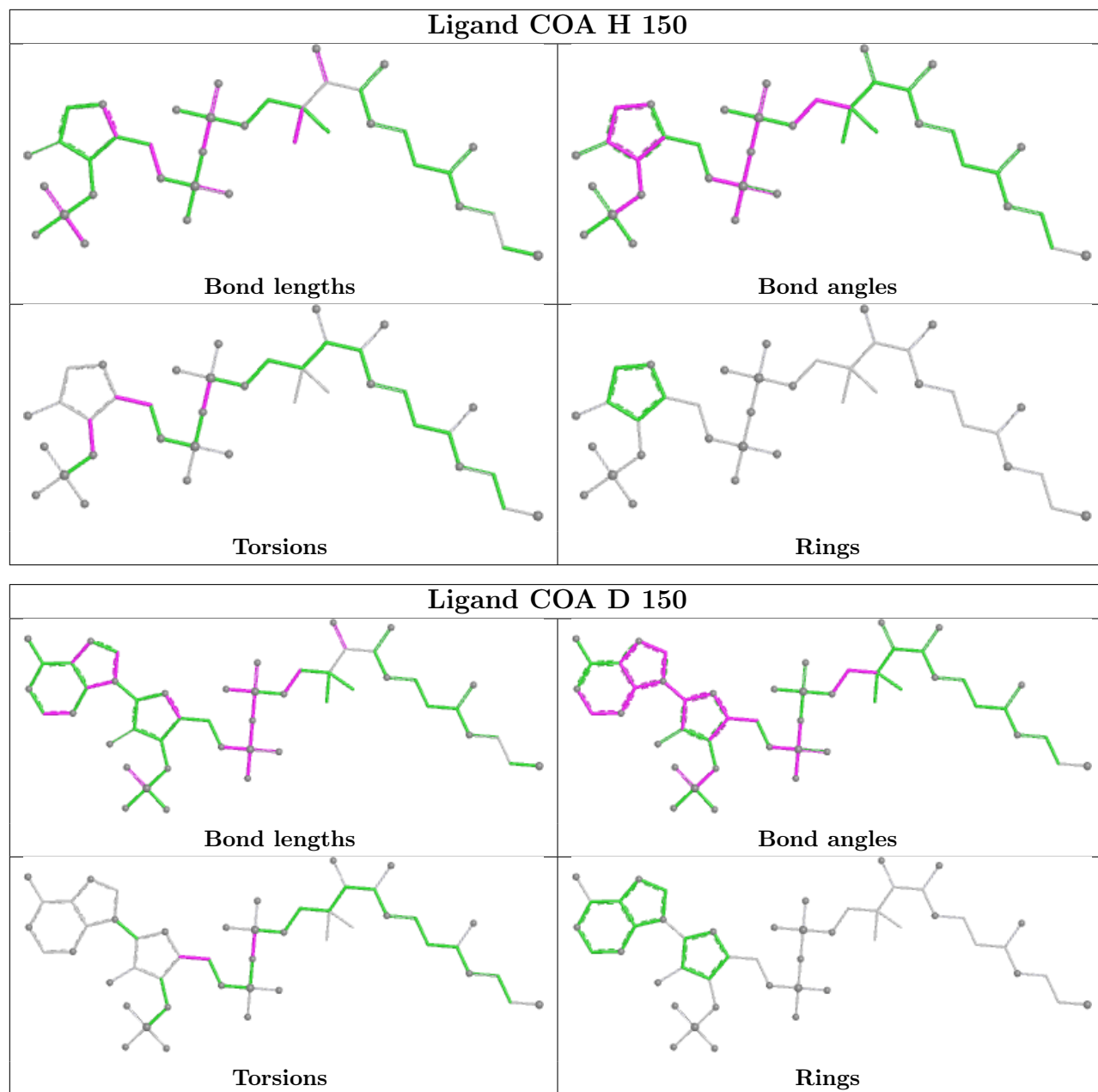
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1001	P6G	1	0
4	A	150	COA	6	0
3	C	149	UOC	1	0
3	D	149	UOC	1	0
3	H	149	UOC	2	0
3	A	149	UOC	6	0
4	B	150	COA	1	0
5	G	1001	P6G	1	0
4	G	150	COA	5	0
4	H	150	COA	3	0
4	E	150	COA	1	0

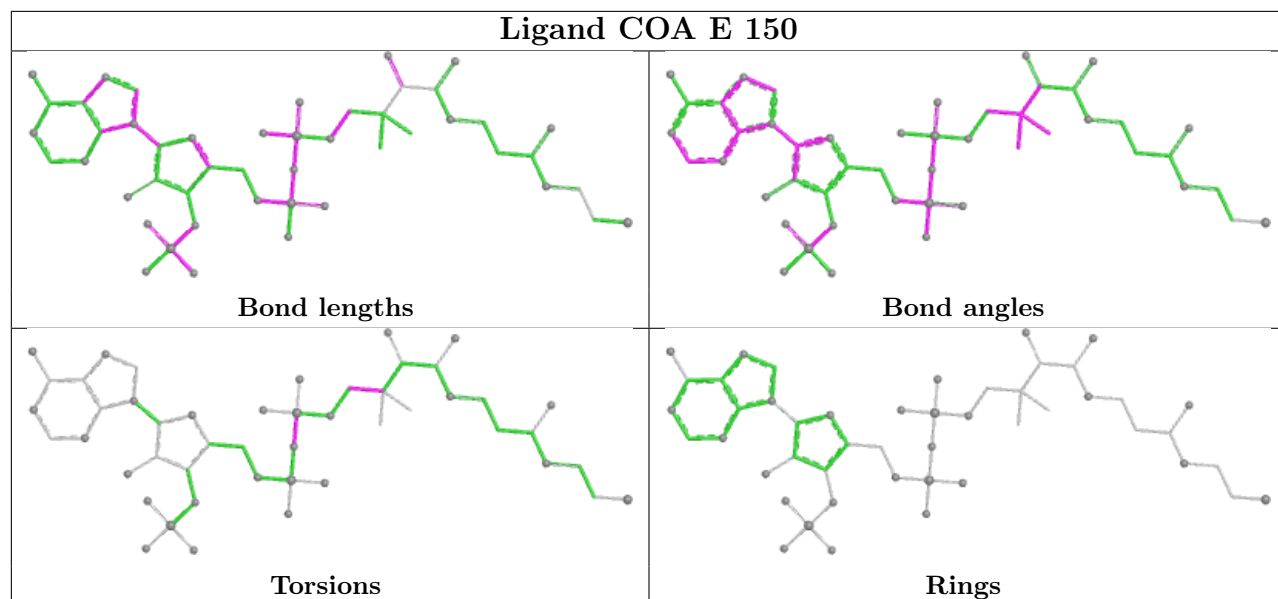
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	138/148 (93%)	-0.01	1 (0%) 84 86	10, 25, 35, 39	7 (5%)
1	B	136/148 (91%)	0.18	4 (2%) 53 58	13, 26, 36, 42	10 (7%)
1	C	137/148 (92%)	-0.08	2 (1%) 72 76	14, 23, 32, 43	10 (7%)
1	D	137/148 (92%)	0.03	1 (0%) 84 86	13, 24, 36, 45	8 (5%)
1	E	138/148 (93%)	0.04	1 (0%) 84 86	18, 24, 34, 40	7 (5%)
1	F	138/148 (93%)	0.09	4 (2%) 53 58	14, 24, 36, 53	12 (8%)
1	G	136/148 (91%)	0.07	0 100 100	13, 25, 33, 38	12 (8%)
1	H	138/148 (93%)	0.16	4 (2%) 53 58	13, 27, 36, 45	6 (4%)
All	All	1098/1184 (92%)	0.06	17 (1%) 72 76	10, 25, 35, 53	72 (6%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	139	GLY	6.2
1	F	2	THR	4.8
1	F	139	GLY	3.7
1	A	139	GLY	3.5
1	H	2	THR	3.5

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 ⓘ

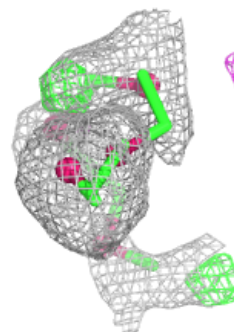
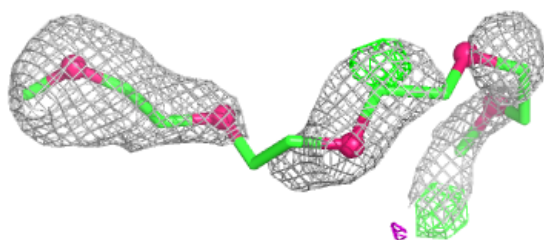
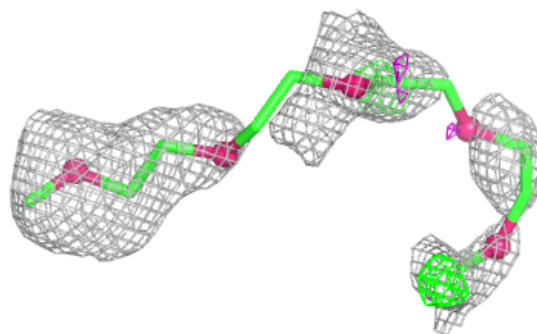
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	UOC	H	149	12/12	0.67	0.16	35,47,53,53	0
3	UOC	F	149	12/12	0.68	0.17	37,46,53,53	0
3	UOC	G	149	12/12	0.69	0.16	37,45,50,51	0
3	UOC	A	149	12/12	0.70	0.20	35,38,45,46	12
3	UOC	B	149	12/12	0.73	0.15	36,46,52,52	0
5	P6G	B	1001	15/19	0.76	0.20	72,77,79,79	0
5	P6G	E	1001	15/19	0.78	0.17	63,67,70,70	0
5	P6G	G	1001	15/19	0.78	0.16	63,67,69,69	0
4	COA	A	150	38/48	0.79	0.16	33,43,54,55	38
5	P6G	C	1001	15/19	0.79	0.14	48,52,53,53	0
4	COA	H	150	38/48	0.81	0.14	33,47,64,64	21
3	UOC	C	149	12/12	0.82	0.12	31,38,42,42	0
3	UOC	D	149	12/12	0.84	0.12	29,38,49,51	0
3	UOC	E	149	12/12	0.86	0.12	26,37,48,49	0
4	COA	B	150	48/48	0.88	0.13	33,43,61,61	33
4	COA	F	150	48/48	0.89	0.13	32,43,56,56	27
4	COA	G	150	48/48	0.90	0.13	28,45,56,57	30
4	COA	C	150	48/48	0.93	0.12	22,34,48,48	17
4	COA	E	150	48/48	0.95	0.10	20,36,52,53	17
4	COA	D	150	48/48	0.95	0.10	21,40,58,60	14
2	CL	A	151	1/1	0.97	0.10	36,36,36,36	0
2	CL	E	151	1/1	0.97	0.10	33,33,33,33	0
2	CL	D	151	1/1	0.98	0.04	27,27,27,27	0
2	CL	G	151	1/1	0.98	0.05	36,36,36,36	0
2	CL	H	151	1/1	0.99	0.06	33,33,33,33	0
2	CL	F	151	1/1	0.99	0.05	25,25,25,25	0
2	CL	C	151	1/1	0.99	0.05	25,25,25,25	0

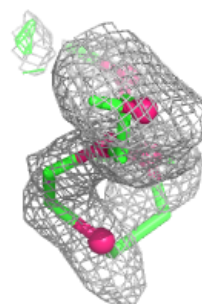
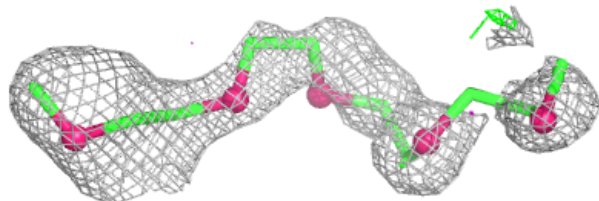
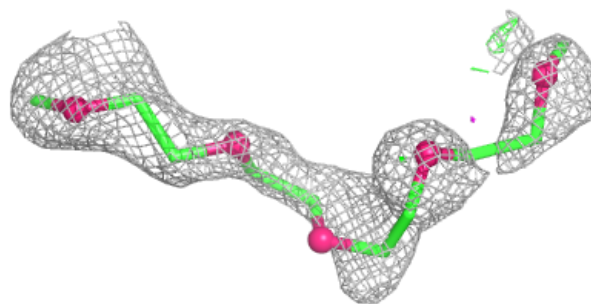
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G B 1001:

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

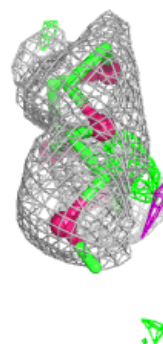
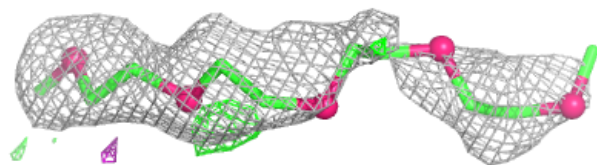
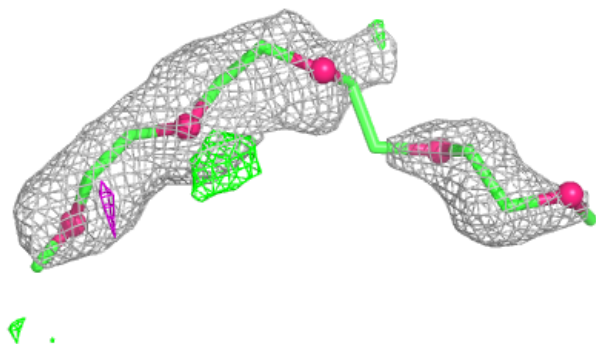
**Electron density around P6G E 1001:**

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

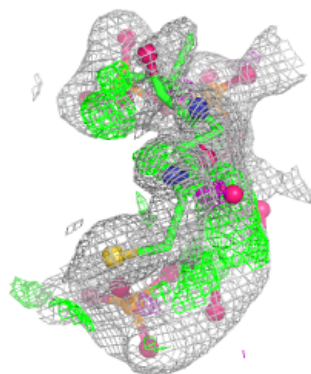
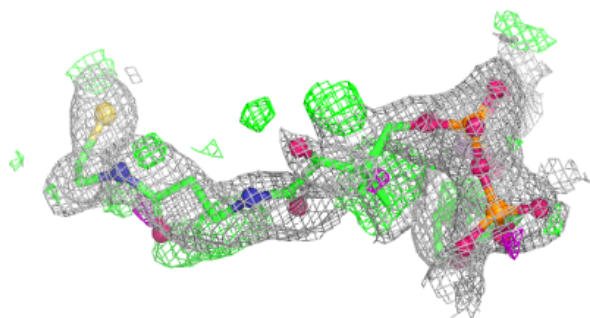
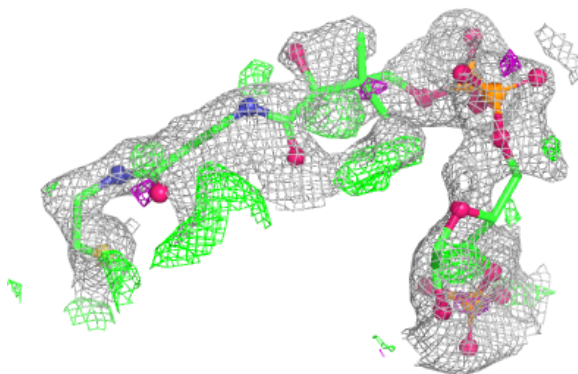


Electron density around P6G G 1001:

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and green (positive)

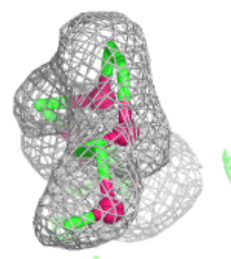
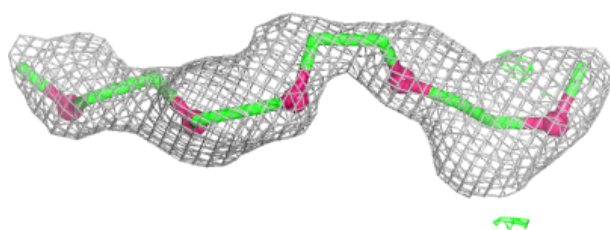
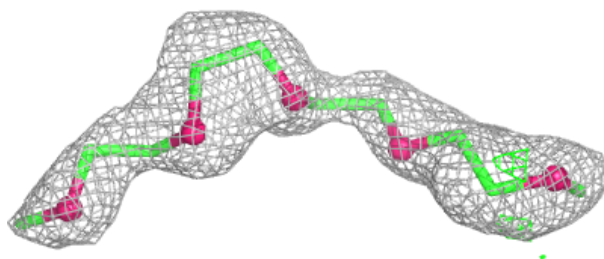
**Electron density around COA A 150:**

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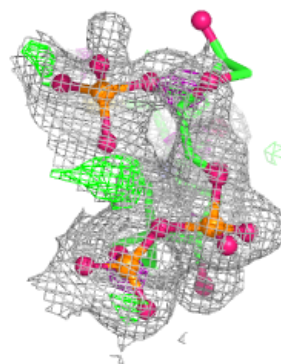
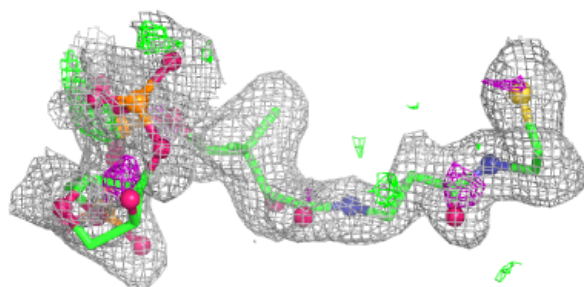
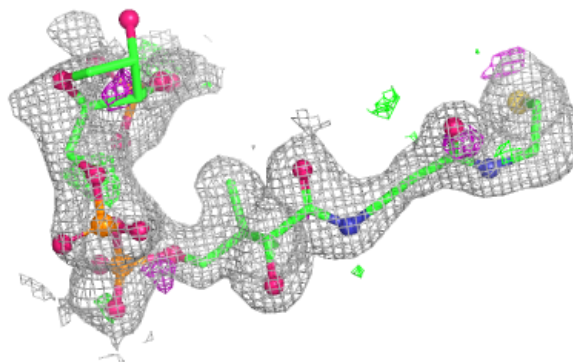


Electron density around P6G C 1001:

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and green (positive)

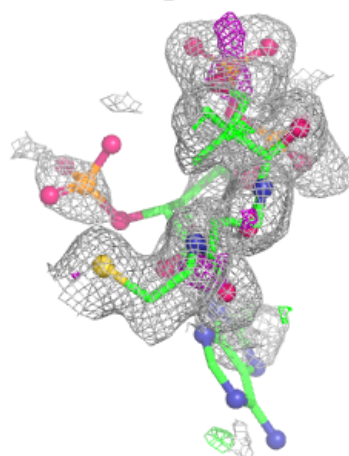
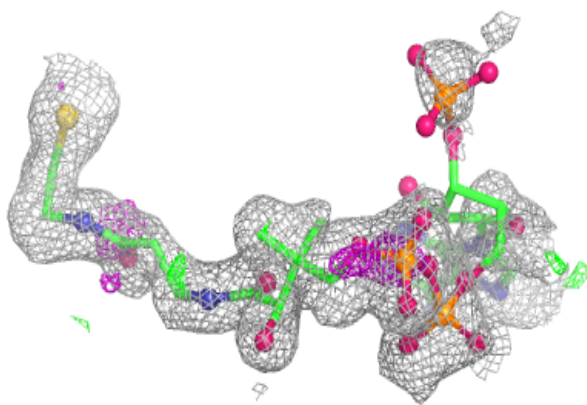
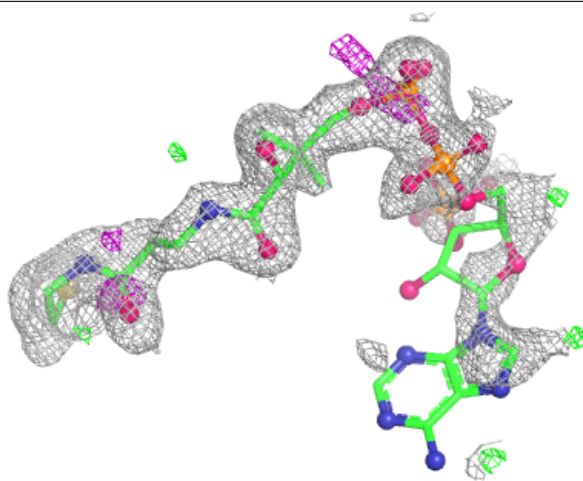
**Electron density around COA H 150:**

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and green (positive)



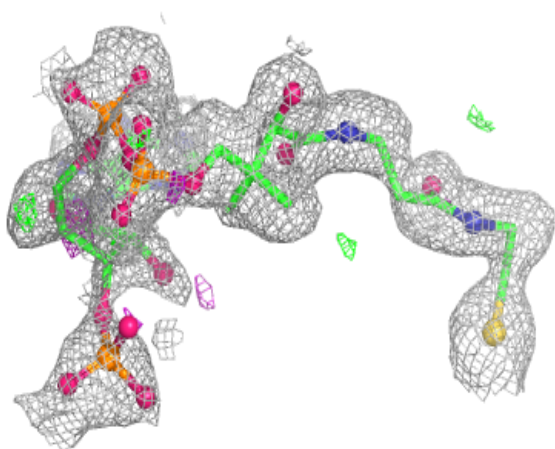
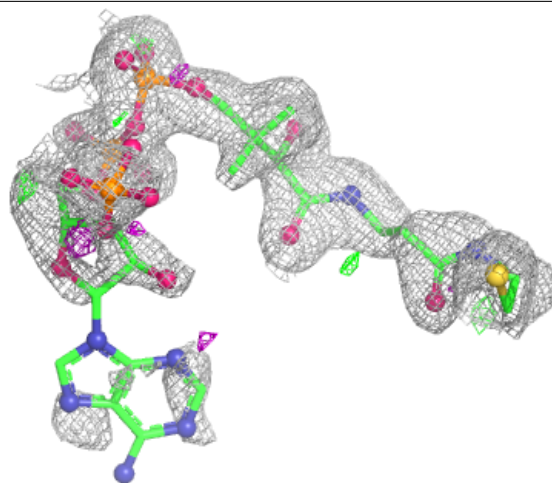
Electron density around COA B 150:

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and green (positive)



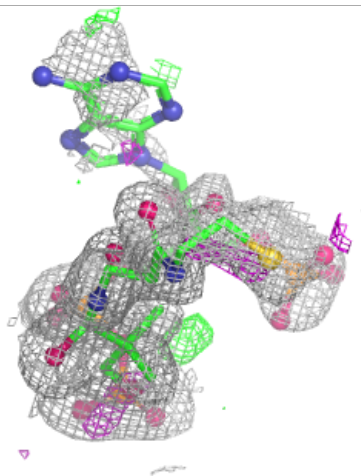
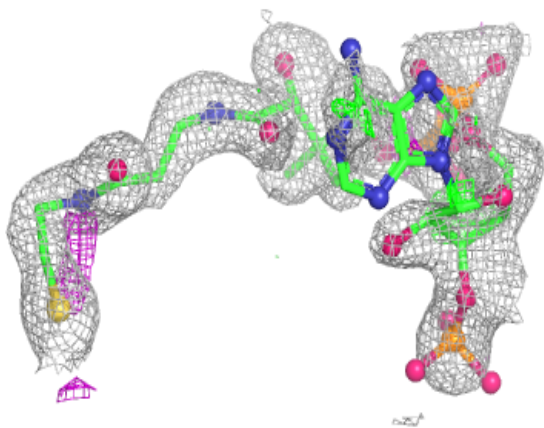
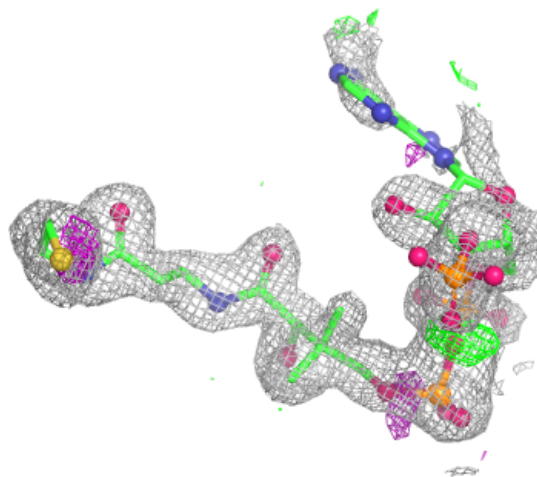
Electron density around COA F 150:

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



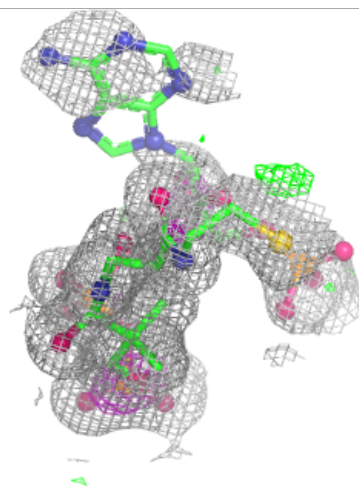
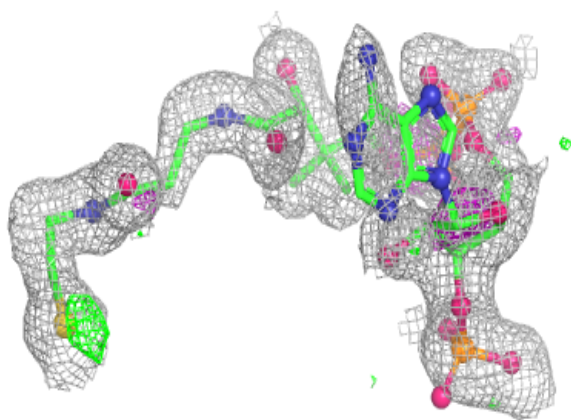
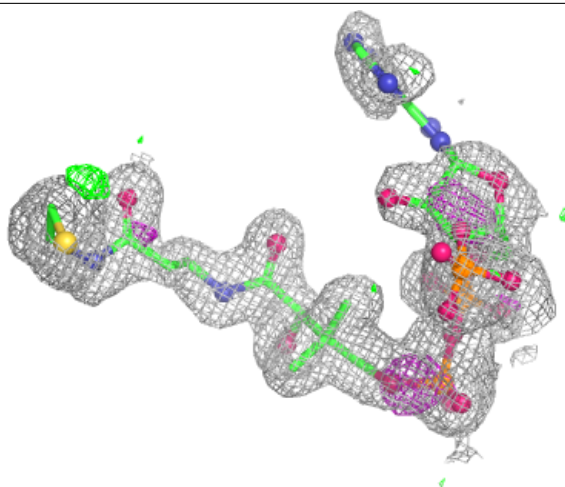
Electron density around COA G 150:

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



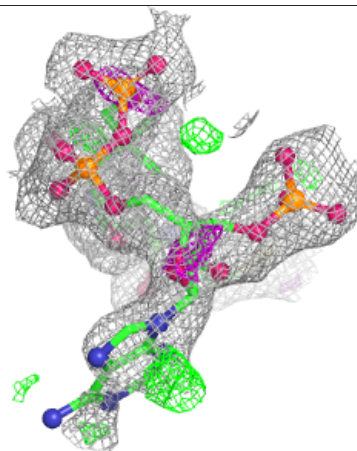
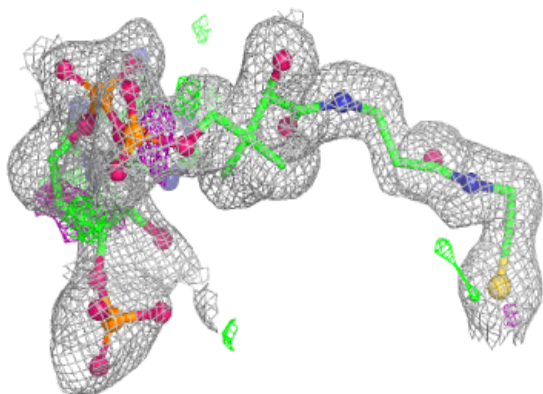
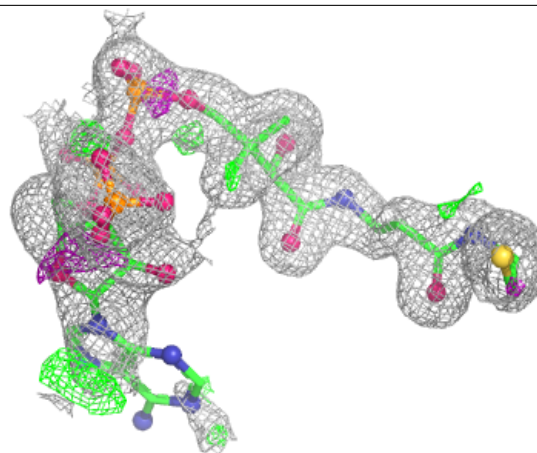
Electron density around COA C 150:

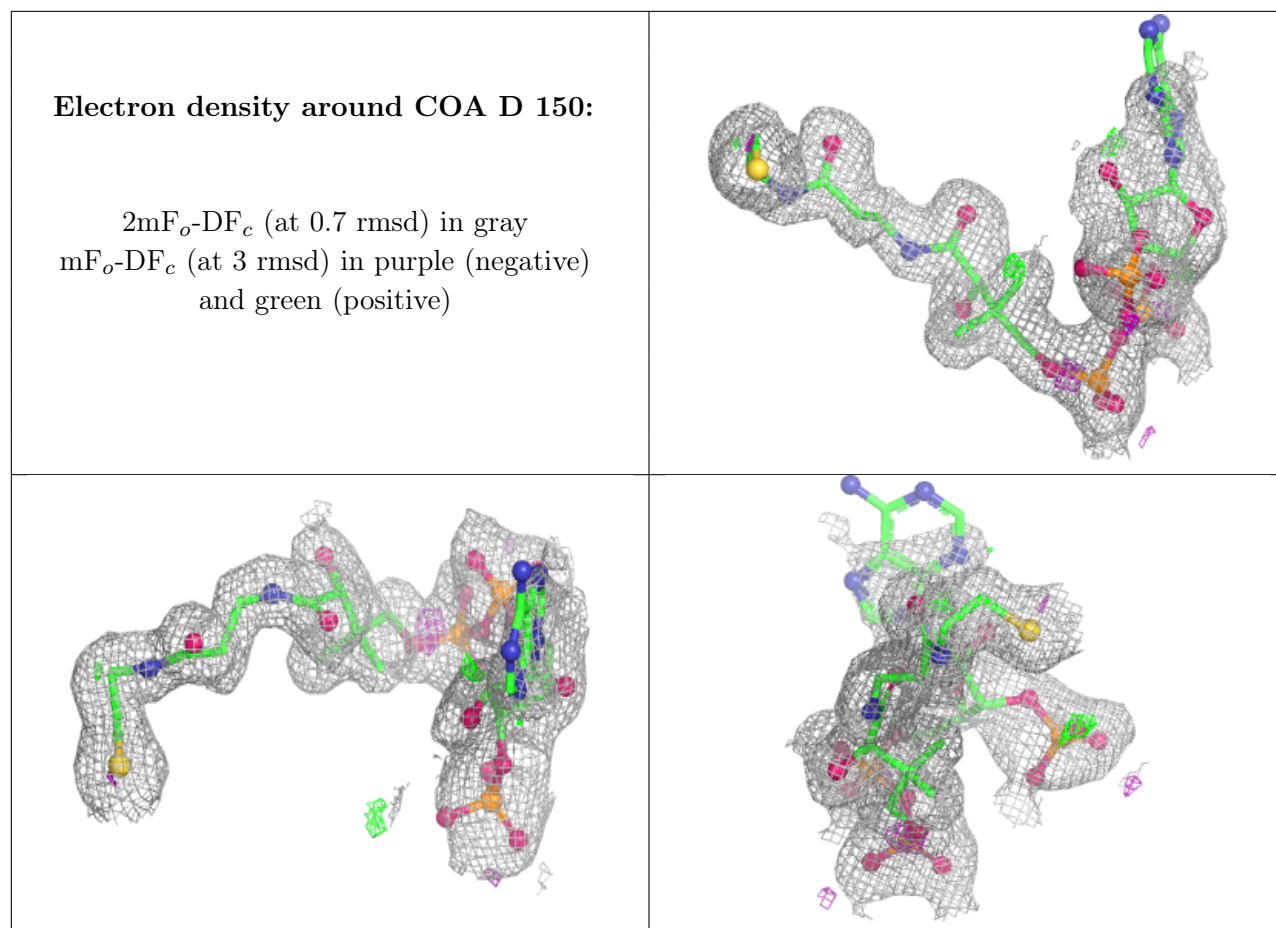
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA E 150:

$2mF_o-DF_c$ (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.