



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 6QKK / pdb_00006qkk
Title : Aplysia californica AChBP in complex with 2-Fluoro-(carbamoylpyridinyl)deschloroepibatidine analogue (1)
Authors : Davis, S.; Bueno, R.V.; Dawson, A.; Hunter, W.N.
Deposited on : 2019-01-29
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

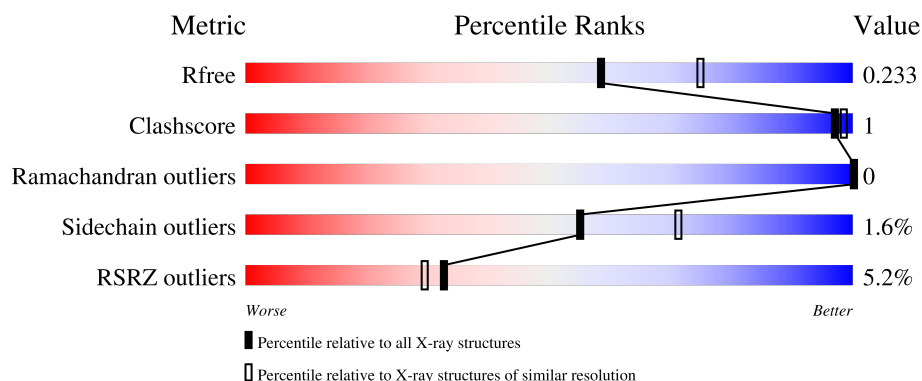
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



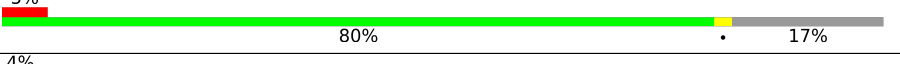
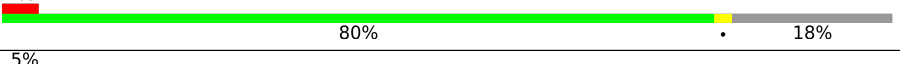
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	249	4% 80% 18%
1	B	249	3% 78% 17%
1	C	249	5% 82% 16%
1	D	249	5% 80% 17%
1	E	249	4% 79% 18%

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Mol	Chain	Length	Quality of chain
1	F	249	
1	G	249	
1	H	249	
1	I	249	
1	J	249	

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
6	OXL	B	403	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18102 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1638	1037	266	325	10			
1	B	206	Total	C	N	O	S	0	1	0
			1649	1043	270	326	10			
1	C	209	Total	C	N	O	S	0	1	0
			1665	1051	274	330	10			
1	D	206	Total	C	N	O	S	0	1	0
			1649	1043	270	326	10			
1	E	205	Total	C	N	O	S	0	1	0
			1638	1037	266	325	10			
1	F	205	Total	C	N	O	S	0	1	0
			1638	1037	266	325	10			
1	G	206	Total	C	N	O	S	0	1	0
			1649	1043	270	326	10			
1	H	206	Total	C	N	O	S	0	1	0
			1649	1043	270	326	10			
1	I	205	Total	C	N	O	S	0	1	0
			1638	1037	266	325	10			
1	J	206	Total	C	N	O	S	0	1	0
			1649	1043	270	326	10			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	VAL	ALA	conflict	UNP Q8WSF8
A	155	VAL	ALA	conflict	UNP Q8WSF8
A	237	GLU	-	expression tag	UNP Q8WSF8
A	238	ASN	-	expression tag	UNP Q8WSF8
A	239	LEU	-	expression tag	UNP Q8WSF8
A	240	TYR	-	expression tag	UNP Q8WSF8
A	241	PHE	-	expression tag	UNP Q8WSF8
A	242	GLN	-	expression tag	UNP Q8WSF8
A	243	GLY	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	244	HIS	-	expression tag	UNP Q8WSF8
A	245	HIS	-	expression tag	UNP Q8WSF8
A	246	HIS	-	expression tag	UNP Q8WSF8
A	247	HIS	-	expression tag	UNP Q8WSF8
A	248	HIS	-	expression tag	UNP Q8WSF8
A	249	HIS	-	expression tag	UNP Q8WSF8
B	60	VAL	ALA	conflict	UNP Q8WSF8
B	155	VAL	ALA	conflict	UNP Q8WSF8
B	237	GLU	-	expression tag	UNP Q8WSF8
B	238	ASN	-	expression tag	UNP Q8WSF8
B	239	LEU	-	expression tag	UNP Q8WSF8
B	240	TYR	-	expression tag	UNP Q8WSF8
B	241	PHE	-	expression tag	UNP Q8WSF8
B	242	GLN	-	expression tag	UNP Q8WSF8
B	243	GLY	-	expression tag	UNP Q8WSF8
B	244	HIS	-	expression tag	UNP Q8WSF8
B	245	HIS	-	expression tag	UNP Q8WSF8
B	246	HIS	-	expression tag	UNP Q8WSF8
B	247	HIS	-	expression tag	UNP Q8WSF8
B	248	HIS	-	expression tag	UNP Q8WSF8
B	249	HIS	-	expression tag	UNP Q8WSF8
C	60	VAL	ALA	conflict	UNP Q8WSF8
C	155	VAL	ALA	conflict	UNP Q8WSF8
C	237	GLU	-	expression tag	UNP Q8WSF8
C	238	ASN	-	expression tag	UNP Q8WSF8
C	239	LEU	-	expression tag	UNP Q8WSF8
C	240	TYR	-	expression tag	UNP Q8WSF8
C	241	PHE	-	expression tag	UNP Q8WSF8
C	242	GLN	-	expression tag	UNP Q8WSF8
C	243	GLY	-	expression tag	UNP Q8WSF8
C	244	HIS	-	expression tag	UNP Q8WSF8
C	245	HIS	-	expression tag	UNP Q8WSF8
C	246	HIS	-	expression tag	UNP Q8WSF8
C	247	HIS	-	expression tag	UNP Q8WSF8
C	248	HIS	-	expression tag	UNP Q8WSF8
C	249	HIS	-	expression tag	UNP Q8WSF8
D	60	VAL	ALA	conflict	UNP Q8WSF8
D	155	VAL	ALA	conflict	UNP Q8WSF8
D	237	GLU	-	expression tag	UNP Q8WSF8
D	238	ASN	-	expression tag	UNP Q8WSF8
D	239	LEU	-	expression tag	UNP Q8WSF8
D	240	TYR	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	241	PHE	-	expression tag	UNP Q8WSF8
D	242	GLN	-	expression tag	UNP Q8WSF8
D	243	GLY	-	expression tag	UNP Q8WSF8
D	244	HIS	-	expression tag	UNP Q8WSF8
D	245	HIS	-	expression tag	UNP Q8WSF8
D	246	HIS	-	expression tag	UNP Q8WSF8
D	247	HIS	-	expression tag	UNP Q8WSF8
D	248	HIS	-	expression tag	UNP Q8WSF8
D	249	HIS	-	expression tag	UNP Q8WSF8
E	60	VAL	ALA	conflict	UNP Q8WSF8
E	155	VAL	ALA	conflict	UNP Q8WSF8
E	237	GLU	-	expression tag	UNP Q8WSF8
E	238	ASN	-	expression tag	UNP Q8WSF8
E	239	LEU	-	expression tag	UNP Q8WSF8
E	240	TYR	-	expression tag	UNP Q8WSF8
E	241	PHE	-	expression tag	UNP Q8WSF8
E	242	GLN	-	expression tag	UNP Q8WSF8
E	243	GLY	-	expression tag	UNP Q8WSF8
E	244	HIS	-	expression tag	UNP Q8WSF8
E	245	HIS	-	expression tag	UNP Q8WSF8
E	246	HIS	-	expression tag	UNP Q8WSF8
E	247	HIS	-	expression tag	UNP Q8WSF8
E	248	HIS	-	expression tag	UNP Q8WSF8
E	249	HIS	-	expression tag	UNP Q8WSF8
F	60	VAL	ALA	conflict	UNP Q8WSF8
F	155	VAL	ALA	conflict	UNP Q8WSF8
F	237	GLU	-	expression tag	UNP Q8WSF8
F	238	ASN	-	expression tag	UNP Q8WSF8
F	239	LEU	-	expression tag	UNP Q8WSF8
F	240	TYR	-	expression tag	UNP Q8WSF8
F	241	PHE	-	expression tag	UNP Q8WSF8
F	242	GLN	-	expression tag	UNP Q8WSF8
F	243	GLY	-	expression tag	UNP Q8WSF8
F	244	HIS	-	expression tag	UNP Q8WSF8
F	245	HIS	-	expression tag	UNP Q8WSF8
F	246	HIS	-	expression tag	UNP Q8WSF8
F	247	HIS	-	expression tag	UNP Q8WSF8
F	248	HIS	-	expression tag	UNP Q8WSF8
F	249	HIS	-	expression tag	UNP Q8WSF8
G	60	VAL	ALA	conflict	UNP Q8WSF8
G	155	VAL	ALA	conflict	UNP Q8WSF8
G	237	GLU	-	expression tag	UNP Q8WSF8

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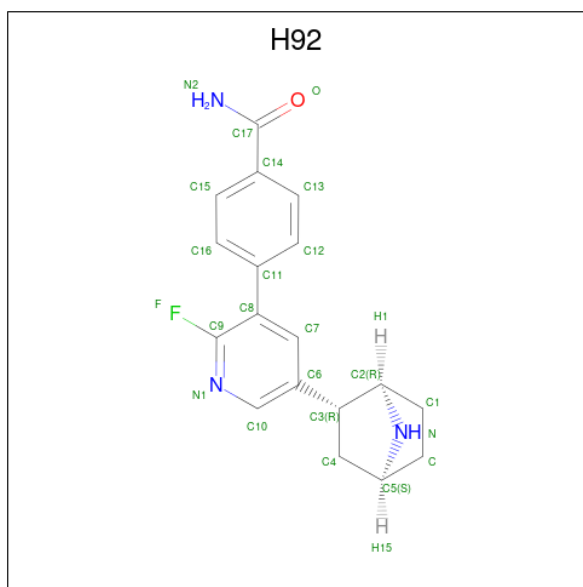
Chain	Residue	Modelled	Actual	Comment	Reference
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G	239	LEU	-	expression tag	UNP Q8WSF8
G	240	TYR	-	expression tag	UNP Q8WSF8
G	241	PHE	-	expression tag	UNP Q8WSF8
G	242	GLN	-	expression tag	UNP Q8WSF8
G	243	GLY	-	expression tag	UNP Q8WSF8
G	244	HIS	-	expression tag	UNP Q8WSF8
G	245	HIS	-	expression tag	UNP Q8WSF8
G	246	HIS	-	expression tag	UNP Q8WSF8
G	247	HIS	-	expression tag	UNP Q8WSF8
G	248	HIS	-	expression tag	UNP Q8WSF8
G	249	HIS	-	expression tag	UNP Q8WSF8
H	60	VAL	ALA	conflict	UNP Q8WSF8
H	155	VAL	ALA	conflict	UNP Q8WSF8
H	237	GLU	-	expression tag	UNP Q8WSF8
H	238	ASN	-	expression tag	UNP Q8WSF8
H	239	LEU	-	expression tag	UNP Q8WSF8
H	240	TYR	-	expression tag	UNP Q8WSF8
H	241	PHE	-	expression tag	UNP Q8WSF8
H	242	GLN	-	expression tag	UNP Q8WSF8
H	243	GLY	-	expression tag	UNP Q8WSF8
H	244	HIS	-	expression tag	UNP Q8WSF8
H	245	HIS	-	expression tag	UNP Q8WSF8
H	246	HIS	-	expression tag	UNP Q8WSF8
H	247	HIS	-	expression tag	UNP Q8WSF8
H	248	HIS	-	expression tag	UNP Q8WSF8
H	249	HIS	-	expression tag	UNP Q8WSF8
I	60	VAL	ALA	conflict	UNP Q8WSF8
I	155	VAL	ALA	conflict	UNP Q8WSF8
I	237	GLU	-	expression tag	UNP Q8WSF8
I	238	ASN	-	expression tag	UNP Q8WSF8
I	239	LEU	-	expression tag	UNP Q8WSF8
I	240	TYR	-	expression tag	UNP Q8WSF8
I	241	PHE	-	expression tag	UNP Q8WSF8
I	242	GLN	-	expression tag	UNP Q8WSF8
I	243	GLY	-	expression tag	UNP Q8WSF8
I	244	HIS	-	expression tag	UNP Q8WSF8
I	245	HIS	-	expression tag	UNP Q8WSF8
I	246	HIS	-	expression tag	UNP Q8WSF8
I	247	HIS	-	expression tag	UNP Q8WSF8
I	248	HIS	-	expression tag	UNP Q8WSF8
I	249	HIS	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	60	VAL	ALA	conflict	UNP Q8WSF8
J	155	VAL	ALA	conflict	UNP Q8WSF8
J	237	GLU	-	expression tag	UNP Q8WSF8
J	238	ASN	-	expression tag	UNP Q8WSF8
J	239	LEU	-	expression tag	UNP Q8WSF8
J	240	TYR	-	expression tag	UNP Q8WSF8
J	241	PHE	-	expression tag	UNP Q8WSF8
J	242	GLN	-	expression tag	UNP Q8WSF8
J	243	GLY	-	expression tag	UNP Q8WSF8
J	244	HIS	-	expression tag	UNP Q8WSF8
J	245	HIS	-	expression tag	UNP Q8WSF8
J	246	HIS	-	expression tag	UNP Q8WSF8
J	247	HIS	-	expression tag	UNP Q8WSF8
J	248	HIS	-	expression tag	UNP Q8WSF8
J	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is 4-[5-[(1 {R},2 {R},4 {S})-7-azabicyclo[2.2.1]heptan-2-yl]-2-fluoranyl-pyridin-3-yl]benzamide (CCD ID: H92) (formula: C₁₈H₁₈FN₃O) (labeled as "Ligand of Interest" by depositor).



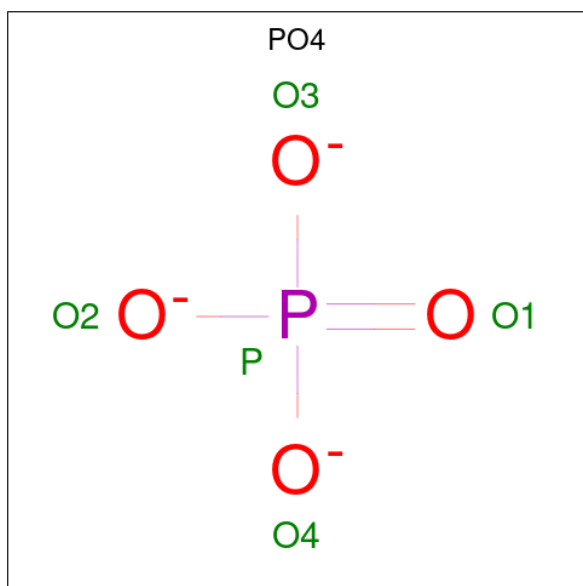
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	B	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	C	1	Total	C	F	N	O	0	0
			23	18	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	E	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	F	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	G	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	H	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	I	1	Total	C	F	N	O	0	0
			23	18	1	3	1		
2	J	1	Total	C	F	N	O	0	0
			23	18	1	3	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



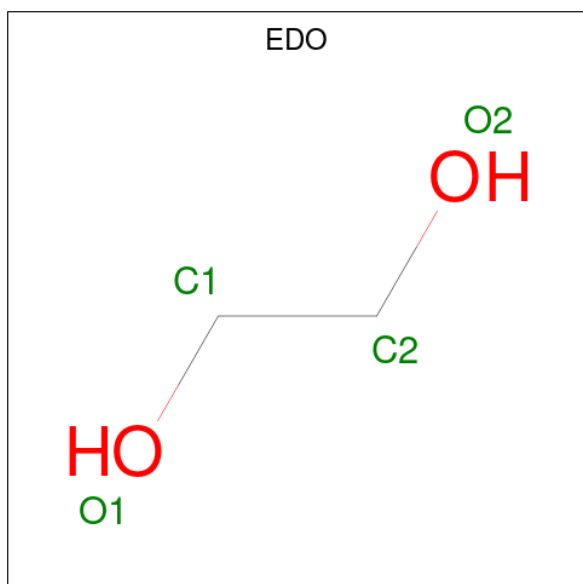
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		
3	I	1	Total	O	P	0	0
			5	4	1		
3	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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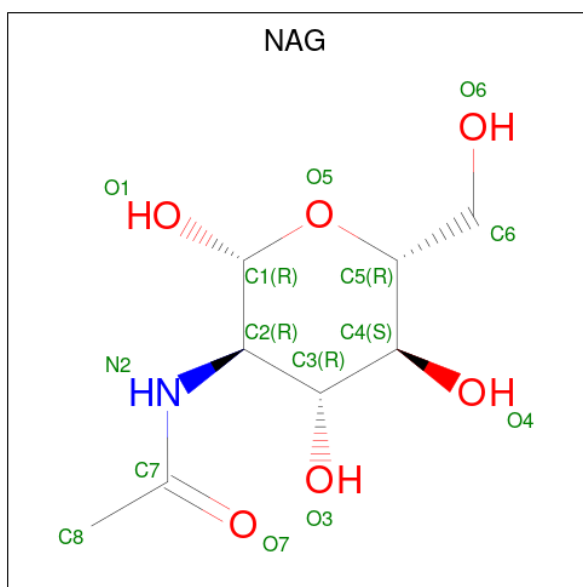
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

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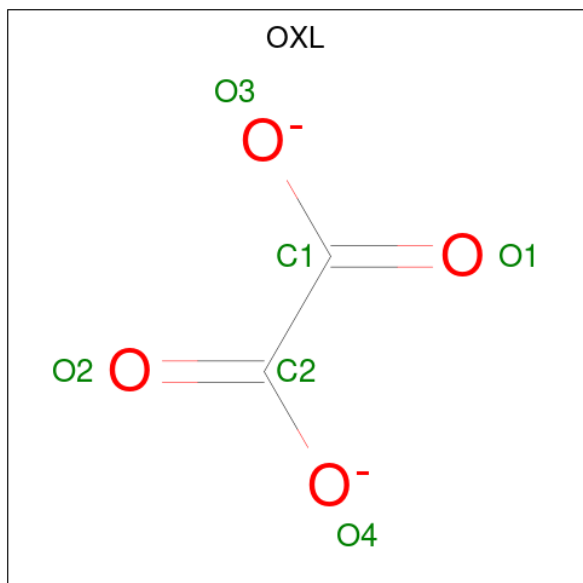
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	2	4		

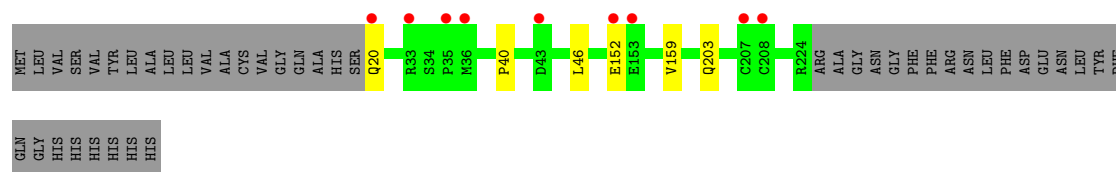
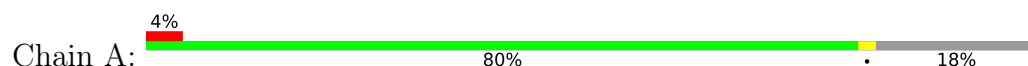
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	115	Total	O	0	0
			115	115		
7	B	135	Total	O	0	0
			135	135		
7	C	127	Total	O	0	0
			127	127		
7	D	104	Total	O	0	0
			104	104		
7	E	124	Total	O	0	0
			124	124		
7	F	112	Total	O	0	0
			112	112		
7	G	113	Total	O	0	0
			113	113		
7	H	104	Total	O	0	0
			104	104		
7	I	92	Total	O	0	0
			92	92		
7	J	112	Total	O	0	0
			112	112		

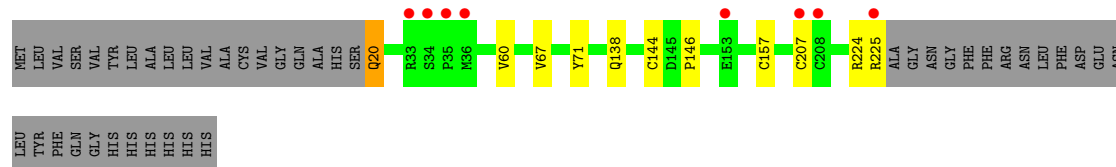
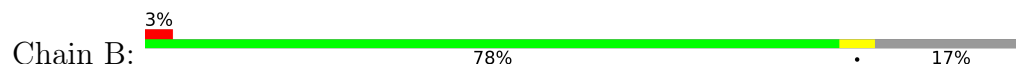
3 Residue-property plots [i](#)

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.

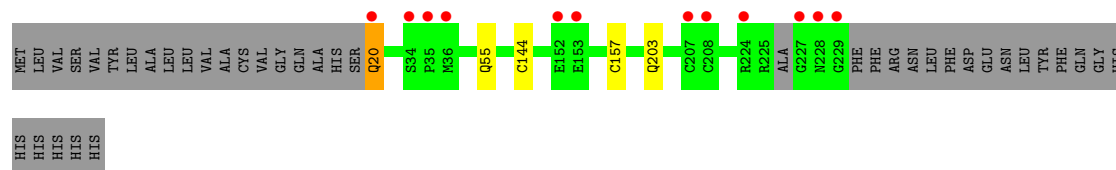
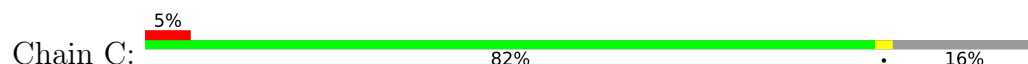
- Molecule 1: Soluble acetylcholine receptor



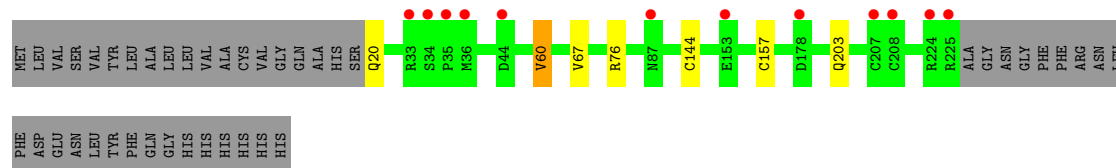
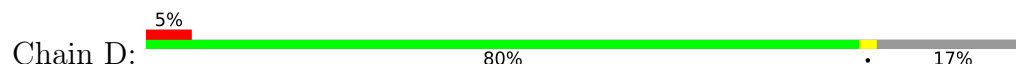
- Molecule 1: Soluble acetylcholine receptor

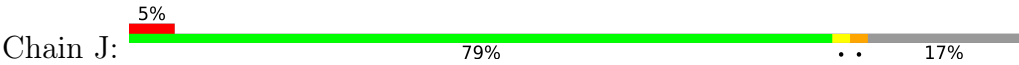


- Molecule 1: Soluble acetylcholine receptor



- Molecule 1: Soluble acetylcholine receptor





MET	LEU	PHE	ASP	GLU	SER	VAL	ASN	TYR	LEU	ALA	LEU	LEU	VAL	ALA	CYS	VAL	GLY	GLN	ALA	HIS	SER	Q20	R33	S34	P35	M36	D43	V60	V67	E88	M133	R139	C144	E153	C157	D178	Q203	C207	C208	R225	ALA	GLY	ASN	GLY	PHE	PHE	ARG	ASN
LEU	PHE	ASP	GLU	SER	VAL	ASN	TYR	LEU	ALA	LEU	LEU	VAL	ALA	CYS	VAL	GLY	GLN	ALA	HIS	SER	Q20	R33	S34	P35	M36	D43	V60	V67	E88	M133	R139	C144	E153	C157	D178	Q203	C207	C208	R225	ALA	GLY	ASN	GLY	PHE	PHE	ARG	ASN	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.00Å 131.58Å 131.82Å 90.00° 102.77° 90.00°	Depositor
Resolution (Å)	48.88 – 2.20 48.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.88-2.20) 99.9 (48.88-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.199 , 0.228 0.204 , 0.233	Depositor DCC
R_{free} test set	8867 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	1.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18102	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG, H92, PO4, OXL

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	0.57	0/1682	0.74	0/2295
1	B	0.58	0/1693	0.75	0/2309
1	C	0.58	0/1708	0.75	0/2327
1	D	0.57	0/1693	0.73	0/2309
1	E	0.58	0/1682	0.75	0/2295
1	F	0.57	0/1682	0.73	0/2295
1	G	0.57	0/1693	0.74	0/2309
1	H	0.57	0/1693	0.74	0/2309
1	I	0.58	0/1682	0.74	0/2295
1	J	0.57	0/1693	0.75	0/2309
All	All	0.57	0/16901	0.74	0/23052

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
1	D	0	1
1	J	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	CYS	Peptide
1	B	224	ARG	Sidechain
1	B	225	ARG	Sidechain
1	D	76	ARG	Sidechain
1	J	139	ARG	Sidechain
1	J	225	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1638	0	1569	1	0
1	B	1649	0	1583	5	0
1	C	1665	0	1594	4	0
1	D	1649	0	1582	2	0
1	E	1638	0	1570	4	0
1	F	1638	0	1570	2	0
1	G	1649	0	1583	3	0
1	H	1649	0	1583	2	0
1	I	1638	0	1569	2	0
1	J	1649	0	1582	4	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
2	E	23	0	0	0	0
2	F	23	0	0	0	0
2	G	23	0	0	0	0
2	H	23	0	0	0	0
2	I	23	0	0	0	0
2	J	23	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
3	G	5	0	0	0	0
3	H	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	5	0	0	0	0
3	J	5	0	0	0	0
4	A	16	0	24	0	0
4	B	16	0	24	0	0
4	C	16	0	24	1	0
4	D	16	0	24	0	0
4	E	16	0	24	0	0
4	F	16	0	24	0	0
4	G	16	0	24	0	0
4	H	12	0	18	0	0
4	I	20	0	30	0	0
4	J	16	0	24	0	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
6	B	6	0	0	0	0
7	A	115	0	0	0	0
7	B	135	0	0	0	0
7	C	127	0	0	0	0
7	D	104	0	0	0	0
7	E	124	0	0	0	0
7	F	112	0	0	0	0
7	G	113	0	0	0	0
7	H	104	0	0	0	0
7	I	92	0	0	0	0
7	J	112	0	0	0	0
All	All	18102	0	16077	28	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 1.

All (28) 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:C:20:GLN:HE21	1:C:20:GLN:HA	1.68	0.57
1:C:20:GLN:HE21	1:C:20:GLN:CA	2.19	0.56
1:B:144:CYS:SG	1:B:157[B]:CYS:HB3	2.48	0.54
1:J:144:CYS:SG	1:J:157[B]:CYS:HB3	2.50	0.52
1:E:144:CYS:SG	1:E:157[B]:CYS:HB3	2.49	0.52
1:G:60:VAL:HG22	1:G:67:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:CYS:SG	1:C:157[B]:CYS:HB3	2.50	0.50
1:D:144:CYS:SG	1:D:157[B]:CYS:HB3	2.52	0.49
1:F:144:CYS:SG	1:F:157[B]:CYS:HB3	2.53	0.48
1:H:144:CYS:SG	1:H:157[B]:CYS:HB3	2.53	0.48
1:B:60:VAL:HG22	1:B:67:VAL:HG22	1.97	0.47
1:H:67:VAL:HG21	1:H:144:CYS:SG	2.55	0.46
1:E:60:VAL:HG22	1:E:67:VAL:HG22	1.98	0.46
1:E:67:VAL:HG21	1:E:144:CYS:SG	2.56	0.45
1:B:71:TYR:OH	1:B:138:GLN:NE2	2.50	0.45
1:I:113:THR:O	1:J:139:ARG:HD2	2.17	0.44
1:G:144:CYS:SG	1:G:157[B]:CYS:HB3	2.58	0.44
1:J:60:VAL:HG22	1:J:67:VAL:HG22	2.01	0.43
1:B:20:GLN:N	1:B:20:GLN:OE1	2.51	0.43
1:A:40:PRO:HB3	1:A:46:LEU:HB2	2.02	0.42
1:I:144:CYS:SG	1:I:157[B]:CYS:HB3	2.60	0.42
1:B:60:VAL:HG13	1:B:146:PRO:HG3	2.02	0.42
1:E:60:VAL:HG13	1:E:146:PRO:HG3	2.02	0.42
1:G:144:CYS:SG	1:G:157[B]:CYS:CB	3.08	0.41
1:D:60:VAL:HG22	1:D:67:VAL:HG22	2.02	0.41
1:F:60:VAL:HG22	1:F:67:VAL:HG22	2.03	0.40
1:C:55:GLN:HE21	4:C:404:EDO:C2	2.35	0.40
1:J:133:MET:HE2	1:J:133:MET:HB2	1.92	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	204/249 (82%)	202 (99%)	2 (1%)	0	100	100
1	B	205/249 (82%)	204 (100%)	1 (0%)	0	100	100
1	C	206/249 (83%)	204 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	205/249 (82%)	204 (100%)	1 (0%)	0	100	100
1	E	204/249 (82%)	202 (99%)	2 (1%)	0	100	100
1	F	204/249 (82%)	201 (98%)	3 (2%)	0	100	100
1	G	205/249 (82%)	204 (100%)	1 (0%)	0	100	100
1	H	205/249 (82%)	202 (98%)	3 (2%)	0	100	100
1	I	204/249 (82%)	203 (100%)	1 (0%)	0	100	100
1	J	205/249 (82%)	204 (100%)	1 (0%)	0	100	100
All	All	2047/2490 (82%)	2030 (99%)	17 (1%)	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	189/224 (84%)	185 (98%)	4 (2%)	47	63
1	B	190/224 (85%)	189 (100%)	1 (0%)	81	90
1	C	191/224 (85%)	189 (99%)	2 (1%)	68	81
1	D	190/224 (85%)	187 (98%)	3 (2%)	55	71
1	E	189/224 (84%)	185 (98%)	4 (2%)	47	63
1	F	189/224 (84%)	186 (98%)	3 (2%)	55	71
1	G	190/224 (85%)	186 (98%)	4 (2%)	47	63
1	H	190/224 (85%)	187 (98%)	3 (2%)	55	71
1	I	189/224 (84%)	187 (99%)	2 (1%)	65	79
1	J	190/224 (85%)	185 (97%)	5 (3%)	40	55
All	All	1897/2240 (85%)	1866 (98%)	31 (2%)	55	71

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	152	GLU
1	A	159	VAL
1	A	203	GLN
1	B	20	GLN
1	C	20	GLN
1	C	203	GLN
1	D	20	GLN
1	D	60	VAL
1	D	203	GLN
1	E	20	GLN
1	E	60	VAL
1	E	201	GLN
1	E	203	GLN
1	F	20	GLN
1	F	201	GLN
1	F	203	GLN
1	G	20	GLN
1	G	60	VAL
1	G	122	GLN
1	G	203	GLN
1	H	20	GLN
1	H	60	VAL
1	H	203	GLN
1	I	20	GLN
1	I	122	GLN
1	J	20	GLN
1	J	60	VAL
1	J	133	MET
1	J	203	GLN
1	J	225	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	74	GLN
1	A	87	ASN
1	A	216	ASN
1	B	20	GLN
1	B	32	ASN
1	B	87	ASN
1	B	91	ASN

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Mol	Chain	Res	Type
1	B	201	GLN
1	B	216	ASN
1	C	20	GLN
1	C	32	ASN
1	C	55	GLN
1	C	216	ASN
1	D	32	ASN
1	D	216	ASN
1	E	32	ASN
1	E	55	GLN
1	E	216	ASN
1	F	32	ASN
1	F	74	GLN
1	F	87	ASN
1	F	138	GLN
1	F	203	GLN
1	F	216	ASN
1	G	32	ASN
1	G	74	GLN
1	G	87	ASN
1	G	138	GLN
1	G	201	GLN
1	G	203	GLN
1	G	216	ASN
1	H	32	ASN
1	H	55	GLN
1	H	87	ASN
1	H	138	GLN
1	H	216	ASN
1	I	32	ASN
1	I	55	GLN
1	I	87	ASN
1	I	138	GLN
1	I	216	ASN
1	J	32	ASN
1	J	74	GLN
1	J	87	ASN
1	J	138	GLN
1	J	216	ASN

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 ⓘ

65 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
6	OXL	B	403	-	5,5,5	2.43	1 (20%)	6,6,6	2.01	2 (33%)
2	H92	C	401	-	26,26,26	0.27	0	30,38,38	0.62	1 (3%)
2	H92	G	401	-	26,26,26	0.21	0	30,38,38	0.58	0
4	EDO	B	404	-	3,3,3	0.38	0	2,2,2	0.34	0
5	NAG	A	406	1	14,14,15	0.42	0	17,19,21	0.92	0
2	H92	B	401	-	26,26,26	0.19	0	30,38,38	0.61	1 (3%)
4	EDO	F	405	-	3,3,3	0.41	0	2,2,2	0.38	0
4	EDO	J	306	-	3,3,3	0.41	0	2,2,2	0.37	0
3	PO4	H	402	-	4,4,4	0.96	0	6,6,6	0.59	0
4	EDO	G	406	-	3,3,3	0.42	0	2,2,2	0.13	0
4	EDO	J	301	-	3,3,3	0.40	0	2,2,2	0.50	0
4	EDO	C	406	-	3,3,3	0.47	0	2,2,2	0.50	0
2	H92	F	401	-	26,26,26	0.31	0	30,38,38	0.52	0
4	EDO	H	404	-	3,3,3	0.41	0	2,2,2	0.33	0
3	PO4	D	402	-	4,4,4	0.87	0	6,6,6	0.59	0
4	EDO	E	301	-	3,3,3	0.37	0	2,2,2	0.69	0
4	EDO	G	405	-	3,3,3	0.42	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	E	303	-	4,4,4	0.97	0	6,6,6	0.58	0
4	EDO	D	404	-	3,3,3	0.39	0	2,2,2	0.39	0
3	PO4	I	402	-	4,4,4	0.94	0	6,6,6	0.47	0
4	EDO	J	304	-	3,3,3	0.53	0	2,2,2	0.23	0
4	EDO	I	408	-	3,3,3	0.38	0	2,2,2	0.58	0
3	PO4	A	402	-	4,4,4	0.87	0	6,6,6	0.84	0
4	EDO	E	306	-	3,3,3	0.42	0	2,2,2	0.23	0
4	EDO	I	406	-	3,3,3	0.45	0	2,2,2	0.25	0
4	EDO	H	403	-	3,3,3	0.48	0	2,2,2	0.32	0
4	EDO	B	402	-	3,3,3	0.46	0	2,2,2	0.20	0
4	EDO	I	404	-	3,3,3	0.42	0	2,2,2	0.32	0
4	EDO	F	403	-	3,3,3	0.51	0	2,2,2	0.25	0
4	EDO	G	403	-	3,3,3	0.44	0	2,2,2	0.34	0
4	EDO	A	404	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	F	404	-	3,3,3	0.40	0	2,2,2	0.30	0
4	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.13	0
4	EDO	D	407	-	3,3,3	0.35	0	2,2,2	0.35	0
4	EDO	C	403	-	3,3,3	0.54	0	2,2,2	0.14	0
5	NAG	D	406	1	14,14,15	0.45	0	17,19,21	0.84	0
5	NAG	I	407	1	14,14,15	0.36	0	17,19,21	0.84	0
2	H92	J	302	-	26,26,26	0.26	0	30,38,38	0.60	1 (3%)
2	H92	A	401	-	26,26,26	0.20	0	30,38,38	0.57	0
5	NAG	J	307	1	14,14,15	0.38	0	17,19,21	1.11	2 (11%)
4	EDO	H	405	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	A	403	-	3,3,3	0.56	0	2,2,2	0.14	0
4	EDO	D	405	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	I	403	-	3,3,3	0.46	0	2,2,2	0.32	0
2	H92	I	401	-	26,26,26	0.24	0	30,38,38	0.59	0
4	EDO	A	407	-	3,3,3	0.39	0	2,2,2	0.57	0
4	EDO	J	305	-	3,3,3	0.47	0	2,2,2	0.07	0
3	PO4	F	402	-	4,4,4	0.93	0	6,6,6	0.60	0
4	EDO	F	406	-	3,3,3	0.41	0	2,2,2	0.48	0
3	PO4	B	406	-	4,4,4	0.88	0	6,6,6	0.62	0
3	PO4	G	402	-	4,4,4	0.98	0	6,6,6	0.62	0
4	EDO	B	407	-	3,3,3	0.42	0	2,2,2	0.51	0
2	H92	E	302	-	26,26,26	0.20	0	30,38,38	0.61	0
3	PO4	C	402	-	4,4,4	1.05	0	6,6,6	0.38	0
4	EDO	G	404	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	E	305	-	3,3,3	0.44	0	2,2,2	0.28	0
2	H92	H	401	-	26,26,26	0.24	0	30,38,38	0.65	1 (3%)
4	EDO	D	403	-	3,3,3	0.48	0	2,2,2	0.26	0
4	EDO	E	304	-	3,3,3	0.50	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	I	405	-	3,3,3	0.41	0	2,2,2	0.36	0
4	EDO	C	404	-	3,3,3	0.43	0	2,2,2	0.34	0
4	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.35	0
3	PO4	J	303	-	4,4,4	0.94	0	6,6,6	0.50	0
2	H92	D	401	-	26,26,26	0.22	0	30,38,38	0.61	0
4	EDO	C	405	-	3,3,3	0.44	0	2,2,2	0.31	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
6	OXL	B	403	-	-	4/4/4/4	-
2	H92	C	401	-	-	2/12/29/29	0/5/4/4
2	H92	G	401	-	-	2/12/29/29	0/5/4/4
4	EDO	B	404	-	-	0/1/1/1	-
5	NAG	A	406	1	-	0/6/23/26	0/1/1/1
2	H92	B	401	-	-	2/12/29/29	0/5/4/4
4	EDO	F	405	-	-	0/1/1/1	-
4	EDO	J	306	-	-	1/1/1/1	-
4	EDO	G	406	-	-	1/1/1/1	-
4	EDO	J	301	-	-	0/1/1/1	-
4	EDO	C	406	-	-	0/1/1/1	-
2	H92	F	401	-	-	2/12/29/29	0/5/4/4
4	EDO	H	404	-	-	0/1/1/1	-
4	EDO	E	301	-	-	0/1/1/1	-
4	EDO	G	405	-	-	0/1/1/1	-
4	EDO	J	304	-	-	0/1/1/1	-
4	EDO	D	404	-	-	0/1/1/1	-
4	EDO	I	408	-	-	0/1/1/1	-
4	EDO	E	306	-	-	0/1/1/1	-
4	EDO	I	406	-	-	1/1/1/1	-
4	EDO	H	403	-	-	1/1/1/1	-
4	EDO	B	402	-	-	1/1/1/1	-
4	EDO	I	404	-	-	1/1/1/1	-
4	EDO	F	403	-	-	1/1/1/1	-
4	EDO	G	403	-	-	1/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	F	404	-	-	0/1/1/1	-
4	EDO	B	405	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	407	-	-	1/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-
5	NAG	D	406	1	-	2/6/23/26	0/1/1/1
5	NAG	I	407	1	-	0/6/23/26	0/1/1/1
2	H92	J	302	-	-	2/12/29/29	0/5/4/4
2	H92	A	401	-	-	2/12/29/29	0/5/4/4
5	NAG	J	307	1	-	4/6/23/26	0/1/1/1
4	EDO	H	405	-	-	0/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	D	405	-	-	1/1/1/1	-
4	EDO	I	403	-	-	1/1/1/1	-
2	H92	I	401	-	-	2/12/29/29	0/5/4/4
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	J	305	-	-	1/1/1/1	-
4	EDO	F	406	-	-	1/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
2	H92	E	302	-	-	2/12/29/29	0/5/4/4
4	EDO	G	404	-	-	0/1/1/1	-
4	EDO	E	305	-	-	1/1/1/1	-
2	H92	H	401	-	-	2/12/29/29	0/5/4/4
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	E	304	-	-	0/1/1/1	-
4	EDO	I	405	-	-	1/1/1/1	-
4	EDO	C	404	-	-	0/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
2	H92	D	401	-	-	2/12/29/29	0/5/4/4
4	EDO	C	405	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	403	OXL	C2-C1	-4.45	1.47	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	403	OXL	O4-C2-C1	3.26	119.15	112.83
6	B	403	OXL	O3-C1-C2	3.23	119.10	112.83
5	J	307	NAG	C2-N2-C7	2.35	126.05	122.90
2	C	401	H92	C10-C6-C3	2.18	125.61	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	307	NAG	O5-C1-C2	-2.10	108.04	111.29
2	H	401	H92	C10-C6-C3	2.05	125.31	120.87
2	B	401	H92	C10-C6-C3	2.02	125.25	120.87
2	J	302	H92	C10-C6-C3	2.01	125.23	120.87

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	307	NAG	C1-C2-N2-C7
5	J	307	NAG	O5-C5-C6-O6
5	J	307	NAG	C4-C5-C6-O6
2	F	401	H92	C2-C3-C6-C10
2	B	401	H92	C2-C3-C6-C7
2	C	401	H92	C2-C3-C6-C7
2	D	401	H92	C2-C3-C6-C7
2	E	302	H92	C2-C3-C6-C7
2	F	401	H92	C2-C3-C6-C7
2	G	401	H92	C2-C3-C6-C7
2	H	401	H92	C2-C3-C6-C7
2	I	401	H92	C2-C3-C6-C7
2	J	302	H92	C2-C3-C6-C7
4	D	407	EDO	O1-C1-C2-O2
4	J	305	EDO	O1-C1-C2-O2
2	A	401	H92	C2-C3-C6-C10
2	A	401	H92	C2-C3-C6-C7
4	A	405	EDO	O1-C1-C2-O2
2	B	401	H92	C2-C3-C6-C10
2	C	401	H92	C2-C3-C6-C10
2	D	401	H92	C2-C3-C6-C10
2	E	302	H92	C2-C3-C6-C10
2	G	401	H92	C2-C3-C6-C10
2	H	401	H92	C2-C3-C6-C10
2	I	401	H92	C2-C3-C6-C10
2	J	302	H92	C2-C3-C6-C10
4	E	305	EDO	O1-C1-C2-O2
5	D	406	NAG	C1-C2-N2-C7
6	B	403	OXL	O3-C1-C2-O4
6	B	403	OXL	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
4	G	406	EDO	O1-C1-C2-O2
4	I	405	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	403	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2
5	D	406	NAG	C3-C2-N2-C7
5	J	307	NAG	C3-C2-N2-C7
6	B	403	OXL	O1-C1-C2-O4
6	B	403	OXL	O3-C1-C2-O2
4	B	402	EDO	O1-C1-C2-O2
4	F	403	EDO	O1-C1-C2-O2
4	G	403	EDO	O1-C1-C2-O2
4	H	403	EDO	O1-C1-C2-O2
4	I	403	EDO	O1-C1-C2-O2
4	I	404	EDO	O1-C1-C2-O2
4	I	406	EDO	O1-C1-C2-O2
4	J	306	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
4	F	406	EDO	O1-C1-C2-O2

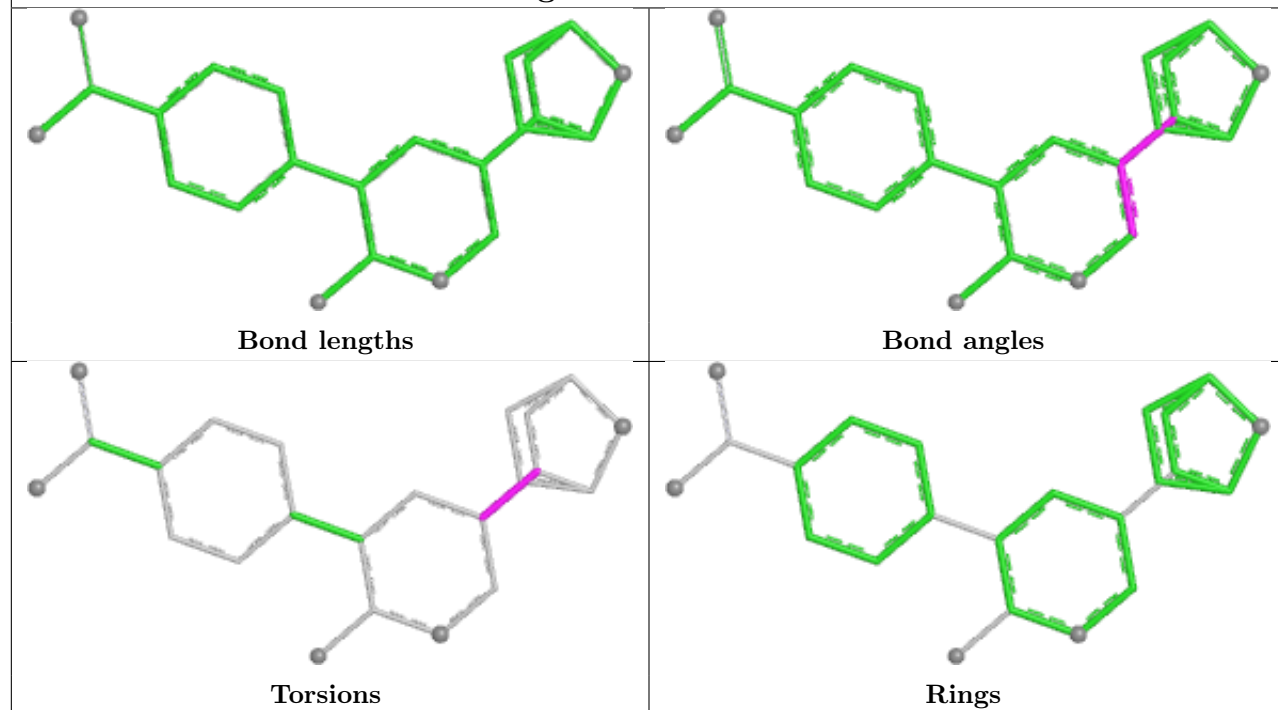
There are no ring outliers.

1 monomer is involved in 1 short contact:

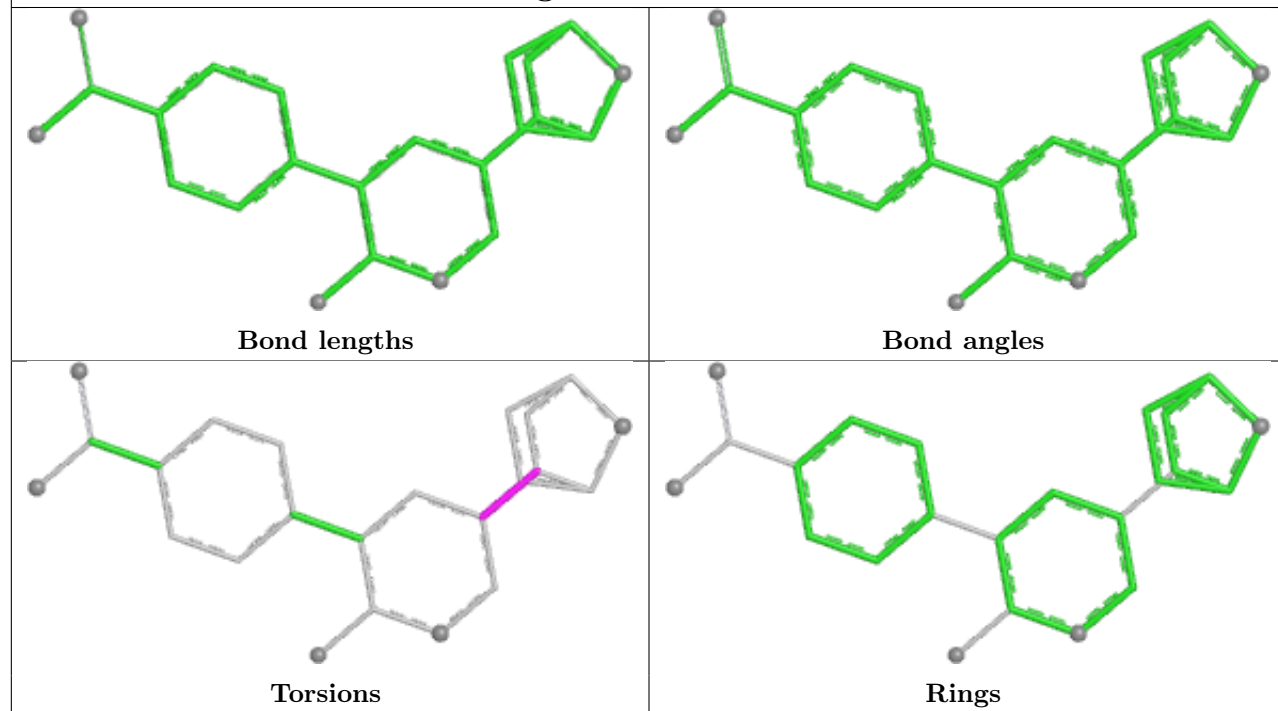
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	EDO	1	0

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

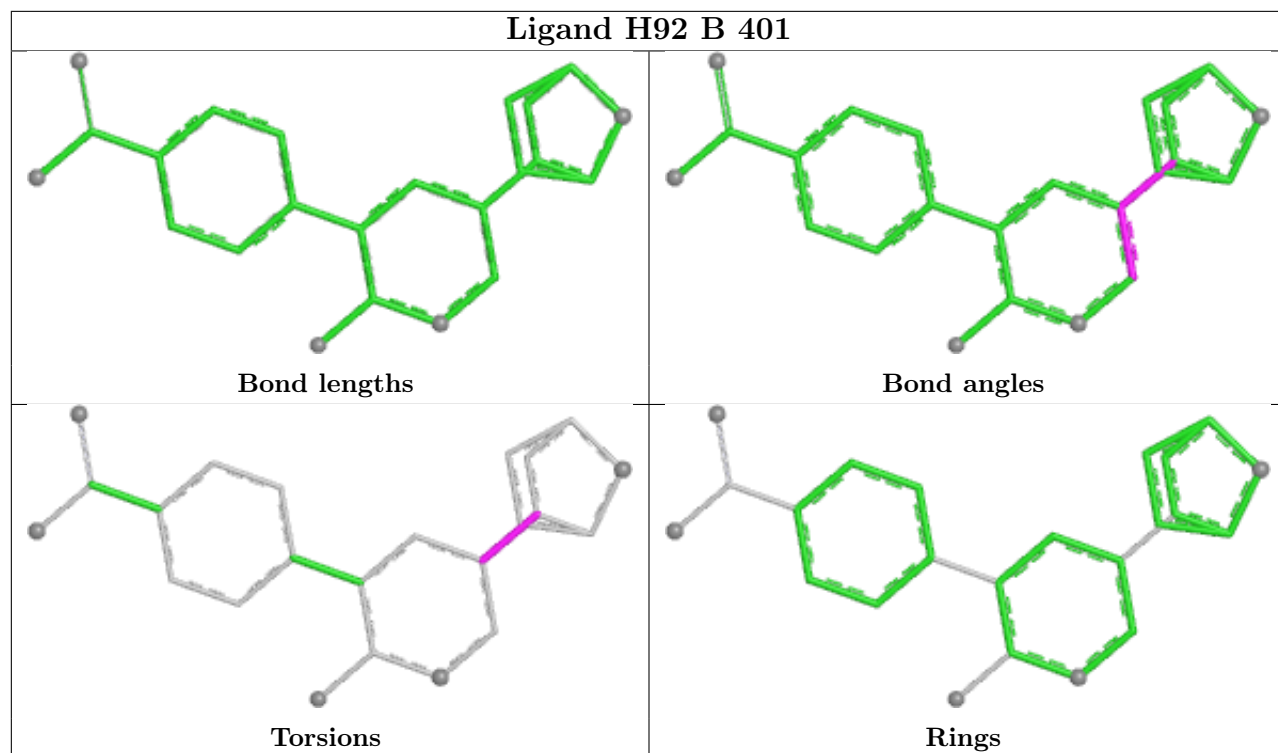
Ligand H92 C 401



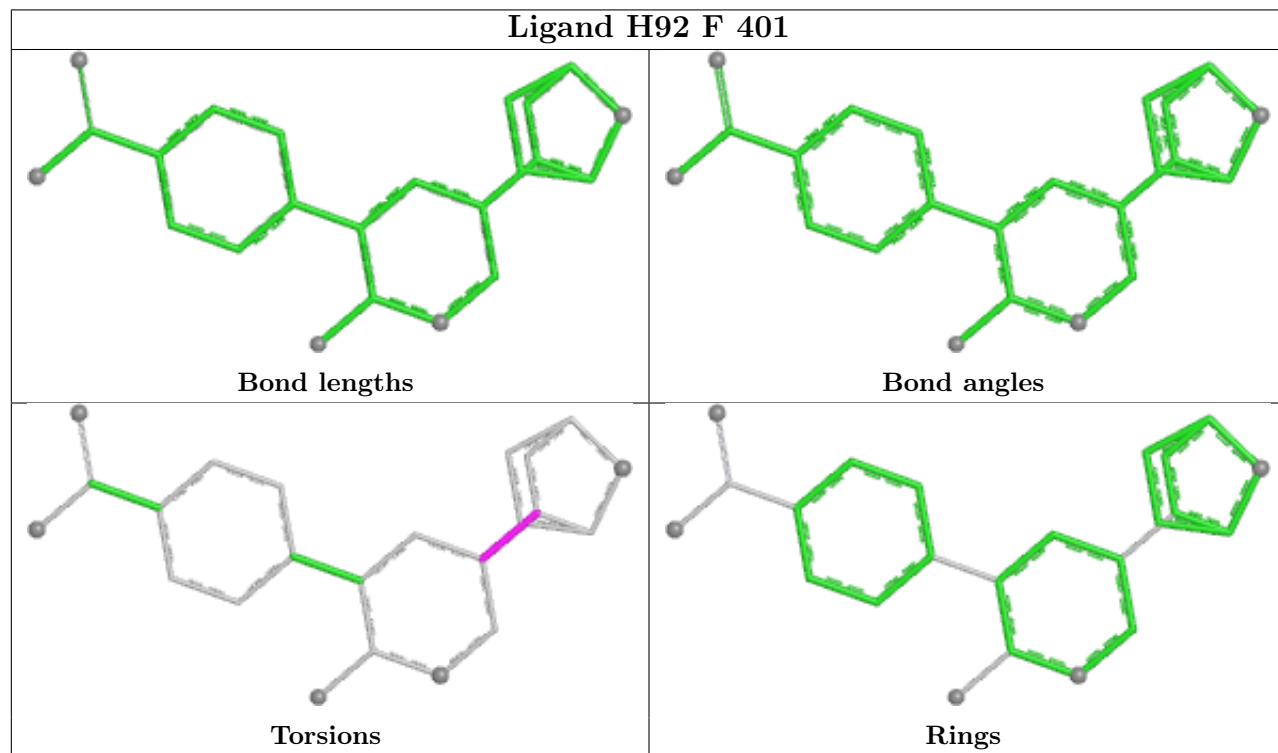
Ligand H92 G 401



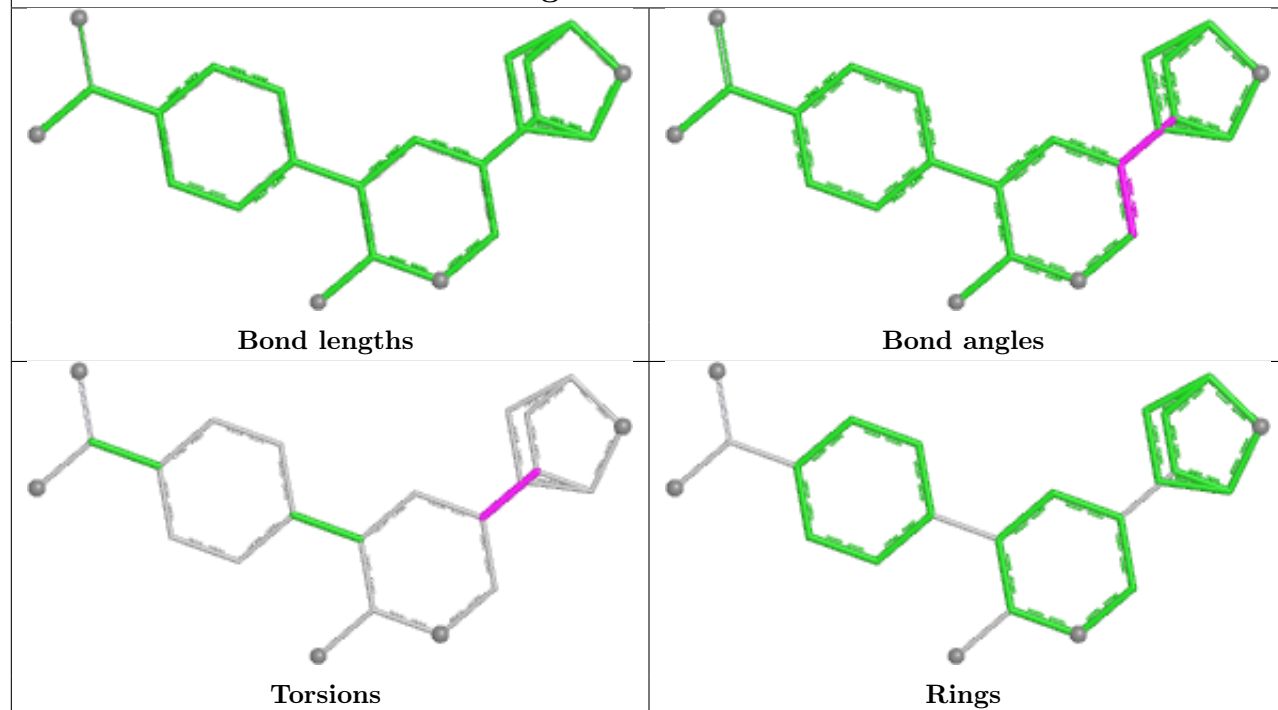
Ligand H92 B 401



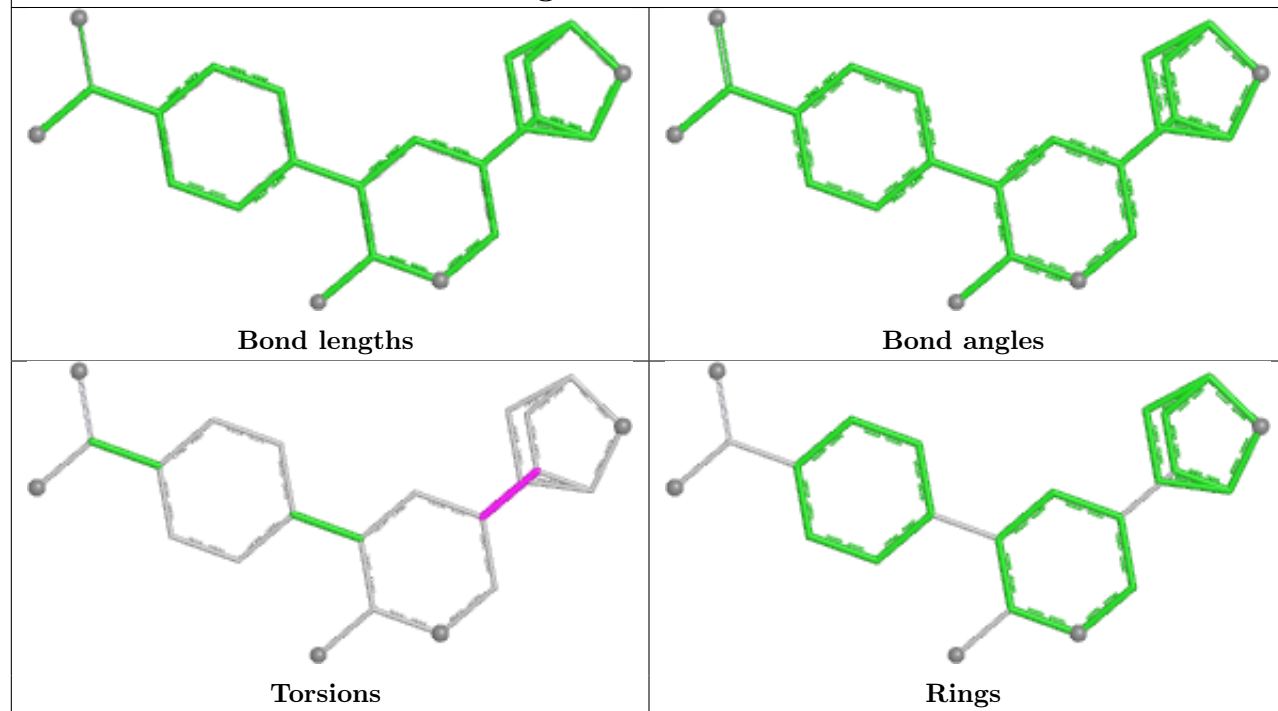
Ligand H92 F 401



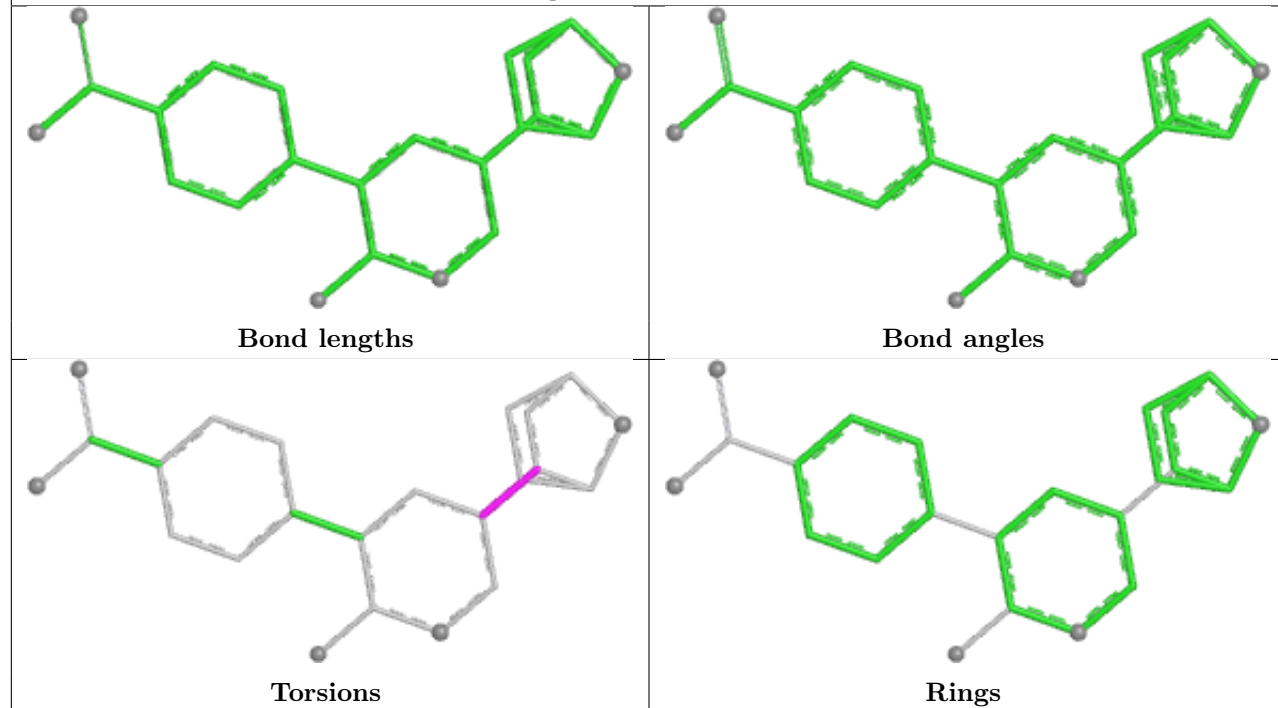
Ligand H92 J 302



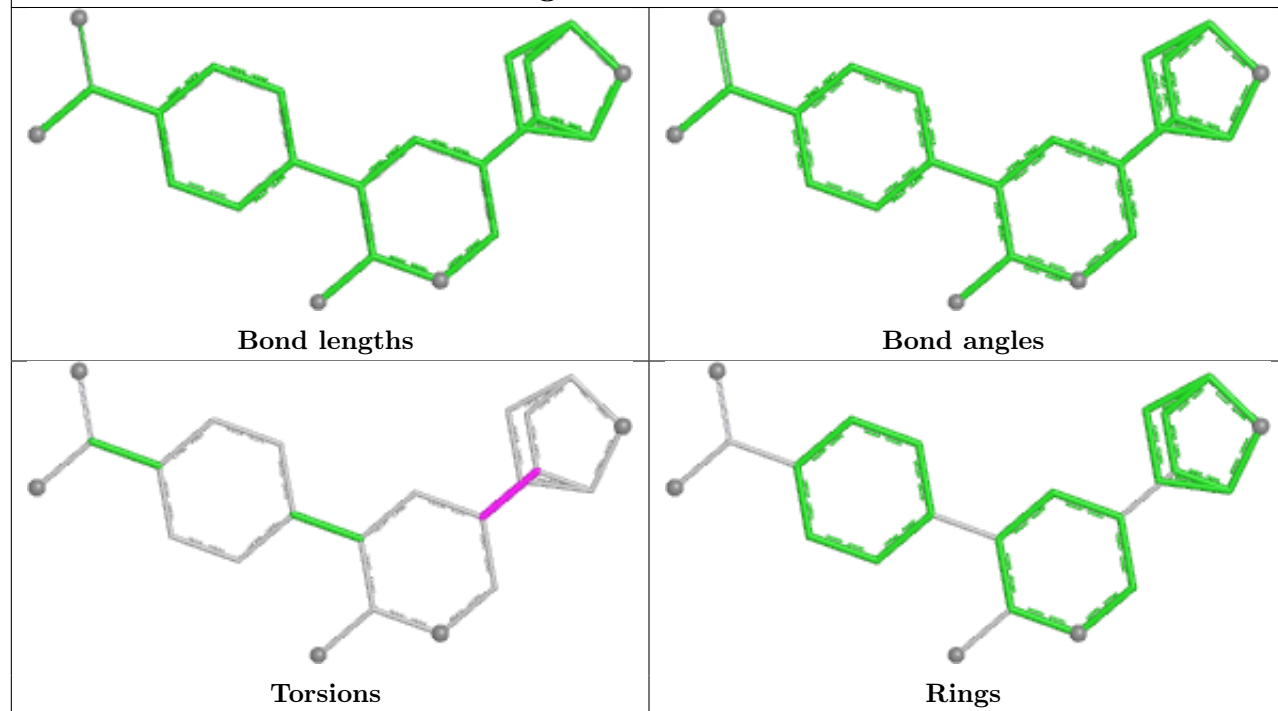
Ligand H92 A 401

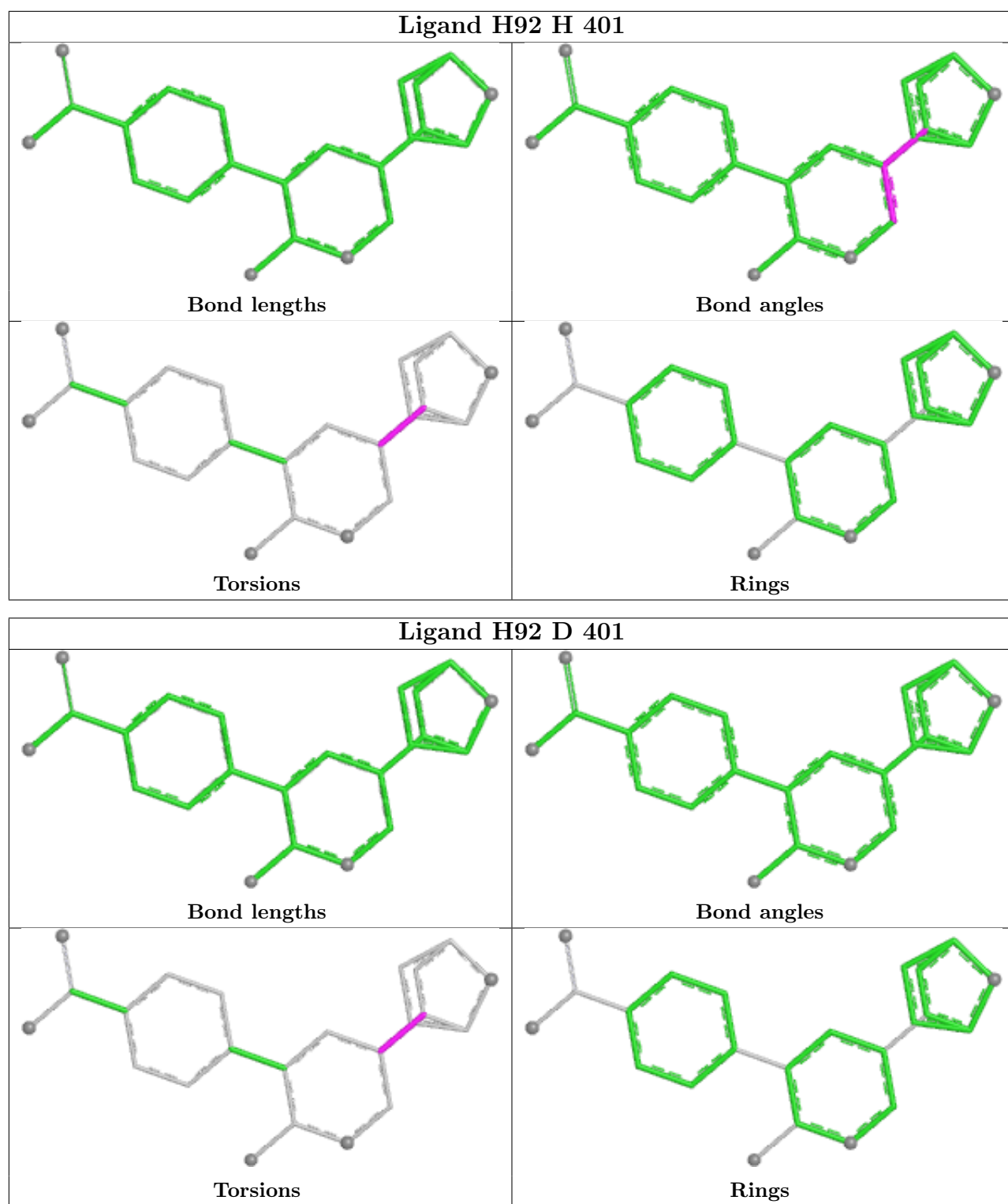


Ligand H92 I 401



Ligand H92 E 302





5.7 Other polymers [i](#)

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	205/249 (82%)	0.05	9 (4%) 39 36	8, 16, 37, 50	1 (0%)
1	B	206/249 (82%)	-0.05	8 (3%) 43 40	7, 14, 31, 48	1 (0%)
1	C	209/249 (83%)	0.16	12 (5%) 29 26	7, 14, 39, 57	1 (0%)
1	D	206/249 (82%)	0.15	12 (5%) 29 25	8, 16, 37, 53	1 (0%)
1	E	205/249 (82%)	0.07	11 (5%) 31 28	8, 14, 34, 59	1 (0%)
1	F	205/249 (82%)	0.09	10 (4%) 35 31	9, 16, 37, 50	1 (0%)
1	G	206/249 (82%)	0.17	11 (5%) 32 29	9, 18, 39, 66	1 (0%)
1	H	206/249 (82%)	0.29	12 (5%) 29 25	10, 19, 43, 64	1 (0%)
1	I	205/249 (82%)	0.22	10 (4%) 35 31	10, 20, 41, 53	1 (0%)
1	J	206/249 (82%)	0.15	12 (5%) 29 25	8, 17, 36, 60	1 (0%)
All	All	2059/2490 (82%)	0.13	107 (5%) 33 29	7, 17, 39, 66	10 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	225	ARG	6.1
1	J	225	ARG	5.8
1	C	227	GLY	5.7
1	C	207	CYS	4.8
1	A	207	CYS	4.6
1	G	207	CYS	4.5
1	C	229	GLY	4.5
1	H	35	PRO	4.5
1	H	36	MET	4.4
1	I	207	CYS	4.3
1	I	208	CYS	4.3
1	J	207	CYS	4.2
1	E	208	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	33	ARG	4.1
1	C	36	MET	4.0
1	G	208	CYS	4.0
1	C	208	CYS	4.0
1	H	225	ARG	3.9
1	H	34	SER	3.9
1	D	225	ARG	3.7
1	D	208	CYS	3.7
1	A	208	CYS	3.6
1	H	207	CYS	3.6
1	F	207	CYS	3.6
1	J	208	CYS	3.6
1	F	208	CYS	3.5
1	J	153	GLU	3.4
1	E	34	SER	3.4
1	E	207	CYS	3.4
1	H	208	CYS	3.3
1	C	228	ASN	3.2
1	B	225	ARG	3.2
1	H	153	GLU	3.2
1	D	35	PRO	3.2
1	G	33	ARG	3.1
1	D	153	GLU	3.1
1	I	87	ASN	3.1
1	B	35	PRO	3.1
1	I	36	MET	3.1
1	G	36	MET	3.1
1	G	153	GLU	3.0
1	C	20	GLN	3.0
1	J	34	SER	3.0
1	D	207	CYS	3.0
1	F	35	PRO	3.0
1	J	36	MET	2.9
1	E	36	MET	2.9
1	D	36	MET	2.8
1	C	152	GLU	2.8
1	F	152	GLU	2.8
1	J	33	ARG	2.8
1	B	153	GLU	2.7
1	E	152	GLU	2.7
1	A	35	PRO	2.7
1	E	209	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	35	PRO	2.7
1	I	33	ARG	2.6
1	C	34	SER	2.6
1	F	34	SER	2.6
1	G	20	GLN	2.6
1	D	33	ARG	2.5
1	G	206	SER	2.5
1	A	153	GLU	2.5
1	E	87	ASN	2.5
1	F	33	ARG	2.5
1	E	33	ARG	2.4
1	J	88	GLU	2.4
1	A	43	ASP	2.4
1	C	35	PRO	2.4
1	D	34	SER	2.4
1	E	20	GLN	2.4
1	F	43	ASP	2.4
1	I	44	ASP	2.4
1	I	34	SER	2.4
1	I	209	PRO	2.3
1	B	36	MET	2.3
1	F	20	GLN	2.3
1	J	178	ASP	2.3
1	G	34	SER	2.3
1	C	224	ARG	2.3
1	I	20	GLN	2.3
1	H	20	GLN	2.3
1	A	36	MET	2.3
1	B	207	CYS	2.2
1	D	87	ASN	2.2
1	E	35	PRO	2.2
1	H	209	PRO	2.2
1	C	153	GLU	2.2
1	F	153	GLU	2.2
1	B	33	ARG	2.2
1	G	152	GLU	2.2
1	H	210	GLU	2.2
1	J	43	ASP	2.2
1	I	35	PRO	2.2
1	A	33	ARG	2.1
1	F	210	GLU	2.1
1	G	35	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.1
1	E	43	ASP	2.1
1	H	224	ARG	2.1
1	J	20	GLN	2.1
1	D	224	ARG	2.1
1	B	34	SER	2.0
1	D	44	ASP	2.0
1	A	20	GLN	2.0
1	B	208	CYS	2.0
1	D	178	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	406	14/15	0.30	0.30	65,69,71,74	0
5	NAG	D	406	14/15	0.47	0.25	60,64,67,67	0
5	NAG	J	307	14/15	0.47	0.24	64,70,73,73	0
5	NAG	I	407	14/15	0.51	0.26	65,69,71,72	0
4	EDO	D	407	4/4	0.74	0.28	34,34,34,37	0
4	EDO	I	406	4/4	0.79	0.22	35,36,37,38	0
4	EDO	C	404	4/4	0.82	0.21	43,43,44,46	0
4	EDO	I	405	4/4	0.83	0.23	50,50,51,51	0
4	EDO	G	406	4/4	0.83	0.23	36,37,39,41	0
4	EDO	F	405	4/4	0.84	0.19	41,42,42,42	0
4	EDO	F	403	4/4	0.84	0.14	21,22,23,24	0
6	OXL	B	403	6/6	0.84	0.16	40,41,41,42	0
4	EDO	I	404	4/4	0.85	0.17	41,41,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	J	304	4/4	0.86	0.14	28,29,29,30	0
4	EDO	J	306	4/4	0.86	0.24	57,58,58,60	0
4	EDO	A	404	4/4	0.86	0.20	39,40,40,40	0
4	EDO	H	403	4/4	0.86	0.13	24,25,26,27	0
4	EDO	A	403	4/4	0.86	0.13	24,24,24,24	0
4	EDO	F	404	4/4	0.86	0.14	39,39,39,41	0
4	EDO	C	406	4/4	0.86	0.14	26,27,27,27	0
4	EDO	E	301	4/4	0.87	0.15	25,25,26,26	0
4	EDO	D	403	4/4	0.87	0.13	19,19,20,20	0
4	EDO	F	406	4/4	0.87	0.13	32,32,32,32	0
4	EDO	G	403	4/4	0.87	0.14	25,25,25,26	0
4	EDO	J	301	4/4	0.88	0.14	28,28,28,29	0
4	EDO	G	404	4/4	0.88	0.13	33,33,33,34	0
4	EDO	G	405	4/4	0.88	0.18	46,47,47,49	0
4	EDO	B	404	4/4	0.88	0.12	28,28,28,28	0
4	EDO	D	404	4/4	0.88	0.15	34,34,35,35	0
3	PO4	B	406	5/5	0.88	0.20	48,49,50,50	0
4	EDO	B	402	4/4	0.88	0.11	21,22,22,22	0
4	EDO	E	305	4/4	0.88	0.15	39,40,41,42	0
4	EDO	A	405	4/4	0.89	0.15	43,43,43,44	0
4	EDO	D	405	4/4	0.89	0.17	45,46,46,46	0
4	EDO	E	304	4/4	0.89	0.12	22,22,22,22	0
4	EDO	H	404	4/4	0.90	0.13	35,35,35,36	0
4	EDO	I	408	4/4	0.90	0.12	27,27,28,28	0
4	EDO	H	405	4/4	0.90	0.15	42,42,43,44	0
3	PO4	J	303	5/5	0.90	0.22	46,47,49,51	0
4	EDO	A	407	4/4	0.90	0.14	33,33,33,34	0
4	EDO	I	403	4/4	0.91	0.12	23,23,23,23	0
4	EDO	C	405	4/4	0.92	0.13	37,38,38,40	0
4	EDO	C	403	4/4	0.92	0.08	17,17,17,17	0
4	EDO	B	407	4/4	0.92	0.11	25,25,26,26	0
4	EDO	E	306	4/4	0.92	0.12	33,34,34,34	0
2	H92	H	401	23/23	0.93	0.08	19,20,21,22	0
2	H92	A	401	23/23	0.93	0.07	13,14,16,17	0
2	H92	C	401	23/23	0.93	0.09	15,15,18,19	0
4	EDO	J	305	4/4	0.93	0.12	42,42,43,43	0
4	EDO	B	405	4/4	0.93	0.12	37,37,37,37	0
2	H92	B	401	23/23	0.94	0.07	12,13,16,17	0
2	H92	I	401	23/23	0.94	0.08	16,16,21,22	0
2	H92	E	302	23/23	0.94	0.08	14,14,16,17	0
3	PO4	D	402	5/5	0.94	0.12	35,36,37,38	0
2	H92	F	401	23/23	0.94	0.08	15,15,19,20	0

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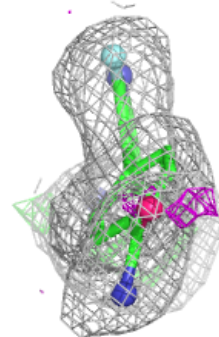
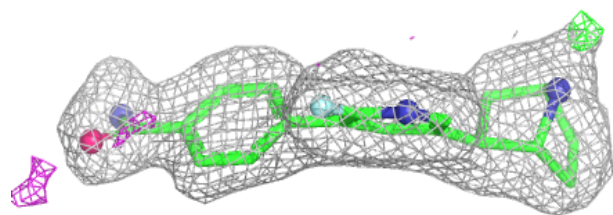
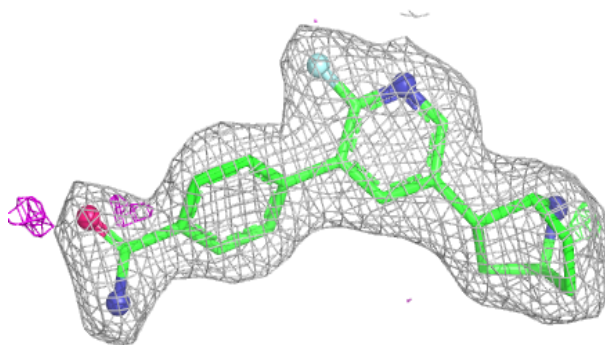
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	H	402	5/5	0.95	0.11	44,44,45,47	0
3	PO4	I	402	5/5	0.95	0.10	43,43,43,44	0
2	H92	J	302	23/23	0.95	0.07	16,17,21,21	0
2	H92	D	401	23/23	0.95	0.07	13,14,15,16	0
2	H92	G	401	23/23	0.95	0.07	16,17,19,20	0
3	PO4	G	402	5/5	0.95	0.12	35,36,36,36	0
3	PO4	A	402	5/5	0.96	0.09	29,29,31,31	0
3	PO4	E	303	5/5	0.96	0.09	41,41,42,44	0
3	PO4	F	402	5/5	0.96	0.09	36,36,37,37	0
3	PO4	C	402	5/5	0.96	0.11	38,39,39,40	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.

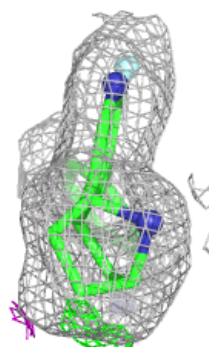
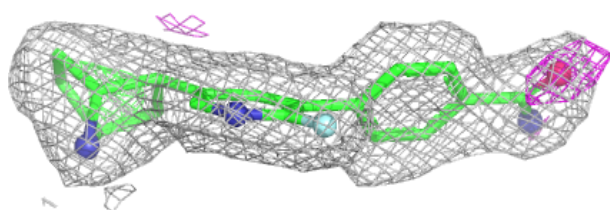
Electron density around H92 H 401:

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

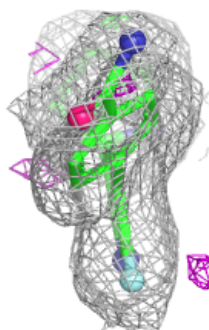
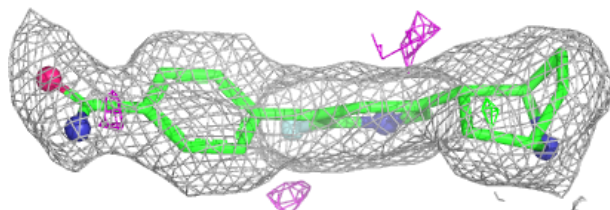
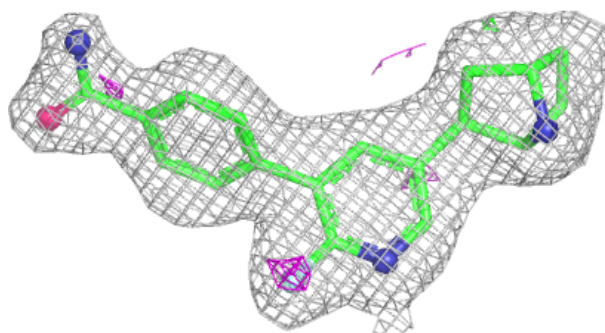


Electron density around H92 A 401:

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

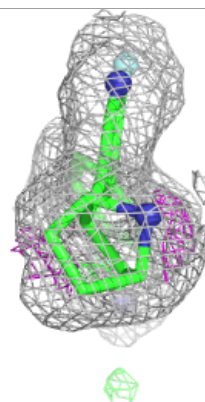
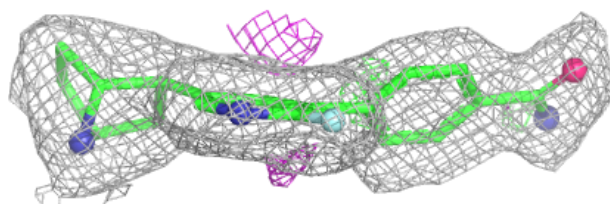
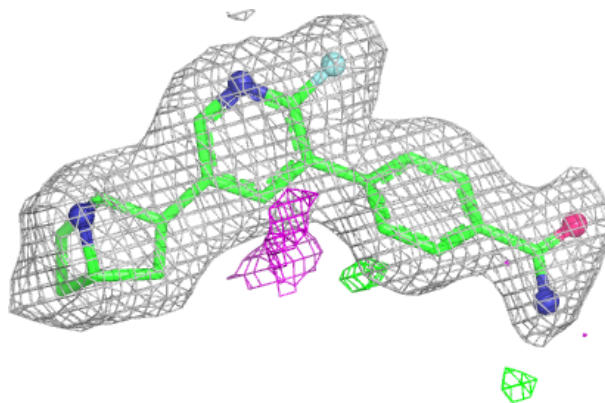
**Electron density around H92 C 401:**

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and green (positive)

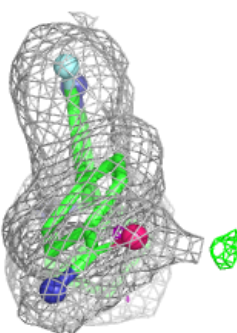
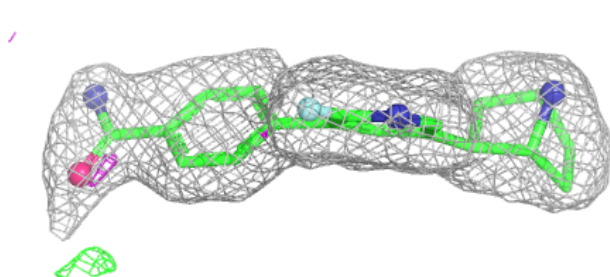
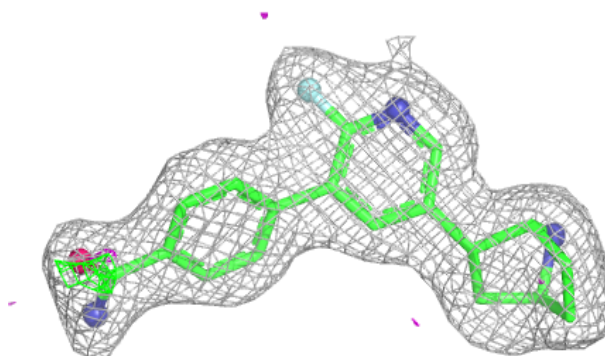


Electron density around H92 B 401:

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

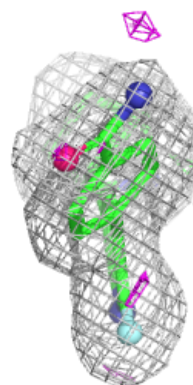
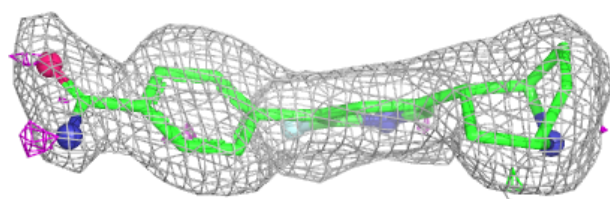
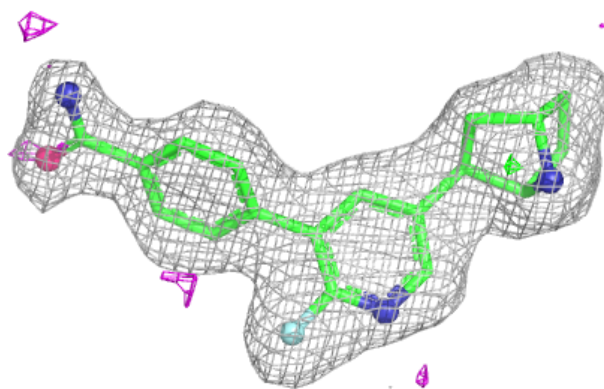
**Electron density around H92 I 401:**

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

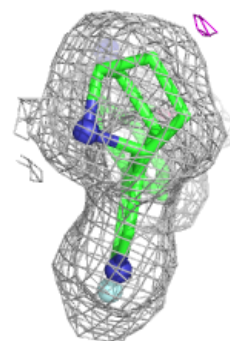
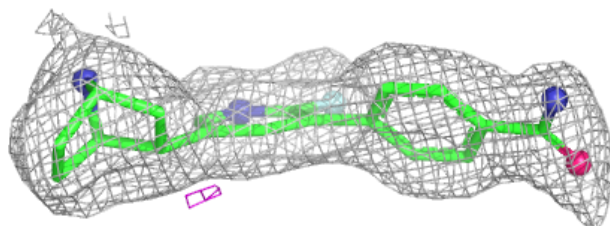
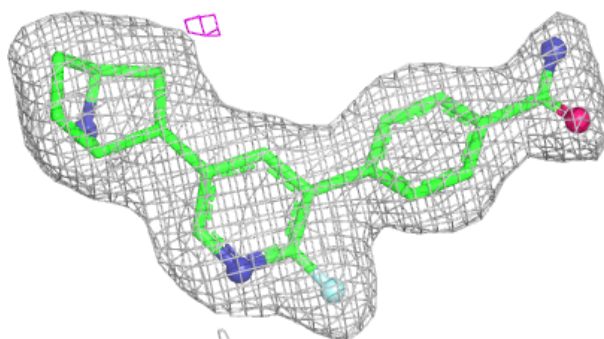


Electron density around H92 E 302:

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

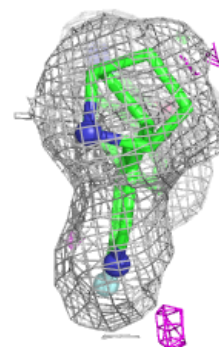
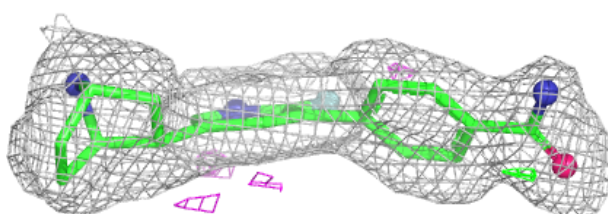
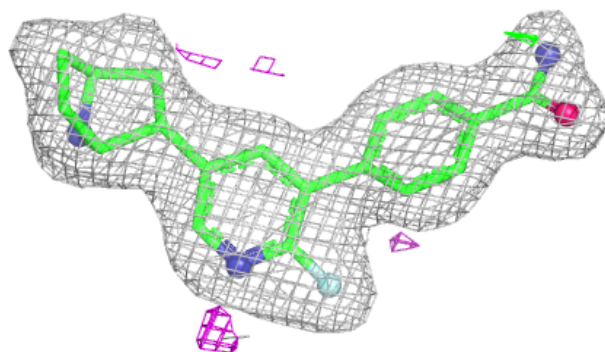
**Electron density around H92 F 401:**

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

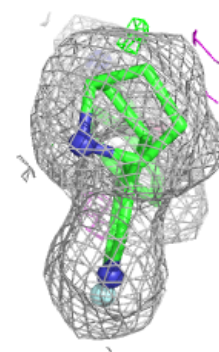
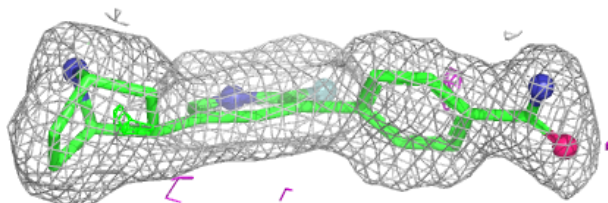
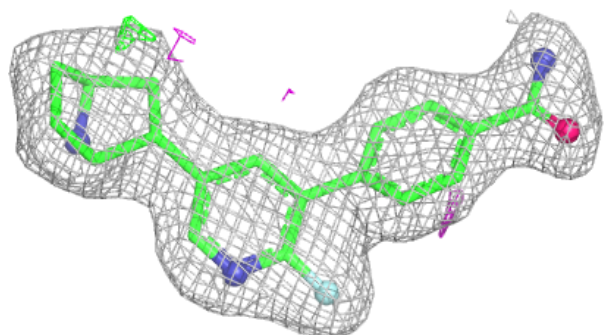


Electron density around H92 J 302:

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and green (positive)

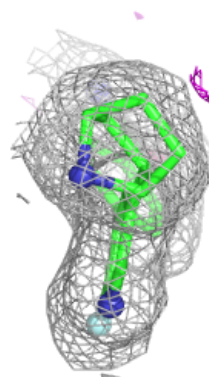
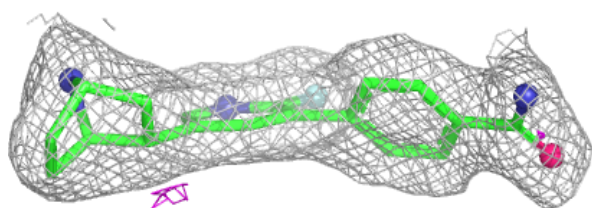
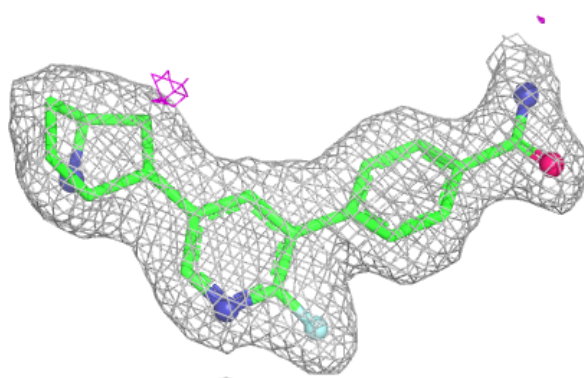
**Electron density around H92 D 401:**

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



Electron density around H92 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.