Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 04:27 AM EDT

PDB ID	:	4FRR
Title	:	X-ray structure of Acetylcholine binding protein from Aplysia californica in presence of 3-((S)-azetidin-2-ylmethoxy)-5-((1S,2R)-2-(2-methoxyethyl)cyclopropyl)pyridine
Authors	:	Mukhopadhyay, S.; Mesecar, A.D.
Deposited on	:	2012-06-26
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:

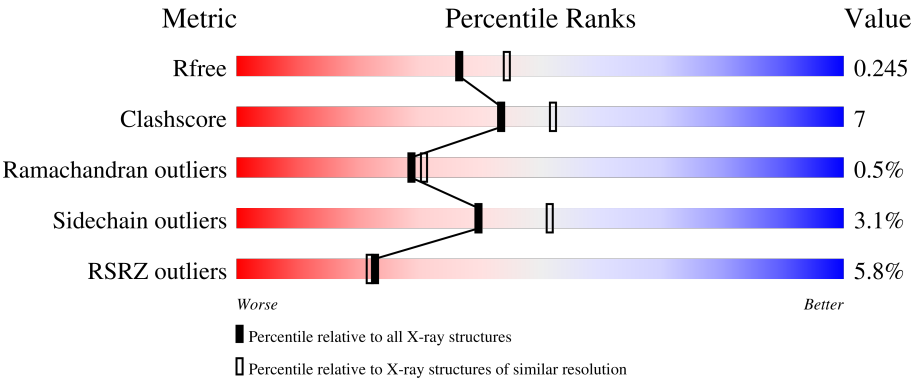
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	232	5% 78% 11% • 10%
1	B	232	3% 74% 15% • 9%
1	C	232	9% 75% 13% • 9%
1	D	232	4% 78% 12% • 9%

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Mol	Chain	Length	Quality of chain
1	E	232	3% 79% 12% 9%
1	F	232	5% 80% 10% 9%
1	G	232	9% 73% 15% 10%
1	H	232	6% 76% 12% 10%
1	I	232	5% 74% 16% 9%
1	J	232	5% 75% 17% 8%

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	GOL	C	303	-	-	X	-
3	GOL	I	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18186 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	208	Total	C	N	O	S	0	1	0
			1670	1054	278	330	8			
1	B	211	Total	C	N	O	S	0	3	0
			1717	1080	290	339	8			
1	C	210	Total	C	N	O	S	0	8	0
			1745	1100	288	347	10			
1	D	211	Total	C	N	O	S	0	2	0
			1704	1074	284	337	9			
1	E	211	Total	C	N	O	S	0	4	0
			1717	1080	287	342	8			
1	F	210	Total	C	N	O	S	0	2	0
			1693	1069	281	334	9			
1	G	208	Total	C	N	O	S	0	1	0
			1671	1054	276	333	8			
1	H	209	Total	C	N	O	S	0	9	0
			1743	1100	288	345	10			
1	I	210	Total	C	N	O	S	0	2	0
			1687	1066	278	334	9			
1	J	214	Total	C	N	O	S	0	4	0
			1747	1097	294	347	9			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q8WSF8
A	-22	SER	-	expression tag	UNP Q8WSF8
A	-21	ALA	-	expression tag	UNP Q8WSF8
A	-20	LEU	-	expression tag	UNP Q8WSF8
A	-19	LEU	-	expression tag	UNP Q8WSF8
A	-18	ILE	-	expression tag	UNP Q8WSF8
A	-17	LEU	-	expression tag	UNP Q8WSF8
A	-16	ALA	-	expression tag	UNP Q8WSF8
A	-15	LEU	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	VAL	-	expression tag	UNP Q8WSF8
A	-13	GLY	-	expression tag	UNP Q8WSF8
A	-12	ALA	-	expression tag	UNP Q8WSF8
A	-11	ALA	-	expression tag	UNP Q8WSF8
A	-10	VAL	-	expression tag	UNP Q8WSF8
A	-9	ALA	-	expression tag	UNP Q8WSF8
A	-8	ASP	-	expression tag	UNP Q8WSF8
A	-7	TYR	-	expression tag	UNP Q8WSF8
A	-6	LYS	-	expression tag	UNP Q8WSF8
A	-5	ASP	-	expression tag	UNP Q8WSF8
A	-4	ASP	-	expression tag	UNP Q8WSF8
A	-3	ASP	-	expression tag	UNP Q8WSF8
A	-2	ASP	-	expression tag	UNP Q8WSF8
A	-1	LYS	-	expression tag	UNP Q8WSF8
A	0	LEU	-	expression tag	UNP Q8WSF8
B	-23	MET	-	expression tag	UNP Q8WSF8
B	-22	SER	-	expression tag	UNP Q8WSF8
B	-21	ALA	-	expression tag	UNP Q8WSF8
B	-20	LEU	-	expression tag	UNP Q8WSF8
B	-19	LEU	-	expression tag	UNP Q8WSF8
B	-18	ILE	-	expression tag	UNP Q8WSF8
B	-17	LEU	-	expression tag	UNP Q8WSF8
B	-16	ALA	-	expression tag	UNP Q8WSF8
B	-15	LEU	-	expression tag	UNP Q8WSF8
B	-14	VAL	-	expression tag	UNP Q8WSF8
B	-13	GLY	-	expression tag	UNP Q8WSF8
B	-12	ALA	-	expression tag	UNP Q8WSF8
B	-11	ALA	-	expression tag	UNP Q8WSF8
B	-10	VAL	-	expression tag	UNP Q8WSF8
B	-9	ALA	-	expression tag	UNP Q8WSF8
B	-8	ASP	-	expression tag	UNP Q8WSF8
B	-7	TYR	-	expression tag	UNP Q8WSF8
B	-6	LYS	-	expression tag	UNP Q8WSF8
B	-5	ASP	-	expression tag	UNP Q8WSF8
B	-4	ASP	-	expression tag	UNP Q8WSF8
B	-3	ASP	-	expression tag	UNP Q8WSF8
B	-2	ASP	-	expression tag	UNP Q8WSF8
B	-1	LYS	-	expression tag	UNP Q8WSF8
B	0	LEU	-	expression tag	UNP Q8WSF8
C	-23	MET	-	expression tag	UNP Q8WSF8
C	-22	SER	-	expression tag	UNP Q8WSF8
C	-21	ALA	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	LEU	-	expression tag	UNP Q8WSF8
C	-19	LEU	-	expression tag	UNP Q8WSF8
C	-18	ILE	-	expression tag	UNP Q8WSF8
C	-17	LEU	-	expression tag	UNP Q8WSF8
C	-16	ALA	-	expression tag	UNP Q8WSF8
C	-15	LEU	-	expression tag	UNP Q8WSF8
C	-14	VAL	-	expression tag	UNP Q8WSF8
C	-13	GLY	-	expression tag	UNP Q8WSF8
C	-12	ALA	-	expression tag	UNP Q8WSF8
C	-11	ALA	-	expression tag	UNP Q8WSF8
C	-10	VAL	-	expression tag	UNP Q8WSF8
C	-9	ALA	-	expression tag	UNP Q8WSF8
C	-8	ASP	-	expression tag	UNP Q8WSF8
C	-7	TYR	-	expression tag	UNP Q8WSF8
C	-6	LYS	-	expression tag	UNP Q8WSF8
C	-5	ASP	-	expression tag	UNP Q8WSF8
C	-4	ASP	-	expression tag	UNP Q8WSF8
C	-3	ASP	-	expression tag	UNP Q8WSF8
C	-2	ASP	-	expression tag	UNP Q8WSF8
C	-1	LYS	-	expression tag	UNP Q8WSF8
C	0	LEU	-	expression tag	UNP Q8WSF8
D	-23	MET	-	expression tag	UNP Q8WSF8
D	-22	SER	-	expression tag	UNP Q8WSF8
D	-21	ALA	-	expression tag	UNP Q8WSF8
D	-20	LEU	-	expression tag	UNP Q8WSF8
D	-19	LEU	-	expression tag	UNP Q8WSF8
D	-18	ILE	-	expression tag	UNP Q8WSF8
D	-17	LEU	-	expression tag	UNP Q8WSF8
D	-16	ALA	-	expression tag	UNP Q8WSF8
D	-15	LEU	-	expression tag	UNP Q8WSF8
D	-14	VAL	-	expression tag	UNP Q8WSF8
D	-13	GLY	-	expression tag	UNP Q8WSF8
D	-12	ALA	-	expression tag	UNP Q8WSF8
D	-11	ALA	-	expression tag	UNP Q8WSF8
D	-10	VAL	-	expression tag	UNP Q8WSF8
D	-9	ALA	-	expression tag	UNP Q8WSF8
D	-8	ASP	-	expression tag	UNP Q8WSF8
D	-7	TYR	-	expression tag	UNP Q8WSF8
D	-6	LYS	-	expression tag	UNP Q8WSF8
D	-5	ASP	-	expression tag	UNP Q8WSF8
D	-4	ASP	-	expression tag	UNP Q8WSF8
D	-3	ASP	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ASP	-	expression tag	UNP Q8WSF8
D	-1	LYS	-	expression tag	UNP Q8WSF8
D	0	LEU	-	expression tag	UNP Q8WSF8
E	-23	MET	-	expression tag	UNP Q8WSF8
E	-22	SER	-	expression tag	UNP Q8WSF8
E	-21	ALA	-	expression tag	UNP Q8WSF8
E	-20	LEU	-	expression tag	UNP Q8WSF8
E	-19	LEU	-	expression tag	UNP Q8WSF8
E	-18	ILE	-	expression tag	UNP Q8WSF8
E	-17	LEU	-	expression tag	UNP Q8WSF8
E	-16	ALA	-	expression tag	UNP Q8WSF8
E	-15	LEU	-	expression tag	UNP Q8WSF8
E	-14	VAL	-	expression tag	UNP Q8WSF8
E	-13	GLY	-	expression tag	UNP Q8WSF8
E	-12	ALA	-	expression tag	UNP Q8WSF8
E	-11	ALA	-	expression tag	UNP Q8WSF8
E	-10	VAL	-	expression tag	UNP Q8WSF8
E	-9	ALA	-	expression tag	UNP Q8WSF8
E	-8	ASP	-	expression tag	UNP Q8WSF8
E	-7	TYR	-	expression tag	UNP Q8WSF8
E	-6	LYS	-	expression tag	UNP Q8WSF8
E	-5	ASP	-	expression tag	UNP Q8WSF8
E	-4	ASP	-	expression tag	UNP Q8WSF8
E	-3	ASP	-	expression tag	UNP Q8WSF8
E	-2	ASP	-	expression tag	UNP Q8WSF8
E	-1	LYS	-	expression tag	UNP Q8WSF8
E	0	LEU	-	expression tag	UNP Q8WSF8
F	-23	MET	-	expression tag	UNP Q8WSF8
F	-22	SER	-	expression tag	UNP Q8WSF8
F	-21	ALA	-	expression tag	UNP Q8WSF8
F	-20	LEU	-	expression tag	UNP Q8WSF8
F	-19	LEU	-	expression tag	UNP Q8WSF8
F	-18	ILE	-	expression tag	UNP Q8WSF8
F	-17	LEU	-	expression tag	UNP Q8WSF8
F	-16	ALA	-	expression tag	UNP Q8WSF8
F	-15	LEU	-	expression tag	UNP Q8WSF8
F	-14	VAL	-	expression tag	UNP Q8WSF8
F	-13	GLY	-	expression tag	UNP Q8WSF8
F	-12	ALA	-	expression tag	UNP Q8WSF8
F	-11	ALA	-	expression tag	UNP Q8WSF8
F	-10	VAL	-	expression tag	UNP Q8WSF8
F	-9	ALA	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	ASP	-	expression tag	UNP Q8WSF8
F	-7	TYR	-	expression tag	UNP Q8WSF8
F	-6	LYS	-	expression tag	UNP Q8WSF8
F	-5	ASP	-	expression tag	UNP Q8WSF8
F	-4	ASP	-	expression tag	UNP Q8WSF8
F	-3	ASP	-	expression tag	UNP Q8WSF8
F	-2	ASP	-	expression tag	UNP Q8WSF8
F	-1	LYS	-	expression tag	UNP Q8WSF8
F	0	LEU	-	expression tag	UNP Q8WSF8
G	-23	MET	-	expression tag	UNP Q8WSF8
G	-22	SER	-	expression tag	UNP Q8WSF8
G	-21	ALA	-	expression tag	UNP Q8WSF8
G	-20	LEU	-	expression tag	UNP Q8WSF8
G	-19	LEU	-	expression tag	UNP Q8WSF8
G	-18	ILE	-	expression tag	UNP Q8WSF8
G	-17	LEU	-	expression tag	UNP Q8WSF8
G	-16	ALA	-	expression tag	UNP Q8WSF8
G	-15	LEU	-	expression tag	UNP Q8WSF8
G	-14	VAL	-	expression tag	UNP Q8WSF8
G	-13	GLY	-	expression tag	UNP Q8WSF8
G	-12	ALA	-	expression tag	UNP Q8WSF8
G	-11	ALA	-	expression tag	UNP Q8WSF8
G	-10	VAL	-	expression tag	UNP Q8WSF8
G	-9	ALA	-	expression tag	UNP Q8WSF8
G	-8	ASP	-	expression tag	UNP Q8WSF8
G	-7	TYR	-	expression tag	UNP Q8WSF8
G	-6	LYS	-	expression tag	UNP Q8WSF8
G	-5	ASP	-	expression tag	UNP Q8WSF8
G	-4	ASP	-	expression tag	UNP Q8WSF8
G	-3	ASP	-	expression tag	UNP Q8WSF8
G	-2	ASP	-	expression tag	UNP Q8WSF8
G	-1	LYS	-	expression tag	UNP Q8WSF8
G	0	LEU	-	expression tag	UNP Q8WSF8
H	-23	MET	-	expression tag	UNP Q8WSF8
H	-22	SER	-	expression tag	UNP Q8WSF8
H	-21	ALA	-	expression tag	UNP Q8WSF8
H	-20	LEU	-	expression tag	UNP Q8WSF8
H	-19	LEU	-	expression tag	UNP Q8WSF8
H	-18	ILE	-	expression tag	UNP Q8WSF8
H	-17	LEU	-	expression tag	UNP Q8WSF8
H	-16	ALA	-	expression tag	UNP Q8WSF8
H	-15	LEU	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-14	VAL	-	expression tag	UNP Q8WSF8
H	-13	GLY	-	expression tag	UNP Q8WSF8
H	-12	ALA	-	expression tag	UNP Q8WSF8
H	-11	ALA	-	expression tag	UNP Q8WSF8
H	-10	VAL	-	expression tag	UNP Q8WSF8
H	-9	ALA	-	expression tag	UNP Q8WSF8
H	-8	ASP	-	expression tag	UNP Q8WSF8
H	-7	TYR	-	expression tag	UNP Q8WSF8
H	-6	LYS	-	expression tag	UNP Q8WSF8
H	-5	ASP	-	expression tag	UNP Q8WSF8
H	-4	ASP	-	expression tag	UNP Q8WSF8
H	-3	ASP	-	expression tag	UNP Q8WSF8
H	-2	ASP	-	expression tag	UNP Q8WSF8
H	-1	LYS	-	expression tag	UNP Q8WSF8
H	0	LEU	-	expression tag	UNP Q8WSF8
I	-23	MET	-	expression tag	UNP Q8WSF8
I	-22	SER	-	expression tag	UNP Q8WSF8
I	-21	ALA	-	expression tag	UNP Q8WSF8
I	-20	LEU	-	expression tag	UNP Q8WSF8
I	-19	LEU	-	expression tag	UNP Q8WSF8
I	-18	ILE	-	expression tag	UNP Q8WSF8
I	-17	LEU	-	expression tag	UNP Q8WSF8
I	-16	ALA	-	expression tag	UNP Q8WSF8
I	-15	LEU	-	expression tag	UNP Q8WSF8
I	-14	VAL	-	expression tag	UNP Q8WSF8
I	-13	GLY	-	expression tag	UNP Q8WSF8
I	-12	ALA	-	expression tag	UNP Q8WSF8
I	-11	ALA	-	expression tag	UNP Q8WSF8
I	-10	VAL	-	expression tag	UNP Q8WSF8
I	-9	ALA	-	expression tag	UNP Q8WSF8
I	-8	ASP	-	expression tag	UNP Q8WSF8
I	-7	TYR	-	expression tag	UNP Q8WSF8
I	-6	LYS	-	expression tag	UNP Q8WSF8
I	-5	ASP	-	expression tag	UNP Q8WSF8
I	-4	ASP	-	expression tag	UNP Q8WSF8
I	-3	ASP	-	expression tag	UNP Q8WSF8
I	-2	ASP	-	expression tag	UNP Q8WSF8
I	-1	LYS	-	expression tag	UNP Q8WSF8
I	0	LEU	-	expression tag	UNP Q8WSF8
J	-23	MET	-	expression tag	UNP Q8WSF8
J	-22	SER	-	expression tag	UNP Q8WSF8
J	-21	ALA	-	expression tag	UNP Q8WSF8

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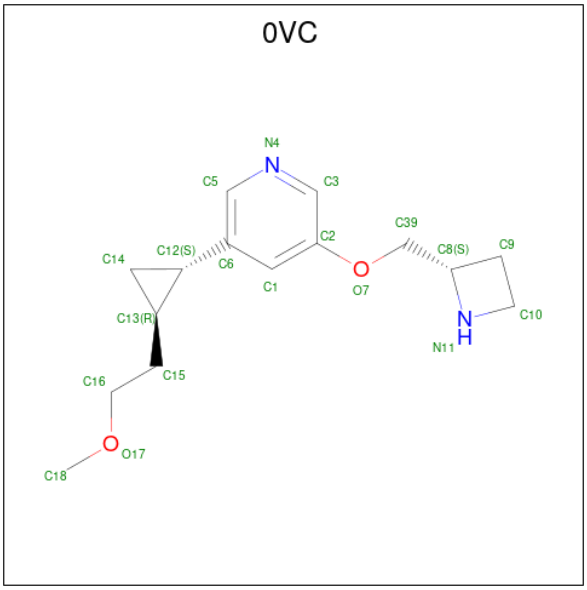
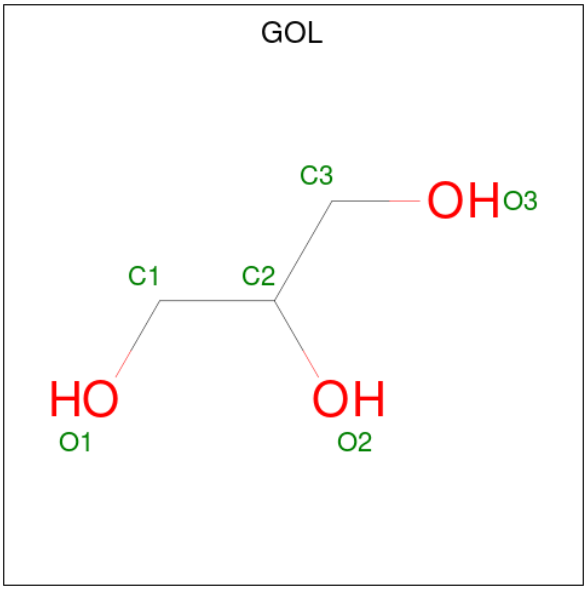
Chain	Residue	Modelled	Actual	Comment	Reference
J	-20	LEU	-	expression tag	UNP Q8WSF8
J	-19	LEU	-	expression tag	UNP Q8WSF8
J	-18	ILE	-	expression tag	UNP Q8WSF8
J	-17	LEU	-	expression tag	UNP Q8WSF8
J	-16	ALA	-	expression tag	UNP Q8WSF8
J	-15	LEU	-	expression tag	UNP Q8WSF8
J	-14	VAL	-	expression tag	UNP Q8WSF8
J	-13	GLY	-	expression tag	UNP Q8WSF8
J	-12	ALA	-	expression tag	UNP Q8WSF8
J	-11	ALA	-	expression tag	UNP Q8WSF8
J	-10	VAL	-	expression tag	UNP Q8WSF8
J	-9	ALA	-	expression tag	UNP Q8WSF8
J	-8	ASP	-	expression tag	UNP Q8WSF8
J	-7	TYR	-	expression tag	UNP Q8WSF8
J	-6	LYS	-	expression tag	UNP Q8WSF8
J	-5	ASP	-	expression tag	UNP Q8WSF8
J	-4	ASP	-	expression tag	UNP Q8WSF8
J	-3	ASP	-	expression tag	UNP Q8WSF8
J	-2	ASP	-	expression tag	UNP Q8WSF8
J	-1	LYS	-	expression tag	UNP Q8WSF8
J	0	LEU	-	expression tag	UNP Q8WSF8

- Molecule 2 is 3-[(2S)-azetidin-2-ylmethoxy]-5-[(1S,2R)-2-(2-methoxyethyl)cyclopropyl]pyridine (three-letter code: 0VC) (formula: $C_{15}H_{22}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 19 15 2 2	0	0
2	C	1	Total C N O 19 15 2 2	0	0
2	E	1	Total C N O 19 15 2 2	0	0
2	F	1	Total C N O 19 15 2 2	0	0
2	H	1	Total C N O 19 15 2 2	0	0
2	J	1	Total C N O 19 15 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

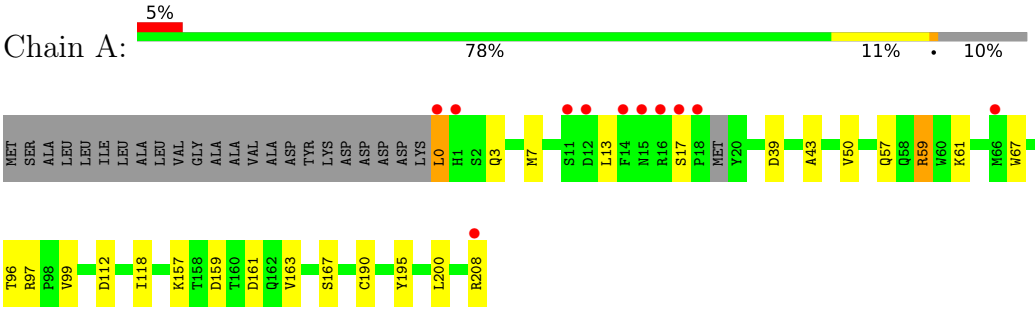
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	91	Total O 91 91	0	0
4	C	90	Total O 90 90	0	0
4	D	84	Total O 84 84	0	0
4	E	79	Total O 79 79	0	0
4	F	82	Total O 82 82	0	0
4	G	72	Total O 72 72	0	0
4	H	63	Total O 63 63	0	0
4	I	93	Total O 93 93	0	0
4	J	78	Total O 78 78	0	0

3 Residue-property plots (i)

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

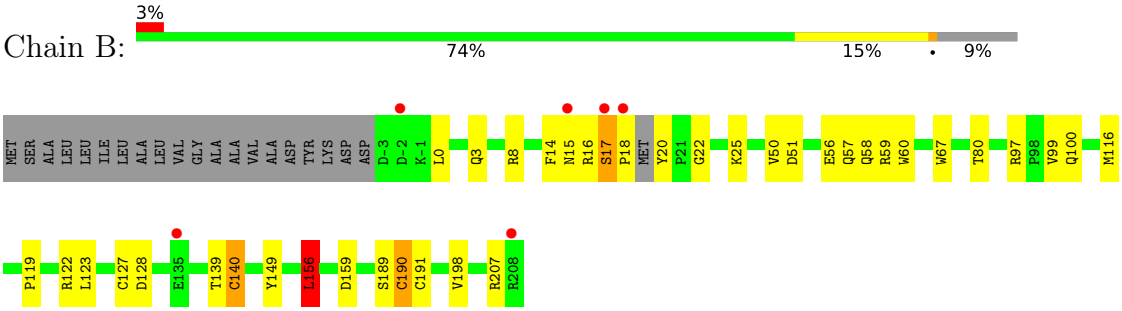
• Molecule 1: Soluble acetylcholine receptor

Chain A:



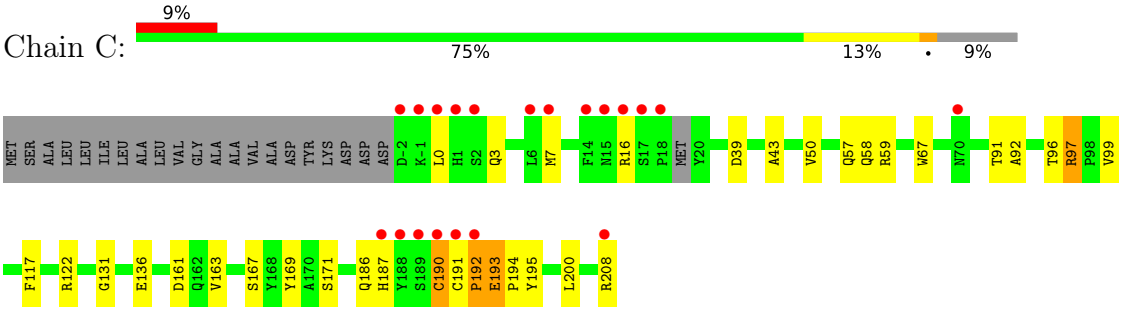
• Molecule 1: Soluble acetylcholine receptor

Chain B:



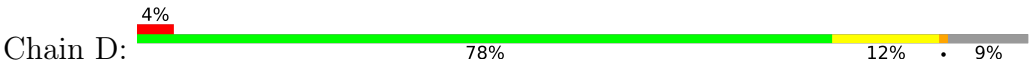
• Molecule 1: Soluble acetylcholine receptor

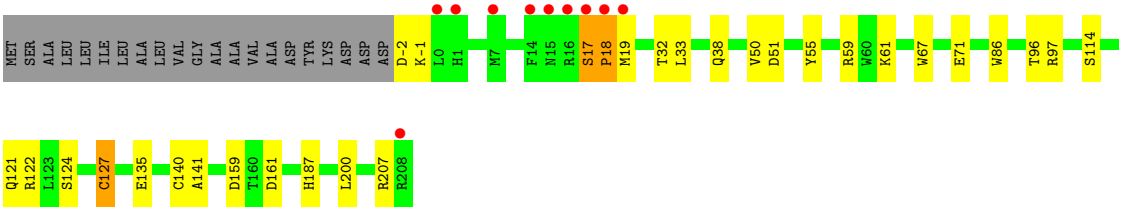
Chain C:



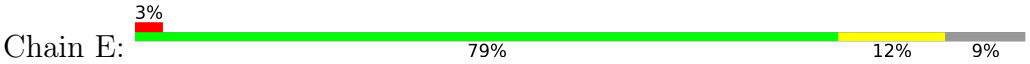
• Molecule 1: Soluble acetylcholine receptor

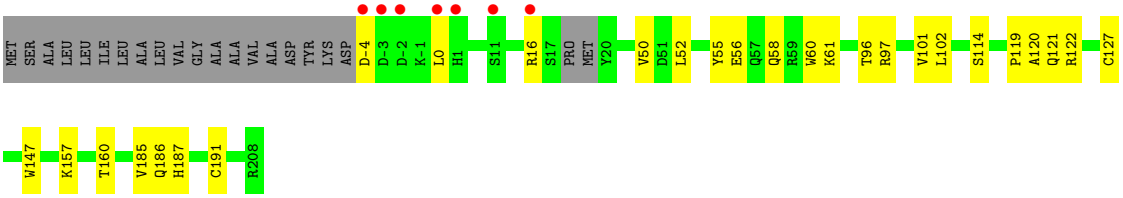
Chain D:



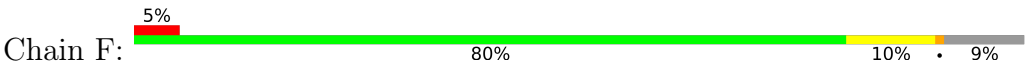


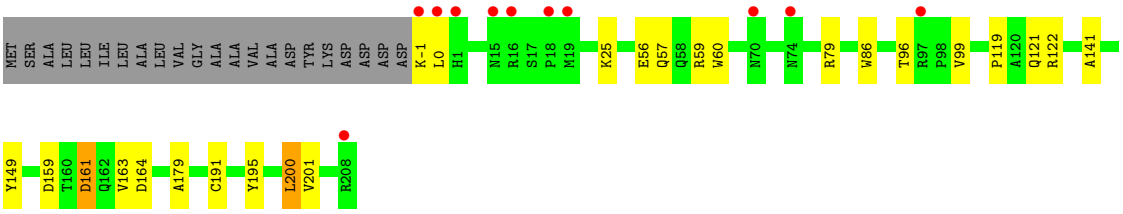
• Molecule 1: Soluble acetylcholine receptor



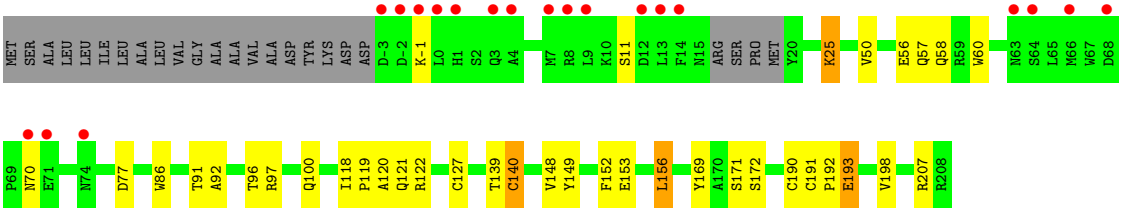


• Molecule 1: Soluble acetylcholine receptor

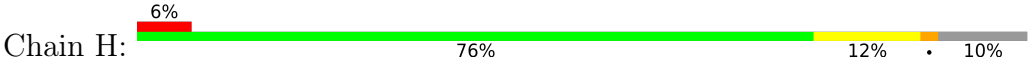


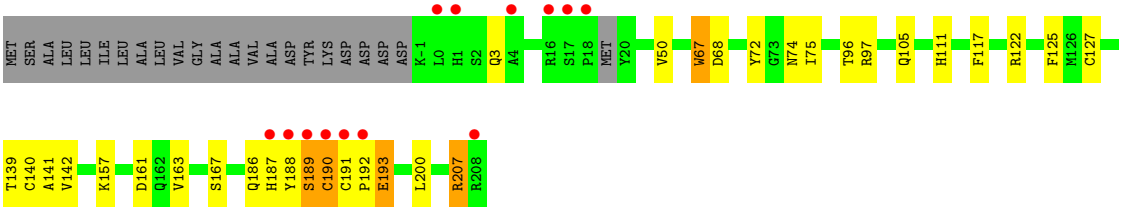


• Molecule 1: Soluble acetylcholine receptor



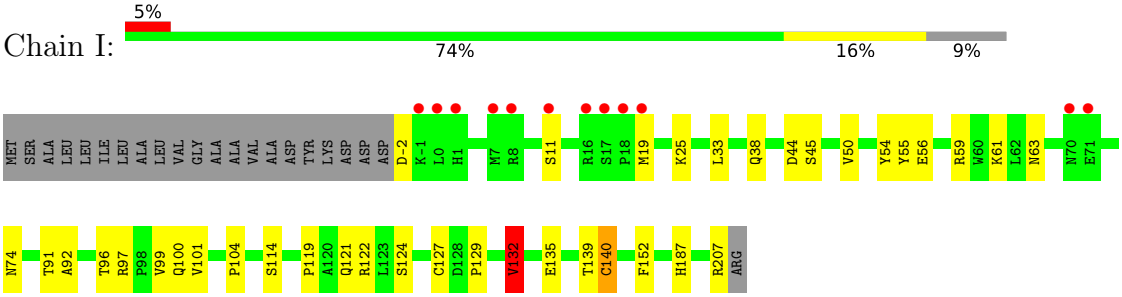
• Molecule 1: Soluble acetylcholine receptor





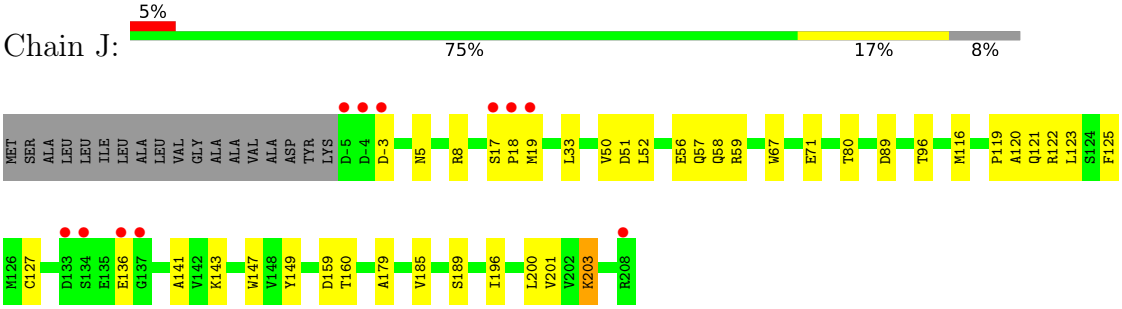
• Molecule 1: Soluble acetylcholine receptor

Chain I:



• Molecule 1: Soluble acetylcholine receptor

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	137.27Å 139.74Å 146.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.08 – 2.20 47.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (101.08-2.20) 99.8 (47.43-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.246 0.197 , 0.245	Depositor DCC
R_{free} test set	7147 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18186	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 45.64 % 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 1.2832e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 0VC

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	0.72	2/1710 (0.1%)	0.85	3/2331 (0.1%)
1	B	0.73	2/1757 (0.1%)	0.82	3/2392 (0.1%)
1	C	0.71	1/1789 (0.1%)	0.82	2/2439 (0.1%)
1	D	0.69	2/1745 (0.1%)	0.84	2/2378 (0.1%)
1	E	0.69	1/1763 (0.1%)	0.80	2/2401 (0.1%)
1	F	0.68	1/1737 (0.1%)	0.79	2/2367 (0.1%)
1	G	0.69	2/1710 (0.1%)	0.77	1/2330 (0.0%)
1	H	0.67	1/1790 (0.1%)	0.79	0/2440
1	I	0.68	0/1734	0.80	4/2364 (0.2%)
1	J	0.72	2/1791 (0.1%)	0.78	0/2439
All	All	0.70	14/17526 (0.1%)	0.81	19/23881 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	2
1	H	0	2
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	TRP	CD2-CE2	5.80	1.48	1.41
1	G	86	TRP	CD2-CE2	5.62	1.48	1.41
1	E	60	TRP	CD2-CE2	5.55	1.48	1.41
1	D	67	TRP	CD2-CE2	5.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	60	TRP	CD2-CE2	5.51	1.48	1.41
1	B	67	TRP	CD2-CE2	5.51	1.48	1.41
1	A	67	TRP	CD2-CE2	5.48	1.48	1.41
1	C	67	TRP	CD2-CE2	5.48	1.48	1.41
1	J	67	TRP	CD2-CE2	5.32	1.47	1.41
1	G	60	TRP	CD2-CE2	5.26	1.47	1.41
1	H	67	TRP	CD2-CE2	5.22	1.47	1.41
1	F	60	TRP	CD2-CE2	5.11	1.47	1.41
1	J	147	TRP	CD2-CE2	5.08	1.47	1.41
1	D	86	TRP	CD2-CE2	5.02	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	140	CYS	CA-CB-SG	-8.18	99.28	114.00
1	D	140	CYS	CA-CB-SG	-7.98	99.63	114.00
1	E	52	LEU	CA-CB-CG	6.16	129.47	115.30
1	F	164	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	97	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	0	LEU	CA-CB-CG	5.79	128.61	115.30
1	I	44	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	D	51	ASP	CB-CG-OD1	5.68	123.42	118.30
1	B	128	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	39	ASP	CB-CG-OD1	5.51	123.26	118.30
1	I	140	CYS	CA-CB-SG	-5.47	104.15	114.00
1	B	140	CYS	CA-CB-SG	-5.43	104.22	114.00
1	A	59	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	E	52	LEU	CB-CA-C	-5.28	100.17	110.20
1	F	200	LEU	CA-CB-CG	5.18	127.23	115.30
1	C	39	ASP	CB-CG-OD1	5.17	122.95	118.30
1	I	132	VAL	CB-CA-C	-5.05	101.81	111.40
1	I	44	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	156	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	CYS	Peptide
1	B	190	CYS	Peptide
1	C	186	GLN	Peptide
1	C	190[A]	CYS	Peptide

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Mol	Chain	Res	Type	Group
1	H	186	GLN	Peptide
1	H	190[A]	CYS	Peptide

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	1670	0	1603	15	0
1	B	1717	0	1648	28	1
1	C	1745	0	1655	38	0
1	D	1704	0	1637	29	0
1	E	1717	0	1641	16	0
1	F	1693	0	1632	20	0
1	G	1671	0	1599	20	0
1	H	1743	0	1659	26	0
1	I	1687	0	1625	26	0
1	J	1747	0	1674	24	1
2	A	19	0	22	1	0
2	C	19	0	22	1	0
2	E	19	0	22	1	0
2	F	19	0	22	3	0
2	H	19	0	22	0	0
2	J	19	0	22	0	0
3	A	30	0	40	3	0
3	B	18	0	24	1	0
3	C	12	0	16	4	0
3	D	12	0	16	0	0
3	E	18	0	24	2	0
3	F	12	0	16	4	0
3	G	18	0	24	2	0
3	H	6	0	8	1	0
3	I	18	0	24	7	0
3	J	12	0	16	1	0
4	A	90	0	0	1	0
4	B	91	0	0	1	1
4	C	90	0	0	6	0
4	D	84	0	0	5	0
4	E	79	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	82	0	0	4	0
4	G	72	0	0	2	0
4	H	63	0	0	0	0
4	I	93	0	0	4	1
4	J	78	0	0	1	0
All	All	18186	0	16713	229	2

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 7.

All (229) 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:H:188[B]:TYR:O	1:H:189[B]:SER:O	1.60	1.15
1:D:17:SER:HB3	1:D:18:PRO:CD	1.75	1.15
1:C:192[B]:PRO:O	1:C:193[B]:GLU:HG2	1.48	1.14
1:D:17:SER:CB	1:D:18:PRO:HD2	1.79	1.13
1:D:97[B]:ARG:HG2	1:D:97[B]:ARG:HH11	1.12	1.10
1:H:207:ARG:HG3	1:H:207:ARG:HH11	0.93	1.09
1:H:207:ARG:HH11	1:H:207:ARG:CG	1.70	1.02
1:D:18:PRO:HB2	1:D:19:MET:HA	1.37	1.00
1:H:189[B]:SER:O	1:H:191[B]:CYS:N	1.95	0.98
1:C:187[B]:HIS:CD2	1:C:193[B]:GLU:H	1.81	0.97
1:A:99:VAL:HG12	3:A:303:GOL:O2	1.64	0.96
1:J:5:ASN:OD1	1:J:8[B]:ARG:NH2	2.01	0.93
1:J:8[A]:ARG:NH2	1:J:71:GLU:O	2.01	0.92
1:C:192[B]:PRO:O	1:C:193[B]:GLU:CG	2.16	0.92
1:H:207:ARG:HG3	1:H:207:ARG:NH1	1.77	0.92
1:I:63:ASN:H	3:I:303:GOL:H12	1.35	0.88
1:A:59:ARG:NH1	1:A:159:ASP:OD1	2.08	0.87
1:J:59[B]:ARG:NH1	1:J:159:ASP:OD2	2.08	0.86
1:I:187:HIS:HD2	4:I:407:HOH:O	1.57	0.85
1:D:97[B]:ARG:HG2	1:D:97[B]:ARG:NH1	1.86	0.84
1:D:17:SER:HB3	1:D:18:PRO:HD2	0.87	0.82
1:F:59:ARG:NH1	1:F:159:ASP:OD1	2.16	0.79
1:I:101:VAL:H	3:I:301:GOL:H2	1.47	0.78
1:F:99:VAL:HG12	4:F:403:HOH:O	1.84	0.77
1:C:3:GLN:HG3	4:D:435:HOH:O	1.83	0.76
1:C:161:ASP:HB3	4:C:485:HOH:O	1.85	0.75
1:C:57:GLN:NE2	1:C:59:ARG:HH22	1.85	0.75
1:C:187[B]:HIS:CD2	1:C:193[B]:GLU:N	2.55	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PRO:HB2	1:D:19:MET:CA	2.18	0.71
1:H:188[B]:TYR:C	1:H:189[B]:SER:O	2.27	0.71
1:B:50:VAL:HG21	1:B:127:CYS:SG	2.30	0.71
1:C:187[B]:HIS:HD2	1:C:193[B]:GLU:H	1.35	0.71
1:C:193[A]:GLU:O	1:C:193[A]:GLU:HG2	1.91	0.70
1:A:97[B]:ARG:CG	1:A:97[B]:ARG:HH21	2.05	0.70
1:J:136:GLU:OE1	1:J:203:LYS:HE2	1.92	0.69
1:D:18:PRO:CB	1:D:19:MET:HA	2.19	0.69
1:H:207:ARG:CG	1:H:207:ARG:NH1	2.38	0.68
1:B:57:GLN:NE2	1:B:59[A]:ARG:HD3	2.10	0.67
1:C:117:PHE:HE2	3:C:303:GOL:H31	1.57	0.67
1:G:100:GLN:HE22	1:H:97:ARG:HH21	1.42	0.67
1:E:56:GLU:O	1:E:119:PRO:HD2	1.95	0.67
1:C:57:GLN:HE21	1:C:59:ARG:NH2	1.94	0.66
1:B:57:GLN:HE21	1:B:59[A]:ARG:HD3	1.60	0.66
1:D:97[B]:ARG:HH11	1:D:97[B]:ARG:CG	1.97	0.65
1:C:57:GLN:NE2	1:C:59:ARG:NH2	2.45	0.65
3:A:303:GOL:H32	1:E:101:VAL:O	1.96	0.64
1:G:192:PRO:HD2	1:G:193:GLU:OE2	1.96	0.64
1:I:129:PRO:O	1:I:132:VAL:HG22	1.98	0.64
1:I:100:GLN:HA	3:I:301:GOL:H11	1.78	0.64
1:J:56:GLU:O	1:J:119:PRO:HD2	1.98	0.64
1:B:14:PHE:C	1:B:16:ARG:H	2.02	0.64
1:D:55:TYR:CE1	1:E:147:TRP:HH2	2.16	0.63
1:B:156:LEU:HD13	1:B:198:VAL:HG23	1.80	0.63
1:I:54:TYR:CE1	1:I:121[A]:GLN:OE1	2.52	0.63
1:C:195:TYR:HE1	4:C:419:HOH:O	1.79	0.63
1:E:185:VAL:HG12	1:E:186:GLN:N	2.15	0.61
3:A:303:GOL:H32	1:E:102:LEU:HA	1.83	0.61
1:J:59[B]:ARG:HD3	1:J:116:MET:HE1	1.82	0.60
1:F:79:ARG:HD3	1:G:149:TYR:CE1	2.37	0.60
1:D:207:ARG:HD2	4:D:432:HOH:O	2.02	0.60
1:F:56[B]:GLU:OE2	3:F:303:GOL:O1	2.19	0.59
1:B:59[A]:ARG:HD2	1:B:116:MET:CE	2.31	0.59
1:B:100:GLN:HE22	1:C:97:ARG:HH21	1.49	0.58
1:G:56:GLU:OE2	1:G:58:GLN:NE2	2.31	0.58
1:B:59[A]:ARG:NH1	1:B:159:ASP:OD2	2.33	0.58
1:D:97[B]:ARG:NH1	1:D:97[B]:ARG:CG	2.59	0.58
1:I:101:VAL:H	3:I:301:GOL:C2	2.15	0.58
1:C:57:GLN:HE21	1:C:59:ARG:HH22	1.50	0.57
1:F:96:THR:O	1:J:122:ARG:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:VAL:HG21	1:G:127:CYS:SG	2.45	0.57
1:I:104:PRO:HG2	1:J:89:ASP:HB2	1.87	0.57
1:B:50:VAL:CG2	1:B:127:CYS:SG	2.92	0.57
1:C:193[B]:GLU:HB2	1:C:194[B]:PRO:HD2	1.87	0.57
1:D:18:PRO:CB	1:D:19:MET:CA	2.81	0.56
1:C:187[B]:HIS:NE2	1:C:193[B]:GLU:HA	2.20	0.56
1:J:56:GLU:OE2	1:J:58:GLN:NE2	2.35	0.56
1:D:187:HIS:HD2	4:D:444:HOH:O	1.87	0.56
4:F:440:HOH:O	1:G:97[B]:ARG:HD3	2.05	0.56
1:C:187[B]:HIS:NE2	1:C:193[B]:GLU:CA	2.69	0.56
1:D:50:VAL:HG21	1:D:127:CYS:SG	2.46	0.56
1:C:99:VAL:HG12	4:C:461:HOH:O	2.06	0.55
1:F:163:VAL:HG21	1:F:200:LEU:CD1	2.37	0.55
1:E:185:VAL:CG1	1:E:186:GLN:N	2.70	0.54
1:E:56:GLU:OE2	1:E:58:GLN:NE2	2.36	0.54
1:B:59[A]:ARG:HD2	1:B:116:MET:HE2	1.89	0.54
1:B:56:GLU:OE2	1:B:58:GLN:NE2	2.36	0.53
1:J:141:ALA:HA	1:J:200:LEU:O	2.07	0.53
1:D:38:GLN:OE1	1:D:55:TYR:CE1	2.62	0.53
1:H:117:PHE:HE2	3:H:302:GOL:H31	1.73	0.53
1:I:54:TYR:HE1	1:I:121[A]:GLN:OE1	1.91	0.53
1:J:185:VAL:HG12	1:J:196:ILE:CD1	2.39	0.53
1:D:59:ARG:NH1	1:D:159:ASP:OD2	2.42	0.53
1:C:192[B]:PRO:O	1:C:193[B]:GLU:CB	2.57	0.52
1:D:50:VAL:CG2	1:D:127:CYS:SG	2.97	0.52
1:D:32:THR:HG21	1:D:59:ARG:HH11	1.75	0.52
1:J:59[B]:ARG:HH21	1:J:116:MET:HE1	1.75	0.52
1:A:97[B]:ARG:HH21	1:A:97[B]:ARG:HG2	1.74	0.52
3:E:303:GOL:H12	4:E:457:HOH:O	2.09	0.52
1:I:50:VAL:HG21	1:I:127:CYS:SG	2.49	0.52
1:J:50:VAL:HG21	1:J:127:CYS:SG	2.50	0.51
1:C:190[B]:CYS:SG	1:C:191[B]:CYS:N	2.83	0.51
1:H:163:VAL:HG21	1:H:200:LEU:CD1	2.41	0.51
1:I:139:THR:O	1:I:140:CYS:SG	2.69	0.51
1:B:20:TYR:CE2	1:B:22:GLY:HA2	2.45	0.51
3:G:303:GOL:H12	4:G:468:HOH:O	2.10	0.51
1:I:91:THR:HG22	1:I:92:ALA:O	2.10	0.51
1:J:57:GLN:NE2	4:J:447:HOH:O	2.45	0.50
1:G:139:THR:O	1:G:140:CYS:SG	2.69	0.50
1:C:7:MET:HE2	1:D:18:PRO:HB3	1.92	0.50
1:C:122:ARG:HD2	1:D:96:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:17:SER:HB3	1:J:18:PRO:HA	1.94	0.49
1:I:56:GLU:O	1:I:119:PRO:HD2	2.13	0.49
1:E:191:CYS:SG	2:E:301:0VC:H8	2.53	0.49
1:C:117:PHE:CE2	3:C:303:GOL:H31	2.44	0.49
1:J:52:LEU:HG	1:J:125:PHE:HE2	1.77	0.49
3:E:303:GOL:C1	4:E:457:HOH:O	2.61	0.49
1:H:207:ARG:NH1	1:H:207:ARG:CB	2.76	0.48
1:B:149:TYR:OH	3:B:303:GOL:H11	2.13	0.48
1:E:120:ALA:C	1:E:121:GLN:HG3	2.33	0.48
1:I:100:GLN:HA	3:I:301:GOL:C1	2.43	0.48
1:F:141:ALA:HA	1:F:200:LEU:O	2.13	0.48
1:H:105:GLN:HA	1:H:105:GLN:NE2	2.28	0.48
1:H:50:VAL:HG21	1:H:127:CYS:SG	2.54	0.48
1:G:25:LYS:HD2	1:G:152:PHE:HB3	1.96	0.48
1:C:58:GLN:HE22	3:C:303:GOL:H11	1.78	0.47
1:C:43:ALA:HA	1:C:50:VAL:HG22	1.95	0.47
1:B:14:PHE:O	1:B:16:ARG:N	2.47	0.47
1:I:25:LYS:HG3	1:I:152:PHE:HB3	1.95	0.47
1:H:122:ARG:HD2	1:I:96:THR:O	2.15	0.47
1:B:97[A]:ARG:NH1	4:B:425:HOH:O	2.48	0.47
1:B:116:MET:HG2	2:C:301:0VC:H6	1.95	0.47
1:H:163:VAL:HG21	1:H:200:LEU:HD11	1.97	0.47
1:I:122:ARG:HD2	1:J:96:THR:O	2.15	0.47
1:A:163:VAL:HG21	1:A:200:LEU:HD12	1.95	0.47
1:G:156:LEU:HD13	1:G:198:VAL:HG23	1.96	0.47
1:J:59[B]:ARG:HD3	1:J:116:MET:CE	2.44	0.47
1:E:61:LYS:HA	1:E:114:SER:HA	1.97	0.47
1:F:161:ASP:HB3	4:F:473:HOH:O	2.13	0.47
1:D:122:ARG:HD2	1:E:96:THR:O	2.15	0.47
1:A:163:VAL:HG21	1:A:200:LEU:CD1	2.45	0.46
1:B:3:GLN:HG2	4:C:418:HOH:O	2.13	0.46
1:B:56:GLU:O	1:B:119:PRO:HD2	2.15	0.46
1:H:193[A]:GLU:O	1:H:193[A]:GLU:HG2	2.14	0.46
1:B:207[A]:ARG:O	1:B:207[A]:ARG:HG3	2.14	0.46
1:F:122:ARG:HD2	1:G:96:THR:O	2.16	0.46
1:C:193[A]:GLU:O	1:C:193[A]:GLU:CG	2.60	0.46
1:F:163:VAL:HG21	1:F:200:LEU:HD12	1.98	0.46
1:G:57:GLN:HG3	1:G:118:ILE:HG12	1.97	0.46
1:I:97[B]:ARG:HD2	1:I:124:SER:OG	2.16	0.46
1:I:99:VAL:HG11	1:I:121[B]:GLN:CD	2.36	0.46
1:G:56:GLU:O	1:G:119:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:ARG:NH1	1:H:207:ARG:HB2	2.30	0.46
1:E:50:VAL:HG21	1:E:127:CYS:SG	2.56	0.45
1:A:97[B]:ARG:HH21	1:A:97[B]:ARG:HG3	1.79	0.45
1:A:43:ALA:HA	1:A:50:VAL:HG22	1.98	0.45
1:I:207:ARG:HD2	4:I:441:HOH:O	2.16	0.45
1:J:185:VAL:HG12	1:J:196:ILE:HD13	1.98	0.45
1:H:141:ALA:HA	1:H:200:LEU:O	2.17	0.45
1:C:58:GLN:HE22	3:C:303:GOL:C1	2.30	0.45
1:I:74:ASN:ND2	4:I:483:HOH:O	2.47	0.45
1:F:86:TRP:HE1	3:F:302:GOL:H12	1.83	0.44
1:B:14:PHE:C	1:B:16:ARG:N	2.68	0.44
1:I:63:ASN:N	3:I:303:GOL:H12	2.17	0.44
1:C:163:VAL:HG21	1:C:200:LEU:HD11	2.00	0.44
1:J:120:ALA:C	1:J:121:GLN:HG3	2.37	0.44
1:F:79:ARG:HG2	1:G:148:VAL:CG2	2.48	0.44
1:H:72:TYR:O	1:H:75:ILE:HD12	2.17	0.44
1:B:57:GLN:HE21	1:B:59[A]:ARG:HH11	1.66	0.43
1:D:161:ASP:OD2	4:D:463:HOH:O	2.21	0.43
1:E:97[B]:ARG:NH1	4:E:448:HOH:O	2.51	0.43
1:B:57:GLN:NE2	1:B:59[A]:ARG:HH11	2.15	0.43
1:J:51:ASP:HA	1:J:123:LEU:O	2.18	0.43
1:D:97[A]:ARG:HD2	1:D:124:SER:CB	2.48	0.43
1:G:91:THR:HG22	1:G:92:ALA:O	2.18	0.43
1:G:120:ALA:O	1:G:121:GLN:HG3	2.19	0.43
1:G:169:TYR:CZ	1:G:171:SER:HB2	2.54	0.43
1:C:187[B]:HIS:HD2	1:C:193[B]:GLU:N	2.04	0.43
1:F:57:GLN:NE2	4:F:446:HOH:O	2.50	0.43
1:G:172:SER:O	1:G:207:ARG:HD3	2.19	0.43
1:A:13:LEU:O	1:A:17:SER:HB2	2.19	0.43
1:A:57:GLN:HG3	1:A:118:ILE:HG12	2.01	0.43
1:D:32:THR:HG21	1:D:59:ARG:NH1	2.33	0.43
1:B:51:ASP:HA	1:B:123:LEU:O	2.19	0.42
1:C:131:GLY:HA2	4:C:449:HOH:O	2.20	0.42
1:F:56[B]:GLU:OE1	3:F:303:GOL:O3	2.28	0.42
1:A:195:TYR:CE1	2:A:301:0VC:H15	2.53	0.42
1:A:161:ASP:HB3	4:A:408:HOH:O	2.20	0.42
1:D:121:GLN:NE2	4:D:481:HOH:O	2.52	0.42
3:I:301:GOL:H32	4:I:480:HOH:O	2.20	0.42
1:F:179:ALA:HA	1:F:201:VAL:O	2.19	0.42
1:I:45:SER:HB3	1:I:129:PRO:HG2	2.02	0.42
2:F:301:0VC:H5	1:J:116:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187[B]:HIS:NE2	1:H:193[B]:GLU:C	2.73	0.42
1:G:190:CYS:SG	1:G:191:CYS:N	2.92	0.42
1:J:149:TYR:OH	3:J:303:GOL:H32	2.20	0.42
1:A:61:LYS:HE3	1:A:112:ASP:O	2.20	0.42
1:F:191:CYS:SG	2:F:301:0VC:H8	2.59	0.42
1:C:91:THR:HG22	1:C:92:ALA:O	2.20	0.41
1:C:163:VAL:HG21	1:C:200:LEU:CD1	2.49	0.41
1:E:55:TYR:HB3	1:E:120:ALA:HA	2.01	0.41
1:H:190[B]:CYS:SG	1:H:191[B]:CYS:N	2.92	0.41
1:J:179:ALA:HA	1:J:201:VAL:O	2.20	0.41
1:B:190:CYS:SG	1:B:191:CYS:N	2.94	0.41
3:G:303:GOL:H12	4:G:466:HOH:O	2.20	0.41
1:H:67:TRP:CE3	1:H:111:HIS:HA	2.56	0.41
1:A:96:THR:O	1:E:122:ARG:HD2	2.21	0.41
1:F:149:TYR:OH	3:F:302:GOL:H11	2.20	0.41
1:I:61:LYS:HA	1:I:114:SER:HA	2.03	0.41
1:B:139:THR:O	1:B:140:CYS:SG	2.78	0.41
1:D:141:ALA:HA	1:D:200:LEU:O	2.19	0.41
1:G:77:ASP:OD2	1:G:77:ASP:N	2.53	0.41
1:G:122:ARG:HD2	1:H:96:THR:O	2.21	0.41
1:H:139:THR:O	1:H:140:CYS:SG	2.78	0.41
1:B:100:GLN:NE2	1:C:97:ARG:HH21	2.18	0.41
1:H:105:GLN:HA	1:H:105:GLN:HE21	1.83	0.41
1:A:7:MET:SD	1:B:18:PRO:HB2	2.61	0.41
1:H:125:PHE:CD1	1:H:142:VAL:HB	2.55	0.41
1:I:38:GLN:OE1	1:I:55:TYR:CE2	2.73	0.41
1:I:25:LYS:HE2	1:I:152:PHE:CD1	2.56	0.41
1:C:169:TYR:CZ	1:C:171:SER:HB2	2.56	0.40
1:D:97[A]:ARG:HD2	1:D:124:SER:OG	2.21	0.40
1:C:187[B]:HIS:NE2	1:C:193[B]:GLU:N	2.66	0.40
1:C:191[B]:CYS:HB3	4:C:419:HOH:O	2.21	0.40
1:D:61:LYS:HA	1:D:114:SER:HA	2.03	0.40
1:B:122:ARG:HD2	1:C:96:THR:O	2.21	0.40
1:F:195:TYR:CE1	2:F:301:0VC:H15	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:430:HOH:O	4:I:493:HOH:O[2_664]	1.88	0.32
1:B:8:ARG:NH1	1:J:8[B]:ARG:NH1[4_455]	2.13	0.07

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	205/232 (88%)	198 (97%)	7 (3%)	0	100 100
1	B	210/232 (90%)	199 (95%)	8 (4%)	3 (1%)	11 8
1	C	215/232 (93%)	207 (96%)	4 (2%)	4 (2%)	8 5
1	D	211/232 (91%)	201 (95%)	8 (4%)	2 (1%)	17 16
1	E	211/232 (91%)	204 (97%)	7 (3%)	0	100 100
1	F	210/232 (90%)	202 (96%)	8 (4%)	0	100 100
1	G	205/232 (88%)	198 (97%)	7 (3%)	0	100 100
1	H	215/232 (93%)	202 (94%)	6 (3%)	7 (3%)	4 2
1	I	210/232 (90%)	204 (97%)	6 (3%)	0	100 100
1	J	216/232 (93%)	208 (96%)	7 (3%)	1 (0%)	29 31
All	All	2108/2320 (91%)	2023 (96%)	68 (3%)	17 (1%)	29 19

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	ASN
1	B	17	SER
1	D	18	PRO
1	H	189[A]	SER
1	H	189[B]	SER
1	H	189[C]	SER
1	J	19	MET
1	B	189	SER
1	C	193[A]	GLU
1	C	193[B]	GLU
1	H	192[A]	PRO
1	H	192[B]	PRO
1	C	192[A]	PRO
1	C	192[B]	PRO

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Mol	Chain	Res	Type
1	D	17	SER
1	H	193[A]	GLU
1	H	193[B]	GLU

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	190/207 (92%)	185 (97%)	5 (3%)	46	58
1	B	195/207 (94%)	189 (97%)	6 (3%)	40	51
1	C	200/207 (97%)	195 (98%)	5 (2%)	47	60
1	D	194/207 (94%)	188 (97%)	6 (3%)	40	51
1	E	196/207 (95%)	191 (97%)	5 (3%)	46	58
1	F	193/207 (93%)	188 (97%)	5 (3%)	46	58
1	G	190/207 (92%)	183 (96%)	7 (4%)	34	43
1	H	200/207 (97%)	192 (96%)	8 (4%)	31	40
1	I	193/207 (93%)	186 (96%)	7 (4%)	35	45
1	J	199/207 (96%)	192 (96%)	7 (4%)	36	46
All	All	1950/2070 (94%)	1889 (97%)	61 (3%)	40	51

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LEU
1	A	3	GLN
1	A	157	LYS
1	A	167	SER
1	A	208	ARG
1	B	0	LEU
1	B	17	SER
1	B	25	LYS
1	B	80	THR
1	B	99	VAL

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Mol	Chain	Res	Type
1	B	156	LEU
1	C	0	LEU
1	C	16	ARG
1	C	136	GLU
1	C	167	SER
1	C	208	ARG
1	D	-2	ASP
1	D	-1	LYS
1	D	33	LEU
1	D	71	GLU
1	D	127	CYS
1	D	135	GLU
1	E	-4	ASP
1	E	0	LEU
1	E	16	ARG
1	E	157	LYS
1	E	160	THR
1	F	-1	LYS
1	F	0	LEU
1	F	25	LYS
1	F	121	GLN
1	F	161	ASP
1	G	-1	LYS
1	G	11	SER
1	G	25	LYS
1	G	70	ASN
1	G	153	GLU
1	G	156	LEU
1	G	193	GLU
1	H	3[A]	GLN
1	H	3[B]	GLN
1	H	68	ASP
1	H	74	ASN
1	H	157	LYS
1	H	161	ASP
1	H	167	SER
1	H	207	ARG
1	I	-2	ASP
1	I	11	SER
1	I	19	MET
1	I	33	LEU
1	I	59	ARG

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Mol	Chain	Res	Type
1	I	132	VAL
1	I	135	GLU
1	J	-3	ASP
1	J	33	LEU
1	J	80	THR
1	J	143	LYS
1	J	160	THR
1	J	189	SER
1	J	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	162	GLN
1	B	57	GLN
1	B	100	GLN
1	C	57	GLN
1	C	58	GLN
1	E	1	HIS
1	E	15	ASN
1	E	63	ASN
1	E	70	ASN
1	F	1	HIS
1	F	58	GLN
1	F	100	GLN
1	G	15	ASN
1	G	100	GLN
1	G	162	GLN
1	H	105	GLN
1	I	57	GLN
1	J	184	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)

32 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	$\#\|Z\| > 2$
3	GOL	D	301	-	5,5,5	0.48	0	5,5,5	0.37	0
2	0VC	C	301	-	20,21,21	1.16	1 (5%)	21,28,28	2.04	6 (28%)
3	GOL	I	302	-	5,5,5	0.47	0	5,5,5	0.61	0
2	0VC	H	301	-	20,21,21	1.09	1 (5%)	21,28,28	2.36	5 (23%)
3	GOL	E	304	-	5,5,5	0.51	0	5,5,5	0.66	0
3	GOL	J	303	-	5,5,5	0.44	0	5,5,5	0.47	0
3	GOL	I	303	-	5,5,5	0.57	0	5,5,5	0.53	0
3	GOL	C	302	-	5,5,5	0.25	0	5,5,5	0.64	0
3	GOL	A	302	-	5,5,5	0.59	0	5,5,5	0.86	0
3	GOL	F	302	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	G	302	-	5,5,5	0.49	0	5,5,5	0.19	0
3	GOL	G	301	-	5,5,5	0.50	0	5,5,5	0.28	0
3	GOL	A	304	-	5,5,5	0.46	0	5,5,5	0.40	0
3	GOL	A	305	-	5,5,5	0.41	0	5,5,5	0.33	0
3	GOL	J	302	-	5,5,5	0.26	0	5,5,5	0.51	0
3	GOL	E	302	-	5,5,5	0.27	0	5,5,5	0.68	0
2	0VC	A	301	-	20,21,21	0.97	0	21,28,28	2.33	8 (38%)
2	0VC	J	301	-	20,21,21	1.00	1 (5%)	21,28,28	2.36	7 (33%)
3	GOL	F	303	-	5,5,5	0.53	0	5,5,5	0.55	0
3	GOL	G	303	-	5,5,5	0.55	0	5,5,5	0.25	0
2	0VC	E	301	-	20,21,21	0.98	1 (5%)	21,28,28	2.25	6 (28%)
3	GOL	H	302	-	5,5,5	0.46	0	5,5,5	0.60	0
3	GOL	B	302	-	5,5,5	0.40	0	5,5,5	0.35	0
3	GOL	A	303	-	5,5,5	1.09	0	5,5,5	1.44	2 (40%)
2	0VC	F	301	-	20,21,21	0.99	0	21,28,28	2.31	9 (42%)
3	GOL	D	302	-	5,5,5	0.31	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	B	303	-	5,5,5	0.15	0	5,5,5	0.75	0
3	GOL	A	306	-	5,5,5	0.60	0	5,5,5	0.87	0
3	GOL	I	301	-	5,5,5	0.49	0	5,5,5	0.90	0
3	GOL	C	303	-	5,5,5	0.81	0	5,5,5	1.00	0
3	GOL	B	301	-	5,5,5	0.41	0	5,5,5	0.25	0
3	GOL	E	303	-	5,5,5	0.40	0	5,5,5	0.50	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	GOL	D	301	-	-	2/4/4/4	-
2	0VC	C	301	-	-	4/12/24/24	0/3/3/3
3	GOL	I	302	-	-	2/4/4/4	-
2	0VC	H	301	-	-	2/12/24/24	0/3/3/3
3	GOL	E	304	-	-	4/4/4/4	-
3	GOL	J	303	-	-	2/4/4/4	-
3	GOL	I	303	-	-	2/4/4/4	-
3	GOL	C	302	-	-	2/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	F	302	-	-	2/4/4/4	-
3	GOL	G	302	-	-	4/4/4/4	-
3	GOL	G	301	-	-	4/4/4/4	-
3	GOL	A	304	-	-	4/4/4/4	-
3	GOL	A	305	-	-	2/4/4/4	-
3	GOL	J	302	-	-	4/4/4/4	-
3	GOL	E	302	-	-	4/4/4/4	-
2	0VC	A	301	-	-	3/12/24/24	0/3/3/3
2	0VC	J	301	-	-	7/12/24/24	0/3/3/3
3	GOL	F	303	-	-	4/4/4/4	-
3	GOL	G	303	-	-	3/4/4/4	-
2	0VC	E	301	-	-	3/12/24/24	0/3/3/3
3	GOL	H	302	-	-	4/4/4/4	-
3	GOL	B	302	-	-	2/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0VC	F	301	-	-	5/12/24/24	0/3/3/3
3	GOL	D	302	-	-	2/4/4/4	-
3	GOL	B	303	-	-	0/4/4/4	-
3	GOL	A	306	-	-	4/4/4/4	-
3	GOL	I	301	-	-	0/4/4/4	-
3	GOL	C	303	-	-	2/4/4/4	-
3	GOL	B	301	-	-	4/4/4/4	-
3	GOL	E	303	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	0VC	C8-N11	-2.78	1.45	1.48
2	J	301	0VC	C14-C12	2.17	1.54	1.50
2	E	301	0VC	C9-C8	-2.15	1.52	1.54
2	H	301	0VC	C8-N11	-2.08	1.46	1.48

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	301	0VC	C6-C12-C13	-6.84	111.09	121.31
2	A	301	0VC	C6-C12-C13	-6.62	111.43	121.31
2	F	301	0VC	C6-C12-C13	-6.44	111.69	121.31
2	J	301	0VC	C6-C12-C13	-5.77	112.69	121.31
2	E	301	0VC	C6-C12-C13	-5.02	113.81	121.31
2	C	301	0VC	C6-C12-C13	-4.90	113.99	121.31
2	E	301	0VC	C15-C13-C12	-4.54	110.15	122.03
2	H	301	0VC	C15-C13-C12	-4.40	110.51	122.03
2	J	301	0VC	C15-C13-C12	-4.25	110.90	122.03
2	C	301	0VC	C14-C12-C6	-4.13	114.31	122.24
2	A	301	0VC	C15-C13-C12	-4.00	111.56	122.03
2	J	301	0VC	C39-O7-C2	3.95	126.31	117.93
2	J	301	0VC	C3-N4-C5	3.95	122.87	117.48
2	E	301	0VC	C14-C12-C6	-3.89	114.76	122.24
2	C	301	0VC	C15-C13-C12	-3.89	111.86	122.03
2	H	301	0VC	C39-O7-C2	3.85	126.09	117.93
2	E	301	0VC	C39-O7-C2	3.75	125.88	117.93
2	J	301	0VC	C14-C12-C6	-3.71	115.11	122.24
2	A	301	0VC	C1-C6-C12	3.52	126.80	120.01
2	H	301	0VC	C14-C12-C6	-3.39	115.71	122.24
2	F	301	0VC	C14-C12-C6	-3.38	115.75	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	0VC	C3-N4-C5	3.28	121.95	117.48
2	A	301	0VC	C3-N4-C5	3.20	121.85	117.48
2	F	301	0VC	C3-N4-C5	3.11	121.72	117.48
2	F	301	0VC	C15-C13-C12	-3.10	113.90	122.03
2	F	301	0VC	C1-C6-C12	3.03	125.86	120.01
2	H	301	0VC	C3-N4-C5	2.88	121.41	117.48
2	F	301	0VC	C2-C3-N4	-2.87	117.95	122.26
2	E	301	0VC	C3-N4-C5	2.70	121.17	117.48
2	C	301	0VC	C39-O7-C2	2.58	123.39	117.93
2	E	301	0VC	C1-C6-C12	2.58	124.98	120.01
2	J	301	0VC	C1-C6-C12	2.35	124.54	120.01
3	A	303	GOL	O2-C2-C3	-2.32	98.91	109.12
2	A	301	0VC	C5-C6-C12	-2.25	115.90	120.92
2	A	301	0VC	C14-C12-C6	-2.20	118.01	122.24
2	F	301	0VC	C1-C2-C3	2.18	121.88	119.28
2	C	301	0VC	C1-C6-C12	2.13	124.12	120.01
3	A	303	GOL	C3-C2-C1	2.12	119.93	111.70
2	J	301	0VC	C6-C5-N4	-2.10	120.84	124.14
2	F	301	0VC	C16-C15-C13	-2.09	109.31	113.17
2	A	301	0VC	C2-C3-N4	-2.06	119.16	122.26
2	F	301	0VC	C39-O7-C2	2.02	122.22	117.93
2	A	301	0VC	C39-O7-C2	2.01	122.19	117.93

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	0VC	C13-C15-C16-O17
3	A	302	GOL	C1-C2-C3-O3
3	A	302	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2
3	A	303	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-C3
3	A	305	GOL	O1-C1-C2-O2
3	A	306	GOL	O1-C1-C2-C3
3	A	306	GOL	C1-C2-C3-O3
3	B	301	GOL	O1-C1-C2-C3
3	B	301	GOL	C1-C2-C3-O3
3	C	302	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-C3
3	E	302	GOL	O1-C1-C2-C3
3	E	304	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	E	304	GOL	O2-C2-C3-O3
3	F	303	GOL	O1-C1-C2-C3
3	G	301	GOL	O1-C1-C2-C3
3	G	301	GOL	C1-C2-C3-O3
3	G	302	GOL	O1-C1-C2-C3
3	G	302	GOL	C1-C2-C3-O3
3	G	303	GOL	O1-C1-C2-C3
3	H	302	GOL	C1-C2-C3-O3
3	H	302	GOL	O2-C2-C3-O3
3	I	303	GOL	O2-C2-C3-O3
3	J	302	GOL	O1-C1-C2-C3
3	J	302	GOL	C1-C2-C3-O3
3	A	306	GOL	O2-C2-C3-O3
3	B	301	GOL	O2-C2-C3-O3
3	C	302	GOL	O2-C2-C3-O3
3	D	301	GOL	O1-C1-C2-O2
3	E	302	GOL	O1-C1-C2-O2
2	F	301	0VC	C13-C15-C16-O17
2	J	301	0VC	C13-C15-C16-O17
3	A	304	GOL	C1-C2-C3-O3
3	A	305	GOL	O1-C1-C2-C3
3	B	302	GOL	C1-C2-C3-O3
3	D	302	GOL	C1-C2-C3-O3
3	E	302	GOL	C1-C2-C3-O3
3	F	302	GOL	O1-C1-C2-C3
3	F	303	GOL	C1-C2-C3-O3
3	H	302	GOL	O1-C1-C2-C3
3	I	302	GOL	O1-C1-C2-C3
3	I	303	GOL	C1-C2-C3-O3
3	J	303	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-O2
3	F	303	GOL	O1-C1-C2-O2
3	G	301	GOL	O1-C1-C2-O2
3	G	301	GOL	O2-C2-C3-O3
3	G	302	GOL	O2-C2-C3-O3
3	G	303	GOL	O1-C1-C2-O2
3	H	302	GOL	O1-C1-C2-O2
3	J	302	GOL	O1-C1-C2-O2
3	J	302	GOL	O2-C2-C3-O3
2	H	301	0VC	C15-C16-O17-C18
2	C	301	0VC	O7-C39-C8-C9
3	E	302	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	J	303	GOL	O1-C1-C2-O2
2	J	301	0VC	C1-C2-O7-C39
3	G	303	GOL	C1-C2-C3-O3
2	J	301	0VC	C15-C16-O17-C18
2	C	301	0VC	C1-C2-O7-C39
3	D	302	GOL	O2-C2-C3-O3
3	E	304	GOL	O1-C1-C2-O2
3	G	302	GOL	O1-C1-C2-O2
2	F	301	0VC	C13-C12-C6-C1
2	F	301	0VC	C15-C16-O17-C18
2	C	301	0VC	C3-C2-O7-C39
2	J	301	0VC	C3-C2-O7-C39
3	A	304	GOL	O2-C2-C3-O3
3	B	302	GOL	O2-C2-C3-O3
3	F	302	GOL	O1-C1-C2-O2
3	I	302	GOL	O1-C1-C2-O2
2	J	301	0VC	O7-C39-C8-C9
2	A	301	0VC	C13-C12-C6-C1
2	E	301	0VC	C13-C12-C6-C1
3	C	303	GOL	O1-C1-C2-C3
2	C	301	0VC	C14-C13-C15-C16
3	B	301	GOL	O1-C1-C2-O2
3	F	303	GOL	O2-C2-C3-O3
2	F	301	0VC	C13-C12-C6-C5
3	A	306	GOL	O1-C1-C2-O2
2	A	301	0VC	C13-C12-C6-C5
2	E	301	0VC	C13-C12-C6-C5
2	H	301	0VC	C13-C12-C6-C1
2	J	301	0VC	C13-C12-C6-C1
3	C	303	GOL	C1-C2-C3-O3
3	E	304	GOL	O1-C1-C2-C3
2	A	301	0VC	C13-C15-C16-O17
2	F	301	0VC	C14-C13-C15-C16
2	J	301	0VC	C12-C13-C15-C16

There are no ring outliers.

15 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	0VC	1	0
3	J	303	GOL	1	0
3	I	303	GOL	2	0

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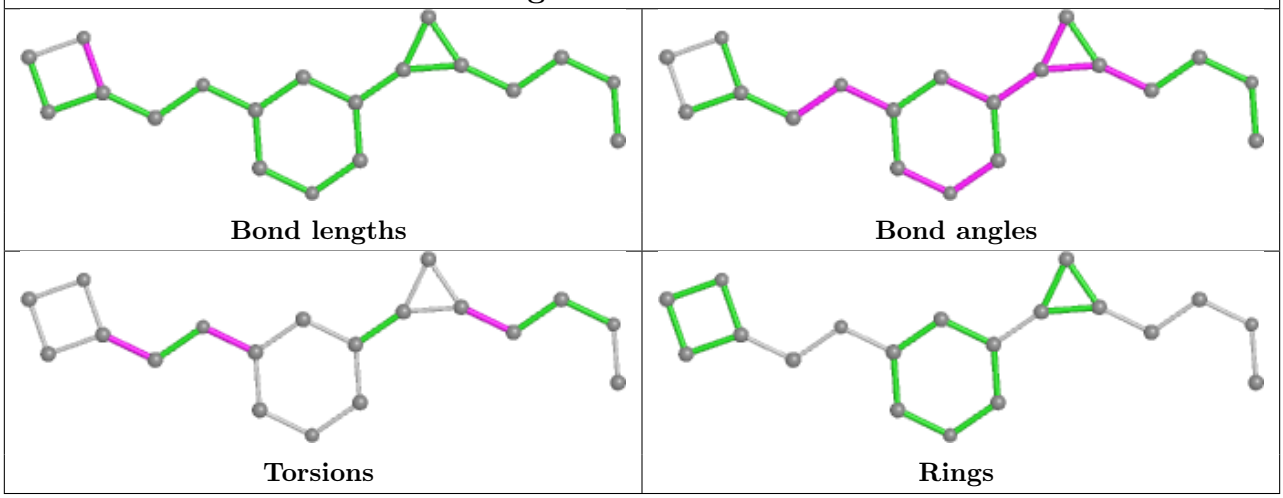
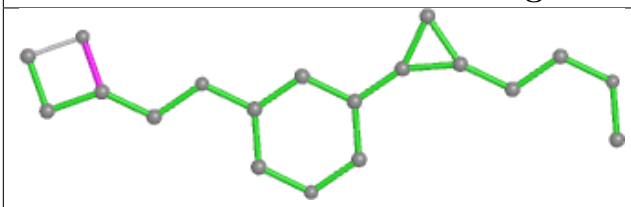
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	GOL	2	0
2	A	301	0VC	1	0
3	F	303	GOL	2	0
3	G	303	GOL	2	0
2	E	301	0VC	1	0
3	H	302	GOL	1	0
3	A	303	GOL	3	0
2	F	301	0VC	3	0
3	B	303	GOL	1	0
3	I	301	GOL	5	0
3	C	303	GOL	4	0
3	E	303	GOL	2	0

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 then 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.

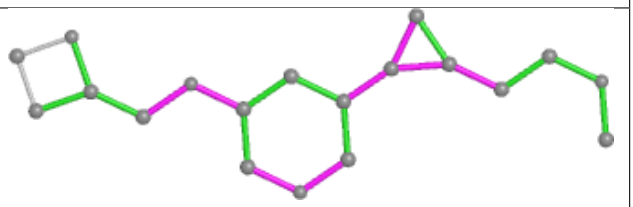
Ligand 0VC C 301



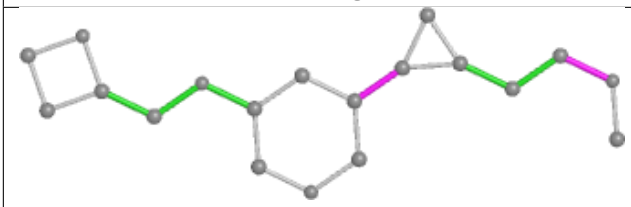
Ligand 0VC H 301



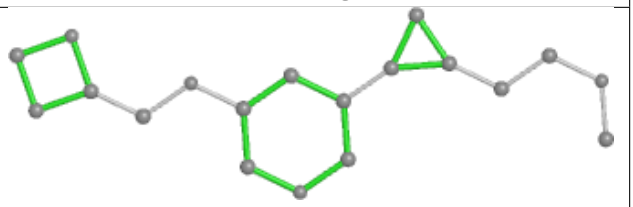
Bond lengths



Bond angles

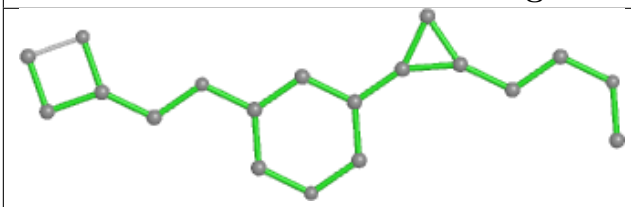


Torsions

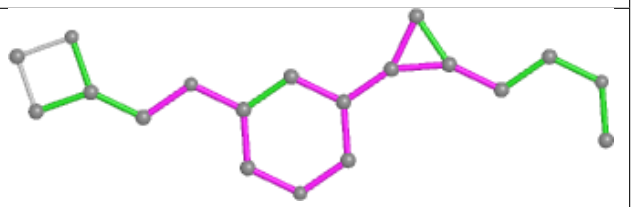


Rings

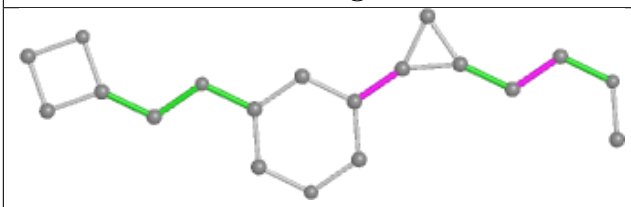
Ligand 0VC A 301



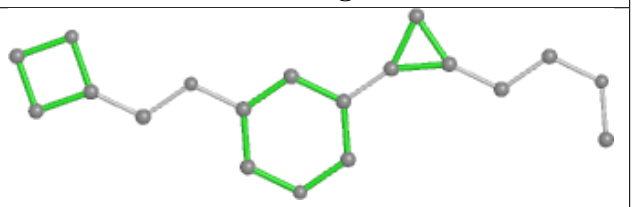
Bond lengths



Bond angles

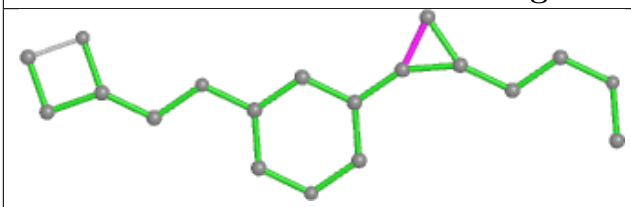


Torsions

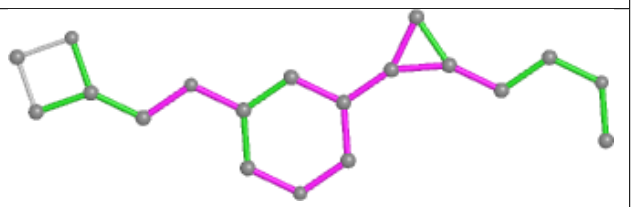


Rings

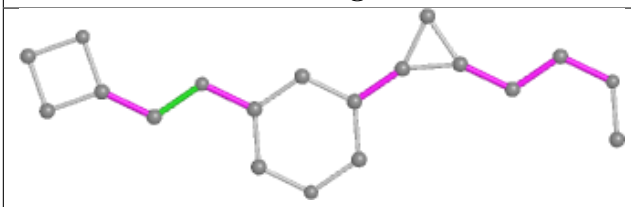
Ligand 0VC J 301



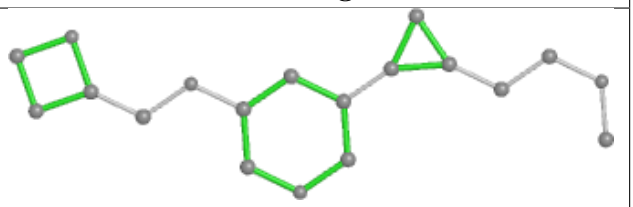
Bond lengths



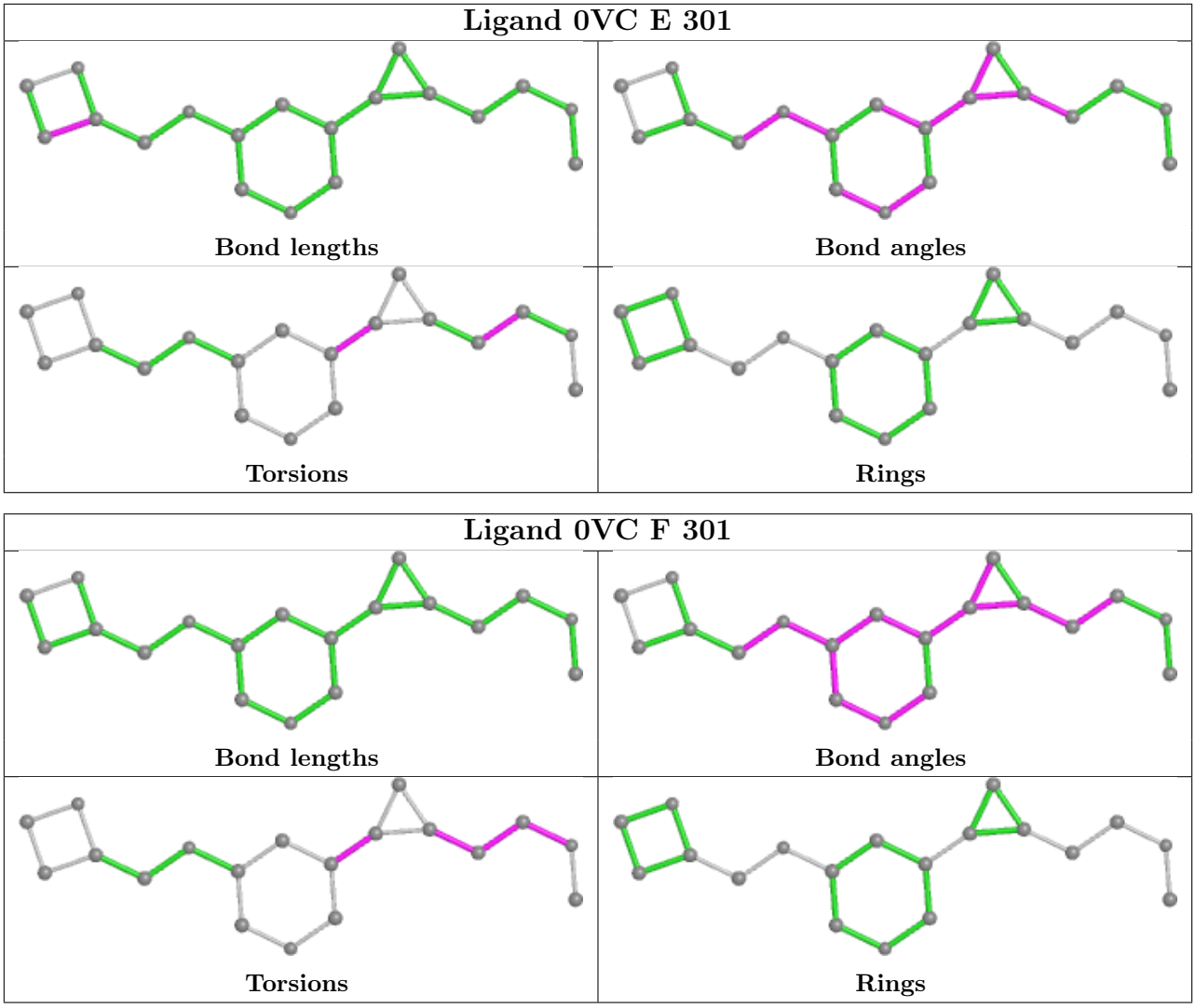
Bond angles



Torsions



Rings



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, 95^{th} 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	208/232 (89%)	-0.02	12 (5%) 23 22	20, 33, 63, 112	1 (0%)
1	B	211/232 (90%)	-0.02	6 (2%) 53 51	22, 34, 67, 122	1 (0%)
1	C	210/232 (90%)	0.25	20 (9%) 8 7	22, 36, 72, 139	3 (1%)
1	D	211/232 (90%)	-0.03	10 (4%) 31 30	22, 38, 79, 110	0
1	E	211/232 (90%)	-0.01	7 (3%) 46 44	22, 36, 69, 113	0
1	F	210/232 (90%)	0.06	11 (5%) 27 26	22, 36, 105, 164	3 (1%)
1	G	208/232 (89%)	0.30	20 (9%) 8 6	26, 40, 90, 129	2 (0%)
1	H	209/232 (90%)	0.15	13 (6%) 20 19	25, 40, 74, 151	2 (0%)
1	I	210/232 (90%)	-0.02	12 (5%) 23 22	23, 37, 72, 114	0
1	J	214/232 (92%)	0.04	11 (5%) 28 26	24, 37, 71, 129	0
All	All	2102/2320 (90%)	0.07	122 (5%) 23 22	20, 37, 81, 164	12 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	17	SER	9.9
1	C	189[A]	SER	7.5
1	D	18	PRO	7.3
1	H	18	PRO	7.2
1	G	0	LEU	6.6
1	B	17	SER	6.5
1	E	-3	ASP	6.3
1	C	190[A]	CYS	6.2
1	J	18	PRO	6.0
1	C	16	ARG	6.0
1	H	190[A]	CYS	5.9
1	F	16	ARG	5.9
1	I	16	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
1	G	7	MET	5.6
1	G	-2	ASP	5.3
1	G	70	ASN	5.2
1	C	18	PRO	5.2
1	A	15	ASN	5.1
1	H	16	ARG	5.1
1	B	18	PRO	5.1
1	H	189[A]	SER	5.0
1	D	16	ARG	5.0
1	A	16	ARG	5.0
1	E	-4	ASP	4.9
1	D	17	SER	4.9
1	I	18	PRO	4.8
1	J	19	MET	4.7
1	A	0	LEU	4.6
1	D	208	ARG	4.6
1	H	188[A]	TYR	4.4
1	C	17	SER	4.4
1	F	0	LEU	4.3
1	G	9	LEU	4.3
1	B	208	ARG	4.3
1	F	70	ASN	4.2
1	C	188[A]	TYR	4.2
1	I	1	HIS	4.2
1	H	0	LEU	4.1
1	G	4	ALA	4.1
1	F	19	MET	4.1
1	G	13	LEU	4.1
1	G	1	HIS	4.1
1	D	19	MET	4.0
1	C	1	HIS	4.0
1	H	1	HIS	3.9
1	C	191[A]	CYS	3.9
1	I	0	LEU	3.7
1	F	74	ASN	3.7
1	I	19	MET	3.6
1	J	-4	ASP	3.5
1	D	0	LEU	3.4
1	J	-3	ASP	3.4
1	A	208	ARG	3.3
1	I	17	SER	3.3
1	J	-5	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	208	ARG	3.3
1	F	1	HIS	3.3
1	G	66	MET	3.2
1	H	191[A]	CYS	3.2
1	B	15	ASN	3.2
1	H	17	SER	3.1
1	E	-2	ASP	3.1
1	G	-1	LYS	3.0
1	C	15	ASN	3.0
1	F	208	ARG	3.0
1	E	16	ARG	3.0
1	H	187[A]	HIS	3.0
1	A	1	HIS	2.9
1	C	-1	LYS	2.9
1	F	-1	LYS	2.8
1	D	7	MET	2.7
1	A	17	SER	2.7
1	F	18	PRO	2.7
1	A	66	MET	2.7
1	C	192[A]	PRO	2.6
1	D	15	ASN	2.6
1	H	192[A]	PRO	2.6
1	D	1	HIS	2.6
1	J	137	GLY	2.6
1	F	15	ASN	2.6
1	I	11	SER	2.6
1	G	-3	ASP	2.5
1	G	12	ASP	2.5
1	G	71	GLU	2.5
1	A	11	SER	2.5
1	I	8	ARG	2.5
1	I	7	MET	2.5
1	G	64	SER	2.5
1	C	6	LEU	2.5
1	G	14	PHE	2.4
1	H	4	ALA	2.4
1	C	-2	ASP	2.4
1	E	1	HIS	2.4
1	A	70	ASN	2.4
1	A	12	ASP	2.4
1	G	3	GLN	2.3
1	H	208	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	208	ARG	2.3
1	G	68	ASP	2.3
1	B	135	GLU	2.3
1	C	2	SER	2.3
1	E	0	LEU	2.3
1	J	134	SER	2.3
1	C	70	ASN	2.3
1	F	97[A]	ARG	2.2
1	G	74	ASN	2.2
1	G	8	ARG	2.2
1	C	7	MET	2.2
1	C	14	PHE	2.2
1	I	70	ASN	2.2
1	I	-1	LYS	2.2
1	C	187[A]	HIS	2.2
1	A	18	PRO	2.2
1	D	14	PHE	2.2
1	C	0	LEU	2.2
1	I	71	GLU	2.1
1	E	11	SER	2.1
1	A	14	PHE	2.1
1	J	133	ASP	2.0
1	J	136	GLU	2.0
1	B	-2	ASP	2.0
1	G	63	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)

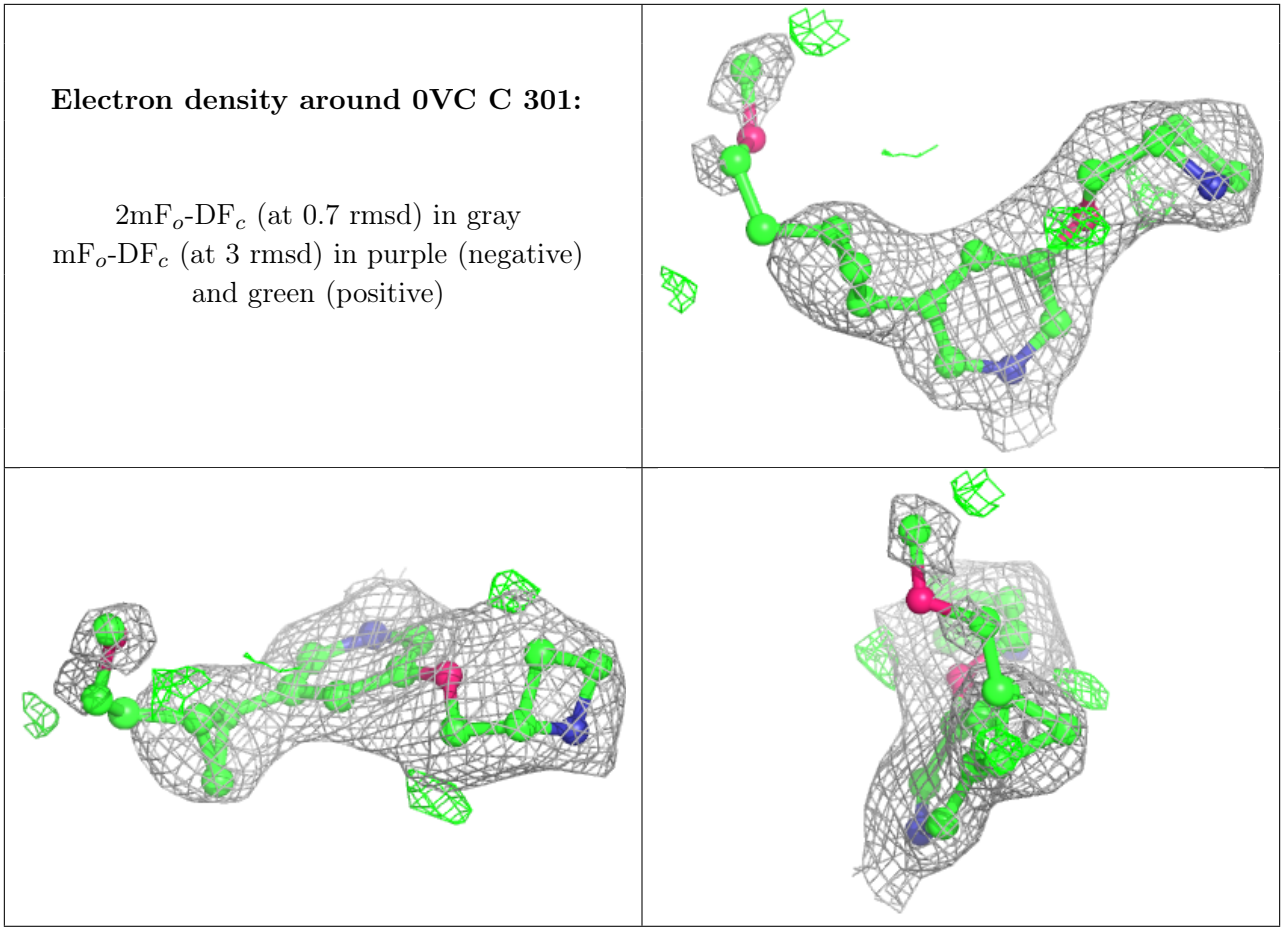
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GOL	B	301	6/6	0.68	0.26	63,74,78,80	0
3	GOL	G	301	6/6	0.68	0.21	51,65,66,72	0
3	GOL	E	304	6/6	0.69	0.19	58,61,65,67	0
3	GOL	G	303	6/6	0.75	0.18	52,58,62,65	0
3	GOL	I	303	6/6	0.75	0.22	43,56,61,65	0
3	GOL	D	301	6/6	0.77	0.25	53,58,64,67	0
3	GOL	I	301	6/6	0.78	0.26	43,51,52,55	0
3	GOL	H	302	6/6	0.79	0.20	39,63,68,73	0
3	GOL	J	303	6/6	0.79	0.22	53,63,68,68	0
3	GOL	B	302	6/6	0.80	0.21	53,64,67,71	0
3	GOL	F	303	6/6	0.81	0.21	53,60,62,64	0
3	GOL	E	303	6/6	0.82	0.19	49,52,52,54	0
3	GOL	I	302	6/6	0.82	0.23	53,58,60,63	0
3	GOL	C	302	6/6	0.83	0.13	73,77,80,80	0
3	GOL	A	302	6/6	0.84	0.18	36,57,63,71	0
3	GOL	A	306	6/6	0.87	0.17	42,52,55,61	0
3	GOL	A	303	6/6	0.87	0.23	32,39,43,46	0
3	GOL	D	302	6/6	0.87	0.18	77,79,80,81	0
3	GOL	G	302	6/6	0.87	0.19	53,64,68,69	0
3	GOL	A	305	6/6	0.87	0.14	52,60,60,65	0
3	GOL	C	303	6/6	0.88	0.16	38,52,55,56	0
2	0VC	C	301	19/19	0.88	0.20	46,59,86,94	0
3	GOL	F	302	6/6	0.90	0.13	55,65,68,69	0
2	0VC	H	301	19/19	0.90	0.13	47,55,83,86	0
3	GOL	A	304	6/6	0.91	0.11	46,63,65,66	0
3	GOL	B	303	6/6	0.91	0.16	50,60,63,67	0
3	GOL	E	302	6/6	0.92	0.20	41,50,51,54	0
3	GOL	J	302	6/6	0.93	0.17	51,54,54,57	0
2	0VC	F	301	19/19	0.96	0.17	27,31,62,69	0
2	0VC	A	301	19/19	0.96	0.15	25,29,50,54	0
2	0VC	E	301	19/19	0.97	0.12	28,34,58,59	0
2	0VC	J	301	19/19	0.98	0.11	29,31,72,75	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.

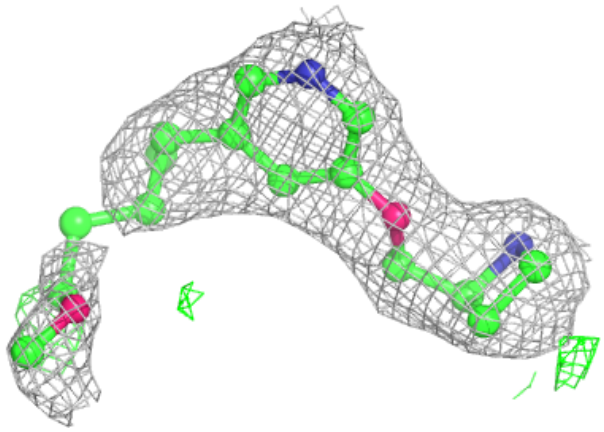
Electron density around 0VC C 301:

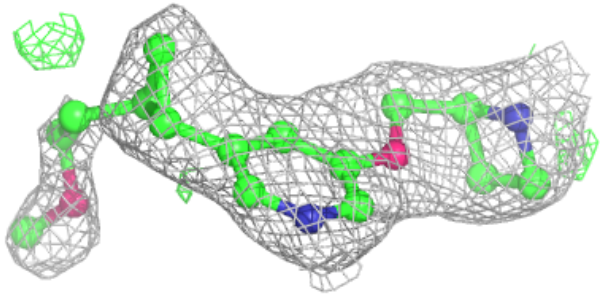
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

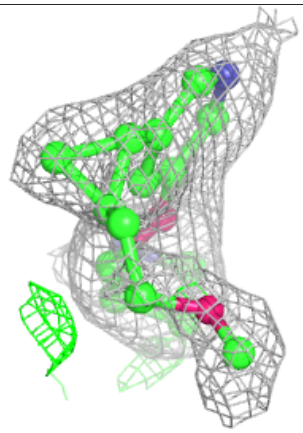


Electron density around 0VC H 301:

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

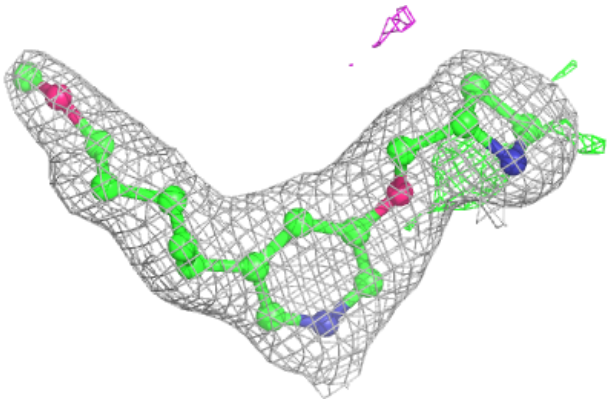


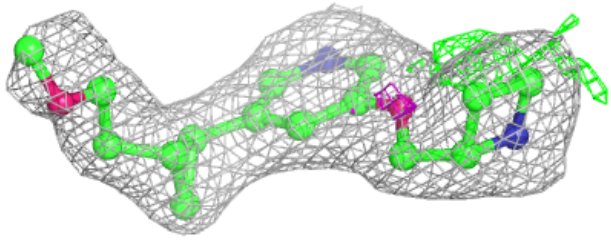


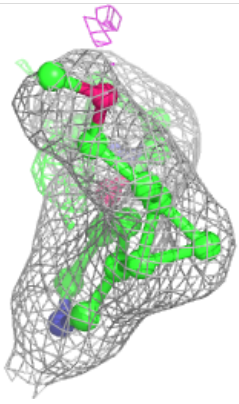


Electron density around 0VC F 301:

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

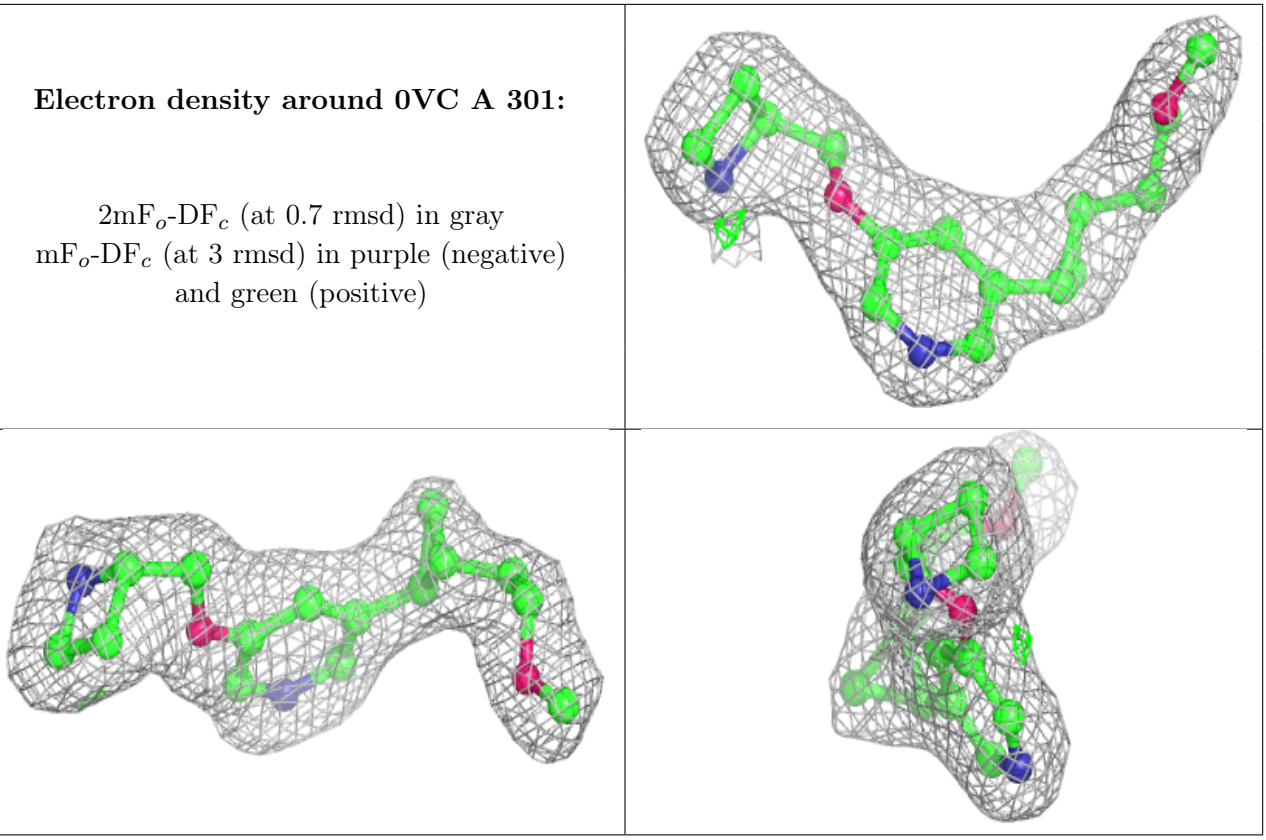






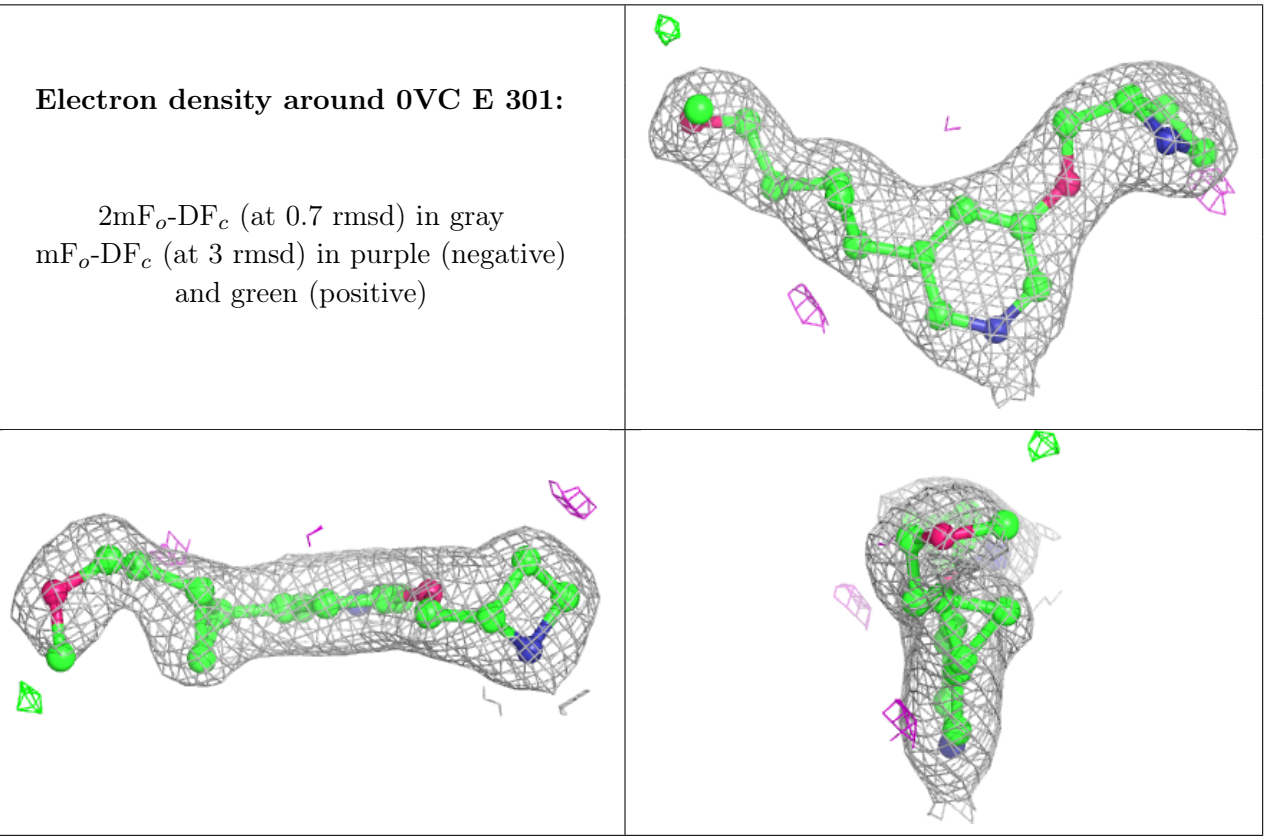
Electron density around 0VC A 301:

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



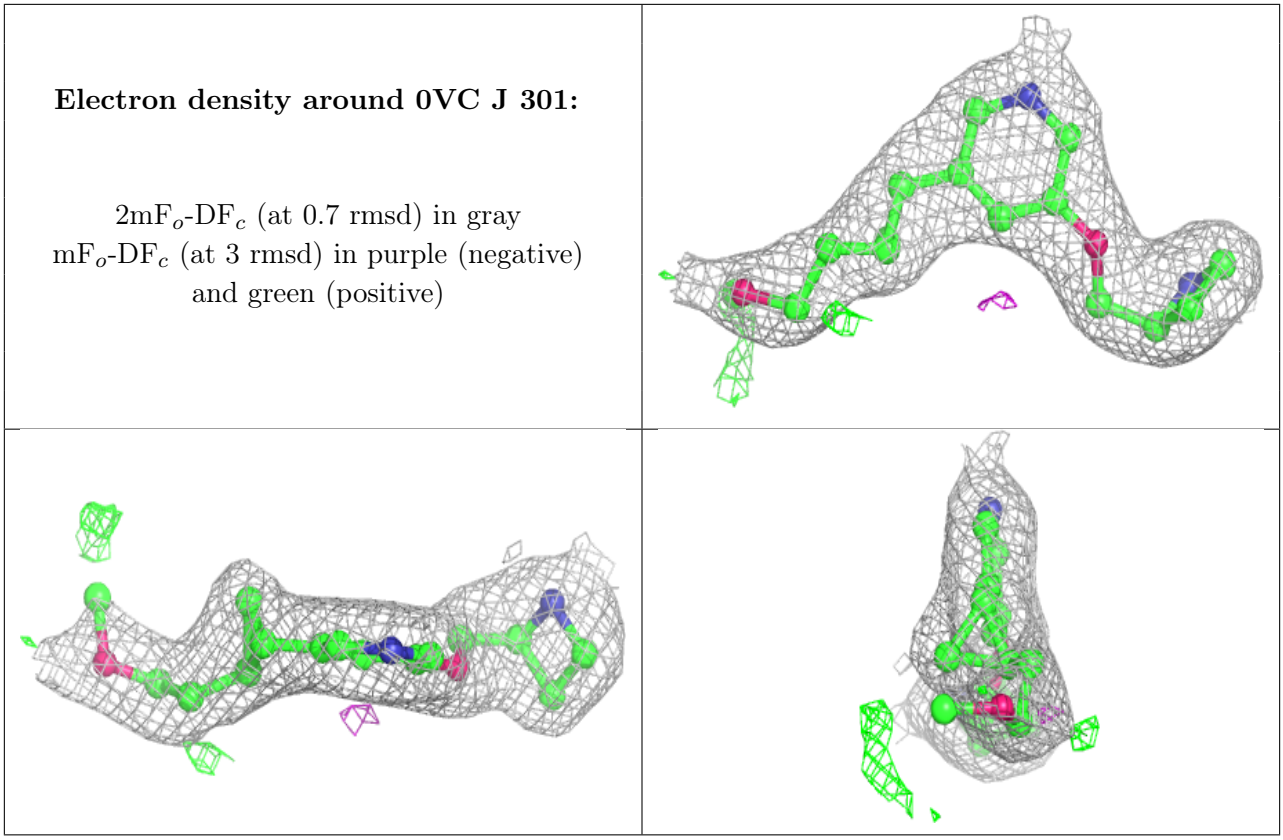
Electron density around 0VC E 301:

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



Electron density around 0VC J 301:

$2mF_o$-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.