Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 05:43 PM EDT

PDB ID	:	7U64
Title	:	Crystal Structure of Anti-Fentanyl Antibody HY6-F9.6 Fab Complexed with Fentanyl
Authors	:	Rodarte, J.V.; Pancera, M.P.
Deposited on	:	2022-03-03
Resolution	:	1.75 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

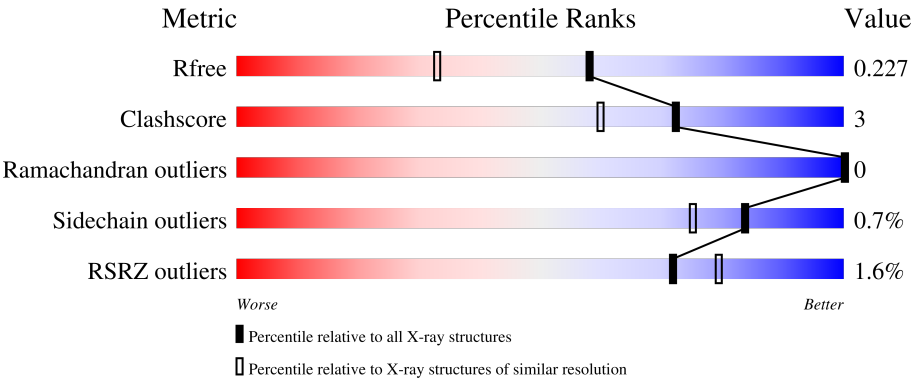
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	226	91% 7% .
1	C	226	3% 89% 8% .
1	E	226	90% 8% .
1	G	226	6% 91% 8% .
1	I	226	% 92% 7% .

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Mol	Chain	Length	Quality of chain
1	K	226	2% 91% 7%
1	M	226	4% 86% 12%
1	O	226	92% 5%
1	Q	226	% 92% 6%
2	B	219	91% 8%
2	D	219	2% 88% 10%
2	F	219	91% 7%
2	H	219	5% 92% 6%
2	J	219	91% 7%
2	L	219	89% 9%
2	N	219	3% 86% 12%
2	P	219	92% 6%
2	R	219	91% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	L	305	-	-	X	-
4	ACT	M	302	-	X	-	-
4	ACT	O	302	-	-	X	-
4	ACT	Q	307	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 33436 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 HY6-F9.6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	C	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	E	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	G	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	I	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	K	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	M	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	O	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			
1	Q	222	Total	C	N	O	S	0	0	0
			1681	1059	276	340	6			

- Molecule 2 is a protein called HY6-F9.6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	D	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	F	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	H	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	J	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			

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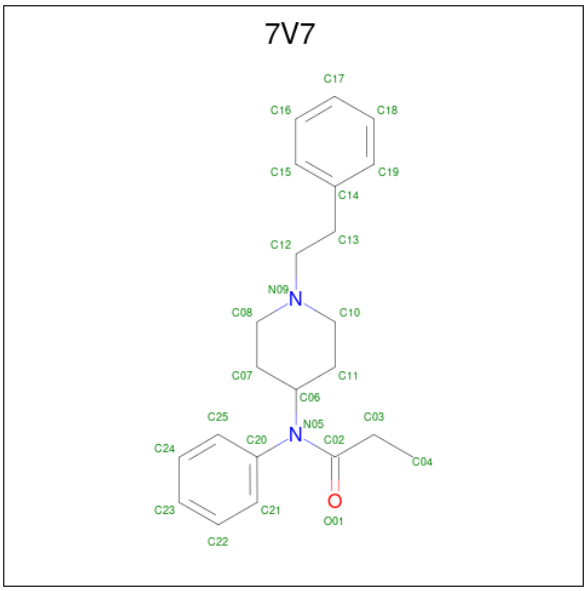
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	N	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	P	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	R	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			

- Molecule 3 is N-phenyl-N-[1-(2-phenylethyl)piperidin-4-yl]propanamide (three-letter code: 7V7) (formula: $C_{22}H_{28}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	22	2	1		
3	C	1	Total	C	N	O	0	0
			25	22	2	1		
3	E	1	Total	C	N	O	0	0
			25	22	2	1		
3	G	1	Total	C	N	O	0	0
			25	22	2	1		
3	I	1	Total	C	N	O	0	0
			25	22	2	1		
3	K	1	Total	C	N	O	0	0
			25	22	2	1		
3	M	1	Total	C	N	O	0	0
			25	22	2	1		

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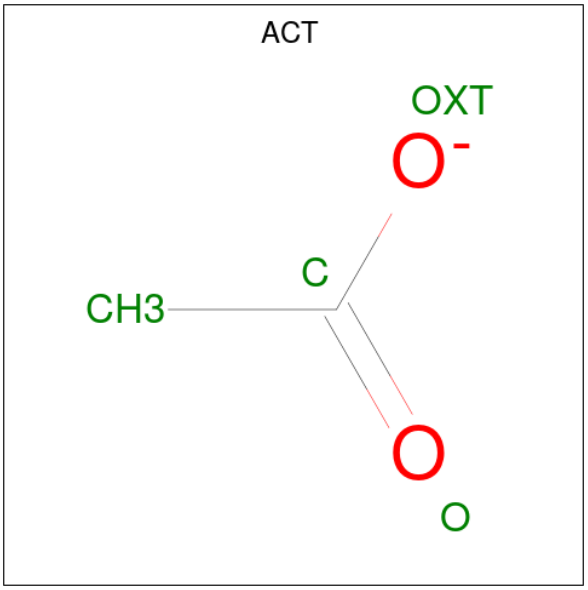
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C N O 25 22 2 1	0	0
3	Q	1	Total C N O 25 22 2 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	1	Total C O 4 2 2	0	0
4	Q	1	Total C O 4 2 2	0	0
4	R	1	Total C O 4 2 2	0	0
4	R	1	Total C O 4 2 2	0	0
4	R	1	Total C O 4 2 2	0	0
4	R	1	Total C O 4 2 2	0	0
4	R	1	Total C O 4 2 2	0	0
4	R	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0
5	H	3	Total Na 3 3	0	0
5	J	2	Total Na 2 2	0	0
5	K	1	Total Na 1 1	0	0
5	L	1	Total Na 1 1	0	0
5	P	2	Total Na 2 2	0	0
5	Q	1	Total Na 1 1	0	0
5	R	1	Total Na 1 1	0	0

- Molecule 6 is water.

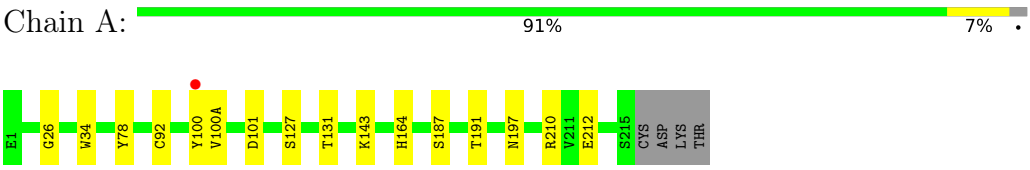
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	192	Total O 192 192	0	0
6	B	157	Total O 157 157	0	0
6	C	118	Total O 118 118	0	0
6	D	113	Total O 113 113	0	0
6	E	184	Total O 184 184	0	0
6	F	154	Total O 154 154	0	0
6	G	174	Total O 174 174	0	0
6	H	124	Total O 124 124	0	0
6	I	203	Total O 203 203	0	0
6	J	149	Total O 149 149	0	0
6	K	185	Total O 185 185	0	0
6	L	148	Total O 148 148	0	0
6	M	120	Total O 120 120	0	0
6	N	122	Total O 122 122	0	0
6	O	177	Total O 177 177	0	0
6	P	161	Total O 161 161	0	0
6	Q	182	Total O 182 182	0	0
6	R	166	Total O 166 166	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.

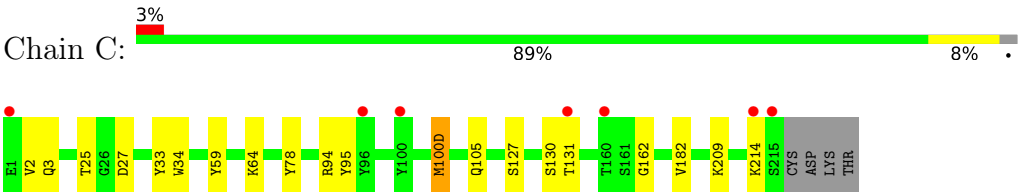
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain A:



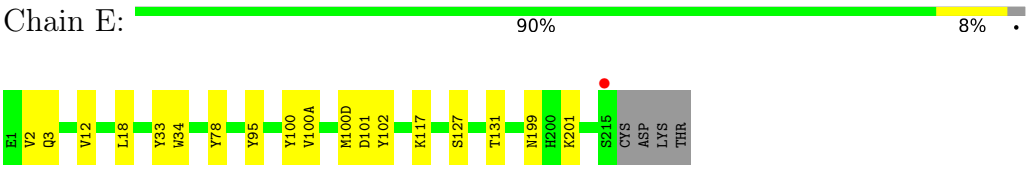
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain C:



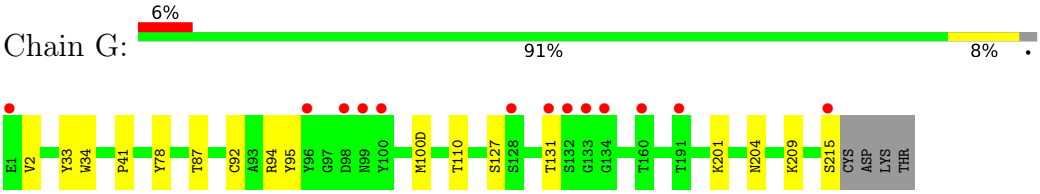
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain E:



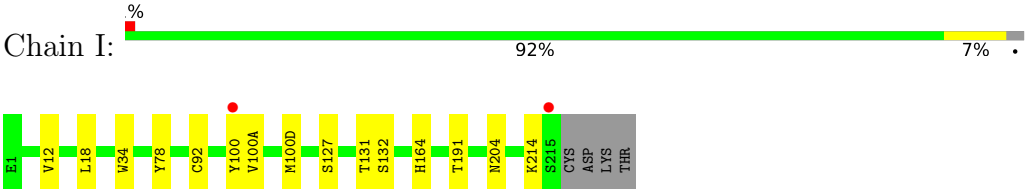
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain G:



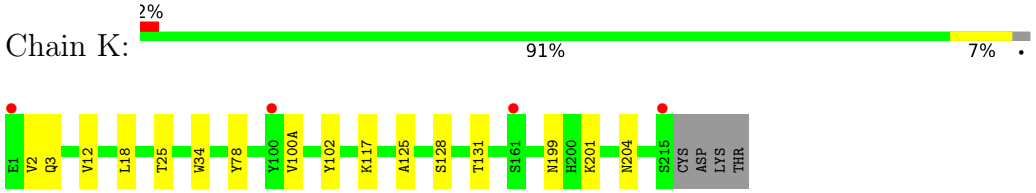
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain I:



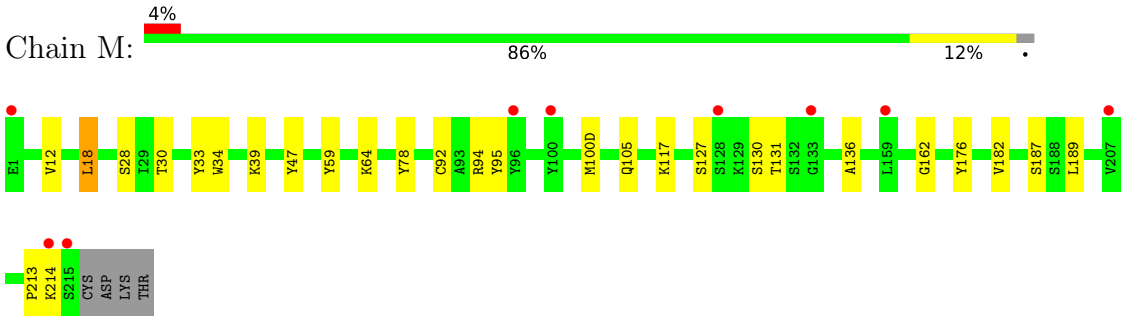
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain K:



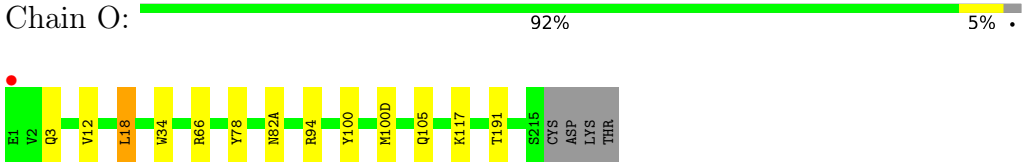
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain M:



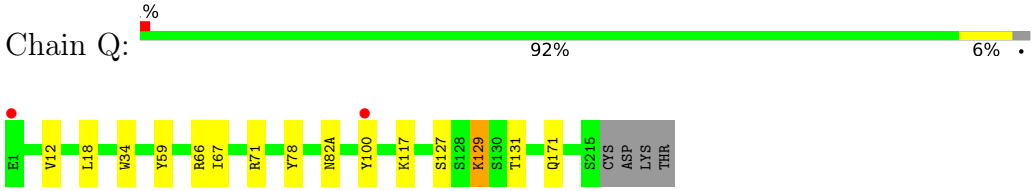
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain O:



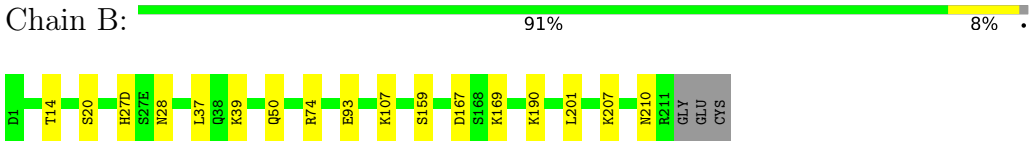
• Molecule 1: HY6-F9.6 Fab heavy chain

Chain Q:



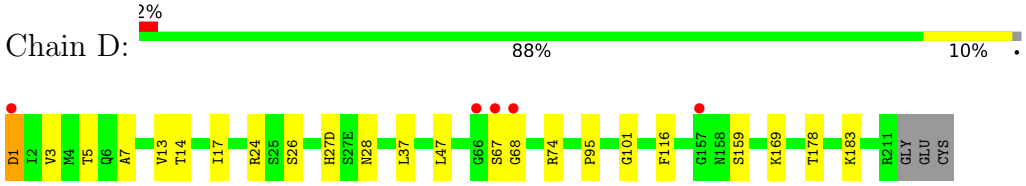
• Molecule 2: HY6-F9.6 Fab light chain

Chain B:



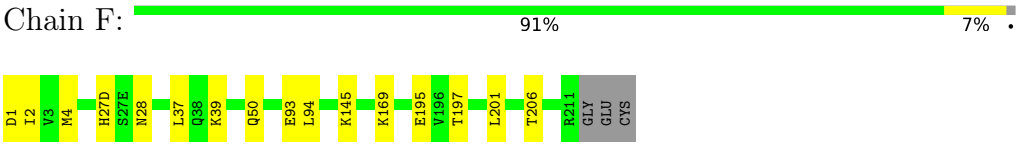
• Molecule 2: HY6-F9.6 Fab light chain

Chain D:



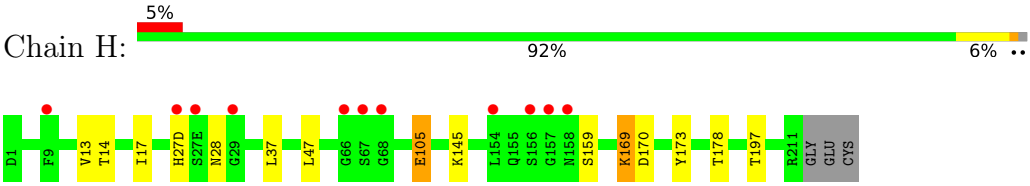
• Molecule 2: HY6-F9.6 Fab light chain

Chain F:



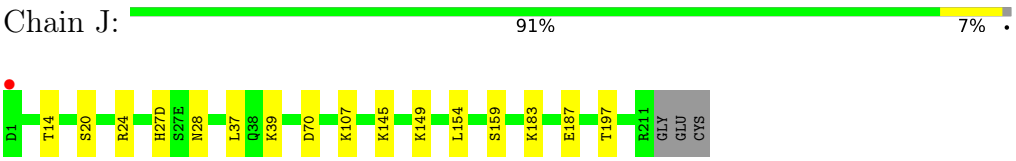
• Molecule 2: HY6-F9.6 Fab light chain

Chain H:



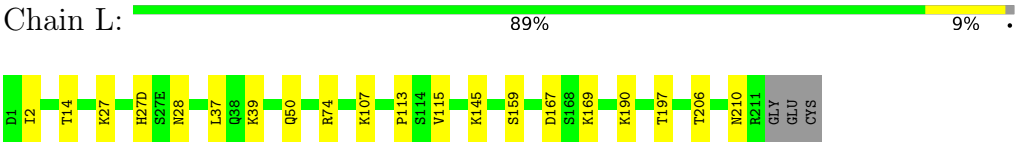
• Molecule 2: HY6-F9.6 Fab light chain

Chain J:



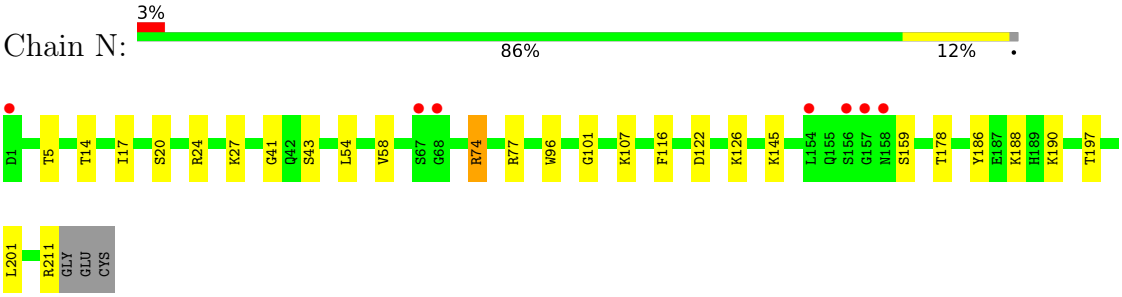
• Molecule 2: HY6-F9.6 Fab light chain

Chain L:



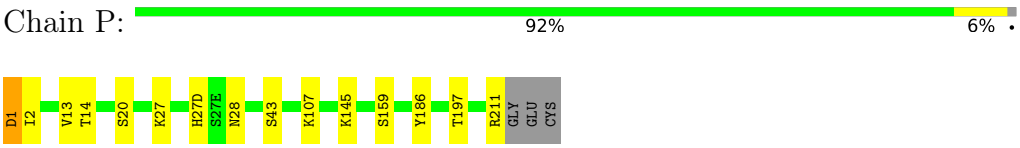
• Molecule 2: HY6-F9.6 Fab light chain

Chain N:



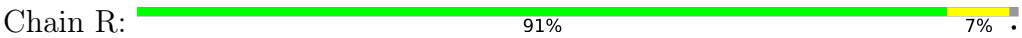
• Molecule 2: HY6-F9.6 Fab light chain

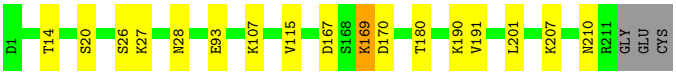
Chain P:



• Molecule 2: HY6-F9.6 Fab light chain

Chain R:




D1
T14
S20
S26
K27
N28
E93
K107
V115
D167
S168
K169
D170
T180
K190
V191
L201
K207
N210
R211
GLY
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	218.14Å 218.14Å 89.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.33 – 1.75 43.33 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.33-1.75) 99.6 (43.33-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.225 0.200 , 0.227	Depositor DCC
R_{free} test set	23996 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.032 for h,-h-k,-l 0.487 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33436	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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 79.73 % 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 5.2369e-07. 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: ACT, NA, 7V7

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	0.36	0/1724	0.62	1/2353 (0.0%)
1	C	0.33	0/1724	0.58	0/2353
1	E	0.37	0/1724	0.64	1/2353 (0.0%)
1	G	0.36	0/1724	0.59	0/2353
1	I	0.40	0/1724	0.64	0/2353
1	K	0.37	0/1724	0.62	0/2353
1	M	0.32	0/1724	0.58	0/2353
1	O	0.37	0/1724	0.63	0/2353
1	Q	0.38	0/1724	0.63	0/2353
2	B	0.38	0/1703	0.61	0/2313
2	D	0.32	0/1703	0.55	0/2313
2	F	0.39	0/1703	0.61	0/2313
2	H	0.36	0/1703	0.58	0/2313
2	J	0.37	0/1703	0.60	0/2313
2	L	0.39	0/1703	0.60	0/2313
2	N	0.33	0/1703	0.55	0/2313
2	P	0.37	0/1703	0.61	0/2313
2	R	0.39	0/1703	0.63	0/2313
All	All	0.36	0/30843	0.60	2/41994 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	101	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	101	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1681	0	1630	11	0
1	C	1681	0	1630	11	0
1	E	1681	0	1629	9	0
1	G	1681	0	1630	10	0
1	I	1681	0	1630	9	0
1	K	1681	0	1629	11	0
1	M	1681	0	1630	18	0
1	O	1681	0	1630	8	0
1	Q	1681	0	1630	10	0
2	B	1667	0	1633	15	0
2	D	1667	0	1633	15	0
2	F	1667	0	1633	13	0
2	H	1667	0	1633	9	0
2	J	1667	0	1633	10	0
2	L	1667	0	1633	14	0
2	N	1667	0	1633	20	0
2	P	1667	0	1633	11	0
2	R	1667	0	1633	12	0
3	A	25	0	0	0	0
3	C	25	0	0	0	0
3	E	25	0	0	0	0
3	G	25	0	0	0	0
3	I	25	0	0	0	0
3	K	25	0	0	0	0
3	M	25	0	0	0	0
3	O	25	0	0	0	0
3	Q	25	0	0	0	0
4	A	20	0	15	2	0
4	B	24	0	18	2	0
4	C	4	0	3	0	0
4	E	8	0	6	0	0
4	F	16	0	12	0	0
4	G	8	0	6	1	0
4	H	28	0	21	0	0
4	I	8	0	6	0	0
4	J	12	0	9	1	0
4	K	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	16	0	12	2	0
4	M	8	0	6	2	0
4	O	12	0	9	3	0
4	P	20	0	15	1	0
4	Q	20	0	15	4	0
4	R	24	0	18	2	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	H	3	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	P	2	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
6	A	192	0	0	2	0
6	B	157	0	0	4	2
6	C	118	0	0	0	0
6	D	113	0	0	4	0
6	E	184	0	0	1	2
6	F	154	0	0	3	2
6	G	174	0	0	1	1
6	H	124	0	0	0	0
6	I	203	0	0	2	2
6	J	149	0	0	3	2
6	K	185	0	0	3	1
6	L	148	0	0	3	0
6	M	120	0	0	2	0
6	N	122	0	0	7	1
6	O	177	0	0	4	1
6	P	161	0	0	3	0
6	Q	182	0	0	1	3
6	R	166	0	0	3	0
All	All	33436	0	29542	206	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (206) 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)
2:R:190:LYS:HE2	2:R:210:ASN:HD21	1.45	0.82
1:E:12:VAL:HG21	1:E:18:LEU:HD23	1.61	0.80
1:I:12:VAL:HG21	1:I:18:LEU:HD23	1.63	0.80
2:L:167:ASP:OD2	2:L:169:LYS:HG2	1.84	0.76
1:A:191:THR:HG21	2:F:93:GLU:OE2	1.86	0.76
1:I:100:TYR:HD1	1:I:100(A):VAL:HG23	1.49	0.76
4:Q:307:ACT:H3	2:R:180:THR:OG1	1.86	0.75
2:J:20:SER:O	6:J:401:HOH:O	2.07	0.73
2:B:93:GLU:OE2	1:I:191:THR:HG21	1.89	0.72
2:N:74:ARG:HH11	2:N:74:ARG:HB3	1.58	0.69
1:A:127:SER:O	1:A:131:THR:HG23	1.93	0.68
1:I:127:SER:O	1:I:131:THR:HG23	1.95	0.67
1:O:12:VAL:HG21	1:O:18:LEU:HD23	1.77	0.66
2:D:13:VAL:HB	2:D:17:ILE:HD11	1.79	0.65
2:B:74:ARG:NH1	6:B:404:HOH:O	2.25	0.65
1:E:127:SER:O	1:E:131:THR:HG23	1.97	0.65
1:O:191:THR:HG21	2:R:93:GLU:OE2	1.96	0.65
1:Q:117:LYS:NZ	6:Q:404:HOH:O	2.30	0.64
1:A:164:HIS:NE2	6:A:404:HOH:O	2.28	0.64
4:O:302:ACT:H1	6:O:558:HOH:O	1.98	0.64
2:B:20:SER:O	6:B:401:HOH:O	2.15	0.63
4:O:302:ACT:H2	6:O:561:HOH:O	2.00	0.62
1:Q:127:SER:O	1:Q:131:THR:HG23	1.99	0.61
2:F:37:LEU:HD21	2:F:39:LYS:HE2	1.83	0.61
2:R:201:LEU:O	6:R:401:HOH:O	2.16	0.61
1:I:164:HIS:NE2	6:I:405:HOH:O	2.29	0.61
2:N:201:LEU:O	6:N:301:HOH:O	2.16	0.60
2:B:159:SER:O	6:B:403:HOH:O	2.17	0.60
2:L:159:SER:O	6:L:401:HOH:O	2.17	0.60
2:B:201:LEU:O	6:B:402:HOH:O	2.16	0.59
2:H:14:THR:O	2:H:17:ILE:HG13	2.02	0.59
2:P:2:ILE:HG12	2:P:27:LYS:HE2	1.85	0.59
2:D:24:ARG:NH2	6:D:405:HOH:O	2.36	0.58
1:E:100(A):VAL:HA	2:F:50:GLN:HE22	1.71	0.56
2:J:37:LEU:HD21	2:J:39:LYS:HE2	1.88	0.56
2:B:167:ASP:OD2	2:B:169:LYS:HG2	2.05	0.56
1:Q:171:GLN:OE1	4:Q:307:ACT:H2	2.05	0.56
2:L:2:ILE:HG12	2:L:27:LYS:HD2	1.88	0.55
1:A:143:LYS:HG3	4:A:306:ACT:H3	1.88	0.55
1:M:176:TYR:OH	4:M:303:ACT:H1	2.07	0.55
2:N:24:ARG:NH1	6:N:314:HOH:O	2.38	0.55
1:M:59:TYR:HB2	1:M:64:LYS:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:190:LYS:HE2	2:L:210:ASN:HD21	1.72	0.55
2:B:210:ASN:HB3	4:B:306:ACT:H2	1.88	0.54
2:L:37:LEU:HD21	2:L:39:LYS:HE2	1.89	0.54
2:B:37:LEU:HD21	2:B:39:LYS:HE2	1.89	0.54
1:M:12:VAL:HG21	1:M:18:LEU:HD23	1.90	0.54
1:E:117:LYS:NZ	6:E:410:HOH:O	2.41	0.53
2:R:169:LYS:HG2	2:R:170:ASP:N	2.24	0.53
2:N:74:ARG:HB3	2:N:74:ARG:NH1	2.22	0.53
1:A:100(A):VAL:HA	2:B:50:GLN:HE22	1.74	0.53
1:Q:100:TYR:OH	2:R:28:ASN:HB2	2.09	0.53
1:K:128:SER:HA	1:K:131:THR:HG22	1.91	0.53
1:M:94:ARG:O	1:M:100(D):MET:HA	2.09	0.53
2:D:101:GLY:O	6:D:401:HOH:O	2.18	0.52
2:H:105:GLU:OE2	2:H:173:TYR:OH	2.17	0.52
2:J:149:LYS:HZ3	2:J:154:LEU:HB2	1.74	0.52
2:P:159:SER:O	6:P:401:HOH:O	2.19	0.52
1:E:100:TYR:OH	2:F:28:ASN:HB2	2.10	0.52
1:G:94:ARG:O	1:G:100(D):MET:HA	2.10	0.52
2:P:13:VAL:HG12	4:P:305:ACT:H2	1.92	0.52
2:P:186:TYR:CZ	2:P:211:ARG:HG3	2.45	0.52
1:Q:129:LYS:HD3	4:R:305:ACT:H2	1.92	0.51
2:L:113:PRO:O	4:L:305:ACT:H2	2.11	0.51
1:A:100:TYR:OH	2:B:28:ASN:HB2	2.10	0.51
2:F:27(D):HIS:HB3	2:F:28:ASN:OD1	2.11	0.51
2:F:201:LEU:O	6:F:401:HOH:O	2.19	0.51
2:H:169:LYS:HG2	2:H:170:ASP:N	2.25	0.51
2:R:20:SER:O	6:R:402:HOH:O	2.19	0.51
1:C:127:SER:O	1:C:131:THR:HG23	2.11	0.51
2:R:26:SER:O	2:R:27:LYS:HE3	2.10	0.51
2:B:207:LYS:NZ	4:B:302:ACT:H2	2.26	0.51
2:B:190:LYS:HE2	2:B:210:ASN:HD21	1.76	0.50
1:C:59:TYR:HB2	1:C:64:LYS:HG3	1.94	0.50
1:Q:12:VAL:HG21	1:Q:18:LEU:HD13	1.92	0.50
2:J:27(D):HIS:HB3	2:J:28:ASN:OD1	2.12	0.50
1:M:127:SER:O	1:M:131:THR:HG23	2.11	0.50
1:O:66:ARG:HD2	1:O:82(A):ASN:O	2.12	0.50
2:P:27(D):HIS:HB3	2:P:28:ASN:OD1	2.12	0.50
1:G:127:SER:O	1:G:131:THR:HG23	2.11	0.50
4:M:302:ACT:OXT	6:M:401:HOH:O	2.18	0.49
2:R:167:ASP:OD1	2:R:169:LYS:HD3	2.12	0.49
2:D:7:ALA:N	6:D:411:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27(D):HIS:HB3	2:B:28:ASN:OD1	2.13	0.49
1:K:12:VAL:HG21	1:K:18:LEU:HD13	1.93	0.49
2:L:145:LYS:HB3	2:L:197:THR:HB	1.93	0.49
4:O:302:ACT:H3	6:O:556:HOH:O	2.12	0.49
1:K:128:SER:HA	1:K:131:THR:CG2	2.43	0.49
1:K:204:ASN:OD1	6:K:402:HOH:O	2.20	0.49
2:N:20:SER:O	6:N:302:HOH:O	2.19	0.49
2:N:186:TYR:CZ	2:N:211:ARG:HG3	2.48	0.49
1:K:117:LYS:NZ	6:K:410:HOH:O	2.46	0.48
1:M:28:SER:HG	1:M:30:THR:HG1	1.61	0.48
1:C:2:VAL:HG22	1:C:27:ASP:HB2	1.96	0.48
2:D:5:THR:HG22	6:D:411:HOH:O	2.13	0.48
2:L:190:LYS:CE	2:L:210:ASN:HD21	2.27	0.48
2:N:145:LYS:HB3	2:N:197:THR:HB	1.96	0.48
2:F:206:THR:O	6:F:402:HOH:O	2.20	0.47
2:P:145:LYS:HB3	2:P:197:THR:HB	1.95	0.47
2:N:14:THR:O	2:N:17:ILE:HG12	2.15	0.47
1:C:33:TYR:HB2	1:C:95:TYR:HB3	1.96	0.47
2:D:14:THR:O	2:D:17:ILE:HG13	2.15	0.47
2:D:67:SER:OG	2:D:68:GLY:N	2.47	0.47
1:E:199:ASN:ND2	1:E:201:LYS:HE3	2.30	0.47
1:M:189:LEU:HB3	1:M:213:PRO:HG3	1.96	0.47
2:N:101:GLY:O	6:N:303:HOH:O	2.20	0.47
2:P:14:THR:HG23	2:P:107:LYS:HE3	1.97	0.47
2:J:159:SER:O	6:J:402:HOH:O	2.21	0.47
2:P:1:ASP:HA	6:P:458:HOH:O	2.14	0.47
1:O:117:LYS:NZ	6:O:415:HOH:O	2.48	0.46
1:O:100:TYR:OH	2:P:28:ASN:HB2	2.14	0.46
1:A:210:ARG:CZ	1:A:212:GLU:OE2	2.63	0.46
2:F:1:ASP:CG	2:F:2:ILE:H	2.18	0.46
1:K:34:TRP:HB3	1:K:78:TYR:CZ	2.51	0.46
1:C:34:TRP:HB3	1:C:78:TYR:CZ	2.51	0.46
2:J:149:LYS:NZ	2:J:154:LEU:HB2	2.31	0.46
2:F:195:GLU:HG3	2:F:206:THR:HG22	1.98	0.45
2:H:13:VAL:HB	2:H:17:ILE:HD11	1.96	0.45
1:G:41:PRO:HB3	4:G:302:ACT:H2	1.98	0.45
1:I:204:ASN:OD1	6:I:401:HOH:O	2.20	0.45
1:M:130:SER:HA	2:N:116:PHE:HD2	1.82	0.45
1:O:34:TRP:HB3	1:O:78:TYR:CZ	2.51	0.45
4:A:303:ACT:H3	6:A:407:HOH:O	2.16	0.45
1:E:34:TRP:HB3	1:E:78:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:GLN:HA	2:N:43:SER:HG	1.81	0.45
1:C:209:LYS:HD3	1:C:209:LYS:HA	1.75	0.45
2:J:183:LYS:HE3	2:J:187:GLU:OE2	2.16	0.45
1:K:125:ALA:O	6:K:403:HOH:O	2.21	0.45
2:P:20:SER:O	6:P:402:HOH:O	2.21	0.45
2:F:145:LYS:HB3	2:F:197:THR:HB	1.98	0.45
1:M:34:TRP:HB3	1:M:78:TYR:CZ	2.52	0.45
2:N:54:LEU:HG	2:N:58:VAL:HB	2.00	0.44
1:C:162:GLY:O	1:C:182:VAL:HA	2.17	0.44
1:I:214:LYS:HA	1:I:214:LYS:HD2	1.70	0.44
1:I:34:TRP:HB3	1:I:78:TYR:CZ	2.53	0.44
1:C:3:GLN:HB2	1:C:25:THR:CG2	2.47	0.44
2:J:24:ARG:HG2	2:J:70:ASP:OD1	2.18	0.44
2:L:27(D):HIS:HB3	2:L:28:ASN:OD1	2.18	0.44
1:M:117:LYS:NZ	6:M:409:HOH:O	2.50	0.44
2:R:115:VAL:HG23	4:R:307:ACT:H3	1.99	0.44
2:D:27(D):HIS:HB3	2:D:28:ASN:OD1	2.18	0.44
2:J:145:LYS:HB3	2:J:197:THR:HB	2.00	0.44
2:R:190:LYS:HG2	2:R:191:VAL:HG23	1.98	0.44
2:F:169:LYS:HD3	2:F:169:LYS:HA	1.78	0.44
1:M:213:PRO:O	1:M:214:LYS:HD2	2.18	0.43
2:L:14:THR:HG23	2:L:107:LYS:HE3	2.00	0.43
1:M:162:GLY:O	1:M:182:VAL:HA	2.18	0.43
1:Q:59:TYR:HB3	1:Q:67:ILE:HD11	1.99	0.43
2:B:14:THR:HG23	2:B:107:LYS:HE3	2.00	0.43
2:F:4:MET:O	6:F:403:HOH:O	2.21	0.43
1:A:78:TYR:OH	1:A:92:CYS:HB2	2.18	0.43
2:J:14:THR:HG23	2:J:107:LYS:HE3	2.00	0.43
1:G:34:TRP:HB3	1:G:78:TYR:CZ	2.53	0.43
2:H:37:LEU:HB2	2:H:47:LEU:HD11	2.01	0.43
1:M:33:TYR:HB2	1:M:95:TYR:HB3	2.00	0.43
2:N:5:THR:HB	2:N:24:ARG:HG3	2.01	0.43
1:C:94:ARG:O	1:C:100(D):MET:HA	2.19	0.43
1:G:87:THR:HG23	1:G:110:THR:HA	1.99	0.43
1:K:3:GLN:HB3	1:K:25:THR:OG1	2.18	0.43
2:L:115:VAL:HG23	4:L:305:ACT:H3	1.99	0.43
2:N:188:LYS:NZ	6:N:312:HOH:O	2.32	0.43
2:R:14:THR:HG23	2:R:107:LYS:HE3	2.01	0.43
1:G:201:LYS:HB3	1:G:201:LYS:HE3	1.78	0.43
2:H:145:LYS:HD3	2:H:145:LYS:HA	1.84	0.43
2:L:74:ARG:HD3	6:L:456:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LYS:HA	1:C:214:LYS:HD3	1.66	0.42
1:G:78:TYR:OH	1:G:92:CYS:HB2	2.19	0.42
1:Q:34:TRP:HB3	1:Q:78:TYR:CZ	2.54	0.42
4:J:305:ACT:H2	6:J:407:HOH:O	2.20	0.42
1:G:204:ASN:ND2	6:G:423:HOH:O	2.53	0.42
2:N:159:SER:HA	2:N:178:THR:O	2.19	0.42
1:Q:66:ARG:HD2	1:Q:82(A):ASN:O	2.19	0.42
1:M:78:TYR:OH	1:M:92:CYS:HB2	2.19	0.42
2:N:14:THR:HG23	2:N:107:LYS:HE3	2.02	0.42
1:G:33:TYR:HB2	1:G:95:TYR:HB3	2.00	0.42
2:H:145:LYS:HB3	2:H:197:THR:HB	2.02	0.42
2:N:122:ASP:O	2:N:126:LYS:HB2	2.20	0.42
4:Q:307:ACT:H1	6:R:453:HOH:O	2.20	0.42
1:C:130:SER:HA	2:D:116:PHE:HD1	1.84	0.41
2:D:37:LEU:HB2	2:D:47:LEU:HD11	2.02	0.41
1:Q:71:ARG:NH2	4:Q:306:ACT:OXT	2.52	0.41
1:A:26:GLY:HA2	1:M:187:SER:O	2.19	0.41
2:B:190:LYS:CE	2:B:210:ASN:HD21	2.33	0.41
1:I:78:TYR:OH	1:I:92:CYS:HB2	2.21	0.41
1:M:47:TYR:CG	2:N:96:TRP:HB2	2.56	0.41
1:O:94:ARG:O	1:O:100(D):MET:HA	2.21	0.41
2:D:159:SER:HA	2:D:178:THR:O	2.20	0.41
2:D:183:LYS:HE2	2:D:183:LYS:HB3	1.86	0.41
2:H:159:SER:HA	2:H:178:THR:O	2.20	0.41
1:K:100(A):VAL:HG23	2:L:50:GLN:OE1	2.21	0.41
1:A:34:TRP:HB3	1:A:78:TYR:CZ	2.56	0.41
1:G:209:LYS:HD3	1:G:209:LYS:HA	1.88	0.41
2:H:27(D):HIS:HB3	2:H:28:ASN:OD1	2.21	0.41
1:K:2:VAL:HG13	1:K:102:TYR:CG	2.56	0.41
2:L:39:LYS:HD3	6:L:448:HOH:O	2.20	0.41
1:E:2:VAL:HG13	1:E:102:TYR:CG	2.56	0.41
1:K:199:ASN:ND2	1:K:201:LYS:HE3	2.35	0.41
1:M:131:THR:HG22	1:M:136:ALA:CB	2.51	0.41
2:N:77:ARG:HD2	6:N:396:HOH:O	2.21	0.41
2:D:1:ASP:OD1	2:D:95:PRO:HD2	2.21	0.41
2:N:41:GLY:O	6:N:304:HOH:O	2.21	0.41
1:A:187:SER:HB3	2:F:94:LEU:HD12	2.03	0.40
2:D:3:VAL:HB	2:D:26:SER:HB3	2.02	0.40
2:D:169:LYS:HD2	2:D:169:LYS:HA	1.80	0.40
1:E:33:TYR:HB2	1:E:95:TYR:HB3	2.02	0.40
1:O:105:GLN:HA	2:P:43:SER:HG	1.86	0.40

All (9) 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)
6:E:539:HOH:O	6:Q:406:HOH:O[2_565]	2.04	0.16
6:B:537:HOH:O	6:Q:564:HOH:O[2_565]	2.14	0.06
6:J:545:HOH:O	6:O:567:HOH:O[3_454]	2.14	0.06
6:G:528:HOH:O	6:I:534:HOH:O[1_545]	2.15	0.05
6:E:444:HOH:O	6:K:532:HOH:O[1_655]	2.16	0.04
6:B:496:HOH:O	6:Q:415:HOH:O[2_565]	2.17	0.03
6:N:406:HOH:O	6:N:417:HOH:O[3_454]	2.17	0.03
6:F:509:HOH:O	6:J:402:HOH:O[3_454]	2.18	0.02
6:F:477:HOH:O	6:I:412:HOH:O[3_454]	2.19	0.01

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	220/226 (97%)	214 (97%)	6 (3%)	0	100	100
1	C	220/226 (97%)	214 (97%)	6 (3%)	0	100	100
1	E	220/226 (97%)	216 (98%)	4 (2%)	0	100	100
1	G	220/226 (97%)	216 (98%)	4 (2%)	0	100	100
1	I	220/226 (97%)	215 (98%)	5 (2%)	0	100	100
1	K	220/226 (97%)	215 (98%)	5 (2%)	0	100	100
1	M	220/226 (97%)	214 (97%)	6 (3%)	0	100	100
1	O	220/226 (97%)	216 (98%)	4 (2%)	0	100	100
1	Q	220/226 (97%)	216 (98%)	4 (2%)	0	100	100
2	B	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
2	D	214/219 (98%)	206 (96%)	8 (4%)	0	100	100
2	F	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
2	H	214/219 (98%)	208 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
2	L	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
2	N	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
2	P	214/219 (98%)	207 (97%)	7 (3%)	0	100	100
2	R	214/219 (98%)	208 (97%)	6 (3%)	0	100	100
All	All	3906/4005 (98%)	3798 (97%)	108 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	194/198 (98%)	193 (100%)	1 (0%)	88	83
1	C	194/198 (98%)	192 (99%)	2 (1%)	76	63
1	E	194/198 (98%)	192 (99%)	2 (1%)	76	63
1	G	194/198 (98%)	192 (99%)	2 (1%)	76	63
1	I	194/198 (98%)	192 (99%)	2 (1%)	76	63
1	K	194/198 (98%)	194 (100%)	0	100	100
1	M	194/198 (98%)	192 (99%)	2 (1%)	76	63
1	O	194/198 (98%)	192 (99%)	2 (1%)	76	63
1	Q	194/198 (98%)	193 (100%)	1 (0%)	88	83
2	B	190/192 (99%)	190 (100%)	0	100	100
2	D	190/192 (99%)	188 (99%)	2 (1%)	73	60
2	F	190/192 (99%)	190 (100%)	0	100	100
2	H	190/192 (99%)	188 (99%)	2 (1%)	73	60
2	J	190/192 (99%)	190 (100%)	0	100	100
2	L	190/192 (99%)	189 (100%)	1 (0%)	88	83
2	N	190/192 (99%)	187 (98%)	3 (2%)	62	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	190/192 (99%)	189 (100%)	1 (0%)	88 83
2	R	190/192 (99%)	188 (99%)	2 (1%)	73 60
All	All	3456/3510 (98%)	3431 (99%)	25 (1%)	84 75

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	ASN
1	C	100(D)	MET
1	C	105	GLN
2	D	1	ASP
2	D	74	ARG
1	E	3	GLN
1	E	100(D)	MET
1	G	2	VAL
1	G	215	SER
2	H	105	GLU
2	H	169	LYS
1	I	100(D)	MET
1	I	132	SER
2	L	206	THR
1	M	18	LEU
1	M	39	LYS
2	N	27	LYS
2	N	74	ARG
2	N	190	LYS
1	O	3	GLN
1	O	18	LEU
2	P	1	ASP
1	Q	129	LYS
2	R	169	LYS
2	R	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	192	GLN
2	B	11	ASN
2	B	199	GLN

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Mol	Chain	Res	Type
2	B	210	ASN
1	C	192	GLN
1	E	5	GLN
2	F	45	GLN
1	I	5	GLN
2	J	45	GLN
1	K	5	GLN
1	K	192	GLN
2	L	45	GLN
2	L	210	ASN
1	M	105	GLN
1	O	82(A)	ASN
1	O	199	ASN
2	P	11	ASN
1	Q	105	GLN
2	R	11	ASN
2	R	45	GLN
2	R	210	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 82 ligands modelled in this entry, 14 are monoatomic - leaving 68 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	J	305	-	3,3,3	1.18	0	3,3,3	1.47	1 (33%)
4	ACT	Q	303	5	3,3,3	1.46	1 (33%)	3,3,3	1.16	0
4	ACT	E	303	-	3,3,3	1.26	0	3,3,3	1.62	1 (33%)
4	ACT	B	301	-	3,3,3	1.21	0	3,3,3	1.75	2 (66%)
4	ACT	H	307	-	3,3,3	1.45	1 (33%)	3,3,3	1.57	0
4	ACT	E	304	-	3,3,3	1.44	1 (33%)	3,3,3	1.40	0
4	ACT	P	305	-	3,3,3	1.28	1 (33%)	3,3,3	1.61	1 (33%)
4	ACT	R	307	-	3,3,3	1.03	0	3,3,3	1.47	0
3	7V7	O	301	-	27,27,27	0.91	1 (3%)	34,35,35	0.89	1 (2%)
4	ACT	H	305	-	3,3,3	1.15	0	3,3,3	1.31	0
4	ACT	I	302	-	3,3,3	1.39	1 (33%)	3,3,3	1.31	0
4	ACT	L	302	5	3,3,3	1.50	1 (33%)	3,3,3	1.28	0
4	ACT	A	305	-	3,3,3	1.43	1 (33%)	3,3,3	1.61	0
4	ACT	Q	304	-	3,3,3	1.41	1 (33%)	3,3,3	1.16	0
4	ACT	R	306	-	3,3,3	1.53	1 (33%)	3,3,3	1.57	1 (33%)
4	ACT	M	302	-	3,3,3	1.38	1 (33%)	3,3,3	1.69	2 (66%)
4	ACT	R	303	-	3,3,3	1.42	1 (33%)	3,3,3	1.43	0
4	ACT	G	303	-	3,3,3	1.34	0	3,3,3	1.56	1 (33%)
4	ACT	L	303	-	3,3,3	1.37	0	3,3,3	1.45	0
4	ACT	J	304	-	3,3,3	1.41	1 (33%)	3,3,3	1.45	0
4	ACT	H	306	-	3,3,3	1.48	1 (33%)	3,3,3	1.56	0
4	ACT	P	304	-	3,3,3	1.53	1 (33%)	3,3,3	1.49	0
4	ACT	A	302	-	3,3,3	1.25	0	3,3,3	1.72	2 (66%)
4	ACT	A	304	-	3,3,3	1.55	1 (33%)	3,3,3	1.53	0
4	ACT	K	304	-	3,3,3	1.58	1 (33%)	3,3,3	1.57	0
3	7V7	K	301	-	27,27,27	0.98	2 (7%)	34,35,35	0.88	1 (2%)
3	7V7	A	301	-	27,27,27	0.87	2 (7%)	34,35,35	0.89	1 (2%)
4	ACT	H	304	5	3,3,3	1.28	0	3,3,3	1.30	0
3	7V7	G	301	-	27,27,27	0.77	1 (3%)	34,35,35	0.92	2 (5%)
4	ACT	H	309	-	3,3,3	1.20	0	3,3,3	1.50	1 (33%)
4	ACT	B	305	-	3,3,3	1.53	1 (33%)	3,3,3	1.50	0
4	ACT	O	303	-	3,3,3	1.51	0	3,3,3	1.42	0
4	ACT	P	307	-	3,3,3	1.51	0	3,3,3	1.46	0
4	ACT	R	305	-	3,3,3	1.25	0	3,3,3	1.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	L	304	-	3,3,3	1.45	0	3,3,3	1.48	0
3	7V7	I	301	-	27,27,27	1.14	2 (7%)	34,35,35	0.88	0
4	ACT	O	302	-	3,3,3	0.70	0	3,3,3	2.02	2 (66%)
4	ACT	B	306	-	3,3,3	1.35	0	3,3,3	1.53	1 (33%)
4	ACT	F	303	-	3,3,3	1.23	0	3,3,3	1.35	0
4	ACT	F	304	-	3,3,3	1.48	0	3,3,3	1.57	1 (33%)
3	7V7	M	301	-	27,27,27	0.86	1 (3%)	34,35,35	0.94	1 (2%)
4	ACT	B	303	-	3,3,3	1.54	1 (33%)	3,3,3	1.46	0
4	ACT	J	303	5	3,3,3	1.59	1 (33%)	3,3,3	1.26	0
4	ACT	O	304	-	3,3,3	1.46	1 (33%)	3,3,3	1.45	0
4	ACT	B	304	-	3,3,3	1.32	1 (33%)	3,3,3	1.46	0
4	ACT	P	303	5	3,3,3	1.51	1 (33%)	3,3,3	1.46	0
4	ACT	P	306	-	3,3,3	1.49	1 (33%)	3,3,3	1.49	0
4	ACT	Q	306	-	3,3,3	1.49	1 (33%)	3,3,3	1.57	0
3	7V7	Q	301	-	27,27,27	0.95	2 (7%)	34,35,35	0.82	1 (2%)
3	7V7	C	301	-	27,27,27	0.79	1 (3%)	34,35,35	0.91	1 (2%)
4	ACT	B	302	-	3,3,3	1.19	0	3,3,3	1.73	2 (66%)
4	ACT	F	302	5	3,3,3	1.57	1 (33%)	3,3,3	1.35	0
4	ACT	L	305	-	3,3,3	1.19	0	3,3,3	1.49	0
4	ACT	Q	307	-	3,3,3	1.10	0	3,3,3	1.84	2 (66%)
4	ACT	A	306	-	3,3,3	1.19	0	3,3,3	1.62	1 (33%)
4	ACT	F	305	-	3,3,3	1.26	0	3,3,3	1.52	0
4	ACT	K	303	-	3,3,3	1.37	0	3,3,3	1.42	0
4	ACT	R	302	5	3,3,3	1.73	1 (33%)	3,3,3	1.24	0
4	ACT	H	308	-	3,3,3	1.39	0	3,3,3	1.44	0
4	ACT	A	303	-	3,3,3	1.38	0	3,3,3	1.67	2 (66%)
4	ACT	M	303	-	3,3,3	0.99	0	3,3,3	1.61	1 (33%)
4	ACT	H	310	-	3,3,3	1.10	0	3,3,3	1.65	1 (33%)
4	ACT	Q	305	-	3,3,3	1.36	0	3,3,3	1.61	1 (33%)
4	ACT	I	303	-	3,3,3	1.35	0	3,3,3	1.67	1 (33%)
4	ACT	G	302	-	3,3,3	1.09	0	3,3,3	1.56	1 (33%)
4	ACT	C	302	-	3,3,3	1.27	0	3,3,3	1.66	2 (66%)
4	ACT	R	304	-	3,3,3	1.34	0	3,3,3	1.37	0
3	7V7	E	301	-	27,27,27	0.76	1 (3%)	34,35,35	0.88	1 (2%)

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	7V7	Q	301	-	-	1/19/29/29	0/3/3/3
3	7V7	I	301	-	-	1/19/29/29	0/3/3/3
3	7V7	K	301	-	-	1/19/29/29	0/3/3/3
3	7V7	O	301	-	-	1/19/29/29	0/3/3/3
3	7V7	M	301	-	-	0/19/29/29	0/3/3/3
3	7V7	A	301	-	-	1/19/29/29	0/3/3/3
3	7V7	C	301	-	-	0/19/29/29	0/3/3/3
3	7V7	G	301	-	-	1/19/29/29	0/3/3/3
3	7V7	E	301	-	-	1/19/29/29	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	7V7	C03-C02	3.83	1.57	1.51
3	O	301	7V7	C02-N05	3.10	1.41	1.37
3	K	301	7V7	C02-N05	2.98	1.41	1.37
3	I	301	7V7	C02-N05	2.96	1.41	1.37
3	M	301	7V7	C02-N05	2.85	1.41	1.37
3	Q	301	7V7	C02-N05	2.82	1.41	1.37
4	R	302	ACT	CH3-C	2.68	1.60	1.49
3	K	301	7V7	C03-C02	2.63	1.55	1.51
3	C	301	7V7	C02-N05	2.53	1.41	1.37
4	J	303	ACT	CH3-C	2.50	1.59	1.49
4	F	302	ACT	CH3-C	2.46	1.59	1.49
4	L	302	ACT	CH3-C	2.41	1.59	1.49
3	E	301	7V7	C02-N05	2.40	1.40	1.37
3	G	301	7V7	C02-N05	2.38	1.40	1.37
3	A	301	7V7	C02-N05	2.37	1.40	1.37
3	Q	301	7V7	C03-C02	2.30	1.55	1.51
4	P	306	ACT	CH3-C	2.27	1.58	1.49
4	K	304	ACT	CH3-C	2.27	1.58	1.49
4	P	303	ACT	CH3-C	2.26	1.58	1.49
4	A	304	ACT	CH3-C	2.26	1.58	1.49
4	Q	303	ACT	CH3-C	2.22	1.58	1.49
4	Q	306	ACT	CH3-C	2.16	1.58	1.49
4	O	304	ACT	CH3-C	2.15	1.58	1.49
4	R	303	ACT	CH3-C	2.11	1.58	1.49
4	P	304	ACT	CH3-C	2.10	1.57	1.49
4	H	306	ACT	CH3-C	2.10	1.57	1.49
4	H	307	ACT	CH3-C	2.10	1.57	1.49
4	B	303	ACT	CH3-C	2.08	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	305	ACT	CH3-C	2.08	1.57	1.49
4	E	304	ACT	CH3-C	2.08	1.57	1.49
4	R	306	ACT	CH3-C	2.08	1.57	1.49
4	B	305	ACT	CH3-C	2.07	1.57	1.49
4	Q	304	ACT	CH3-C	2.07	1.57	1.49
3	A	301	7V7	C03-C02	2.07	1.54	1.51
4	J	304	ACT	CH3-C	2.03	1.57	1.49
4	I	302	ACT	CH3-C	2.03	1.57	1.49
4	B	304	ACT	CH3-C	2.01	1.57	1.49
4	P	305	ACT	CH3-C	2.01	1.57	1.49
4	M	302	ACT	CH3-C	2.01	1.57	1.49

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	302	ACT	O-C-CH3	-2.54	112.44	122.33
4	Q	307	ACT	OXT-C-O	2.44	131.03	122.05
3	G	301	7V7	C04-C03-C02	-2.40	108.28	112.72
3	M	301	7V7	C04-C03-C02	-2.38	108.32	112.72
4	O	302	ACT	OXT-C-O	2.37	130.77	122.05
3	A	301	7V7	C04-C03-C02	-2.37	108.35	112.72
3	C	301	7V7	C04-C03-C02	-2.36	108.36	112.72
4	B	301	ACT	O-C-CH3	-2.23	113.65	122.33
3	E	301	7V7	C04-C03-C02	-2.19	108.67	112.72
4	G	302	ACT	OXT-C-O	2.19	130.11	122.05
3	K	301	7V7	C04-C03-C02	-2.17	108.70	112.72
3	O	301	7V7	C04-C03-C02	-2.14	108.77	112.72
3	Q	301	7V7	C04-C03-C02	-2.13	108.79	112.72
4	B	302	ACT	O-C-CH3	-2.12	114.08	122.33
4	M	303	ACT	OXT-C-O	2.12	129.86	122.05
4	E	303	ACT	OXT-C-O	2.12	129.86	122.05
4	P	305	ACT	O-C-CH3	-2.11	114.10	122.33
4	A	302	ACT	O-C-CH3	-2.11	114.11	122.33
4	I	303	ACT	O-C-CH3	-2.11	114.13	122.33
4	F	304	ACT	OXT-C-O	2.10	129.80	122.05
4	B	302	ACT	OXT-C-O	2.10	129.78	122.05
4	M	302	ACT	O-C-CH3	-2.09	114.20	122.33
4	A	302	ACT	OXT-C-O	2.09	129.75	122.05
4	J	305	ACT	OXT-C-O	2.08	129.70	122.05
4	A	303	ACT	OXT-C-O	2.07	129.66	122.05
4	Q	305	ACT	OXT-C-O	2.06	129.65	122.05
4	H	310	ACT	O-C-CH3	-2.06	114.31	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	306	ACT	OXT-C-O	2.06	129.63	122.05
4	Q	307	ACT	O-C-CH3	-2.05	114.34	122.33
4	H	309	ACT	OXT-C-O	2.05	129.59	122.05
4	C	302	ACT	O-C-CH3	-2.04	114.39	122.33
4	M	302	ACT	OXT-C-O	2.03	129.53	122.05
4	A	303	ACT	O-C-CH3	-2.02	114.45	122.33
4	B	301	ACT	OXT-C-O	2.02	129.50	122.05
4	B	306	ACT	OXT-C-O	2.02	129.50	122.05
4	A	306	ACT	OXT-C-O	2.02	129.49	122.05
4	G	303	ACT	OXT-C-O	2.00	129.43	122.05
4	C	302	ACT	OXT-C-O	2.00	129.43	122.05
3	G	301	7V7	O01-C02-N05	-2.00	119.09	121.58

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	301	7V7	N09-C12-C13-C14
3	Q	301	7V7	N09-C12-C13-C14
3	E	301	7V7	N09-C12-C13-C14
3	A	301	7V7	N09-C12-C13-C14
3	O	301	7V7	N09-C12-C13-C14
3	I	301	7V7	N09-C12-C13-C14
3	G	301	7V7	N09-C12-C13-C14

There are no ring outliers.

15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	305	ACT	1	0
4	P	305	ACT	1	0
4	R	307	ACT	1	0
4	M	302	ACT	1	0
4	R	305	ACT	1	0
4	O	302	ACT	3	0
4	B	306	ACT	1	0
4	Q	306	ACT	1	0
4	B	302	ACT	1	0
4	L	305	ACT	2	0
4	Q	307	ACT	3	0
4	A	306	ACT	1	0

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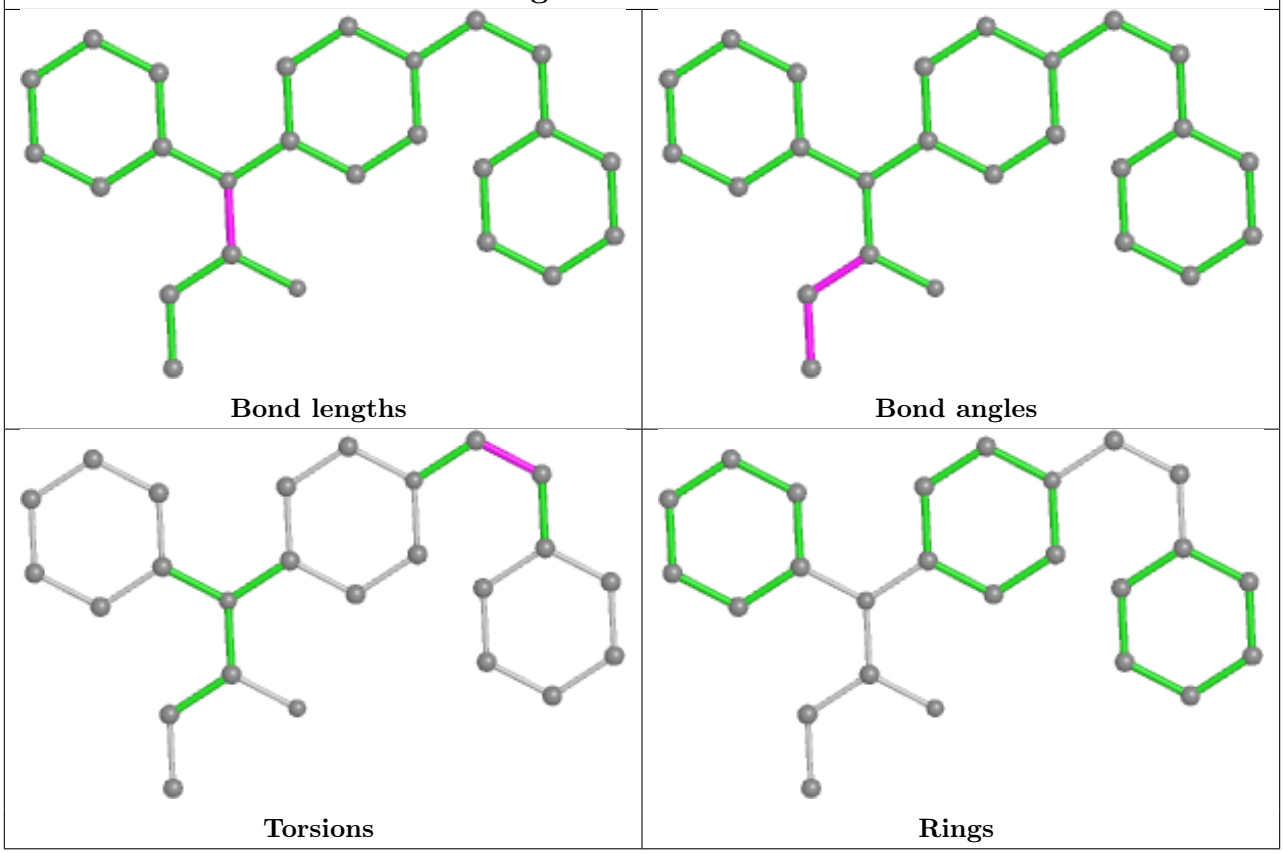
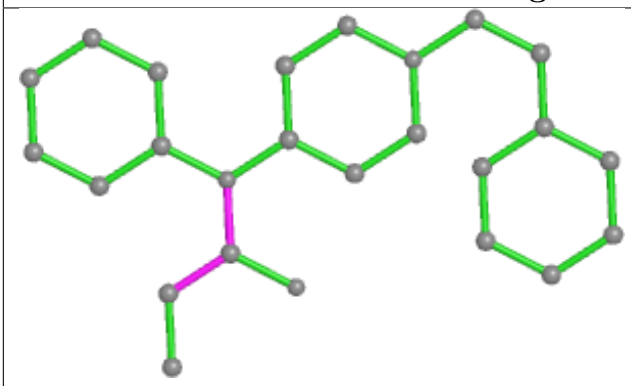
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	ACT	1	0
4	M	303	ACT	1	0
4	G	302	ACT	1	0

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 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.

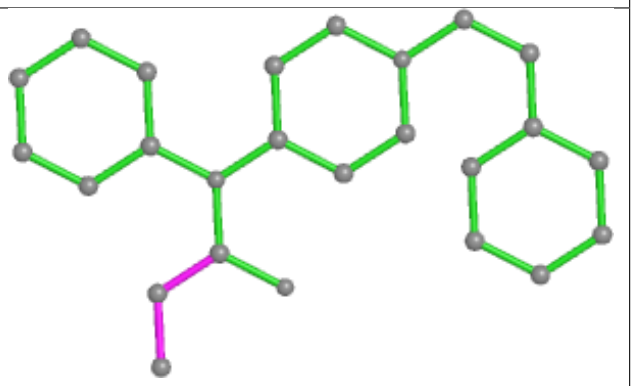
Ligand 7V7 O 301



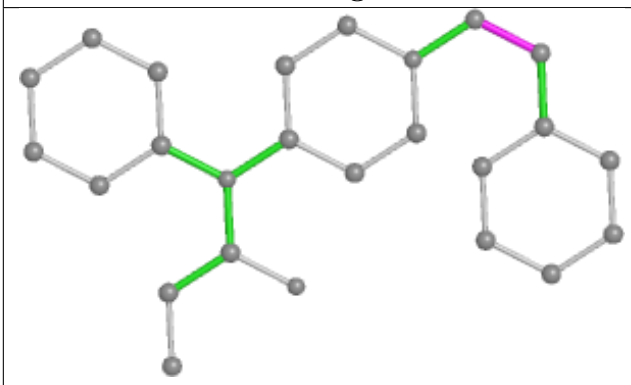
Ligand 7V7 K 301



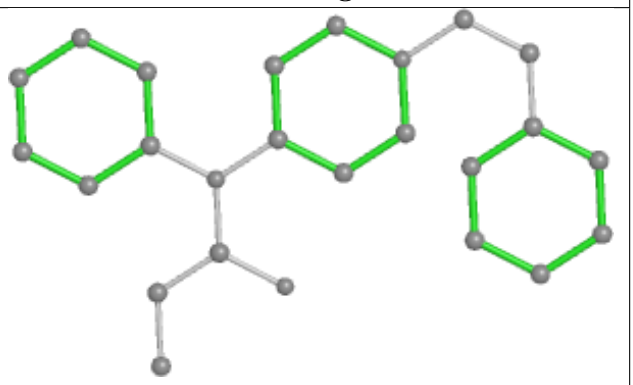
Bond lengths



Bond angles

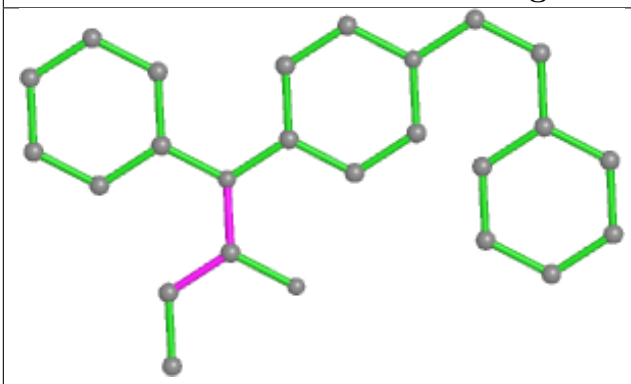


Torsions

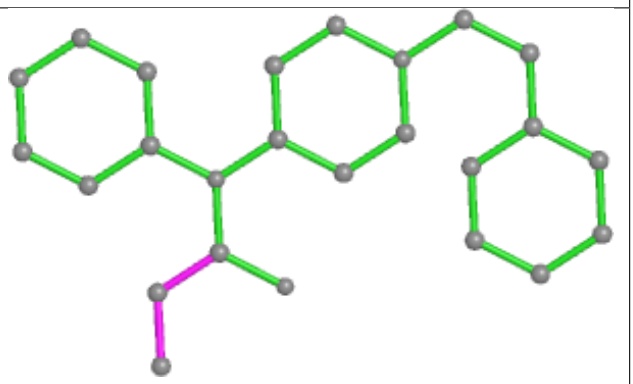


Rings

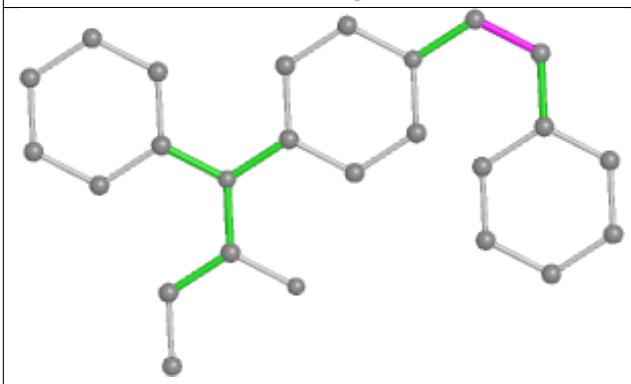
Ligand 7V7 A 301



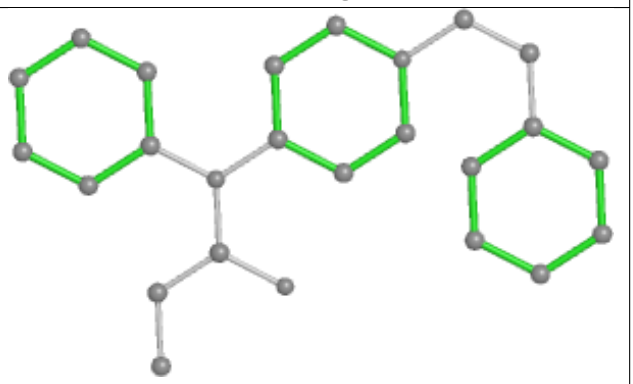
Bond lengths



Bond angles

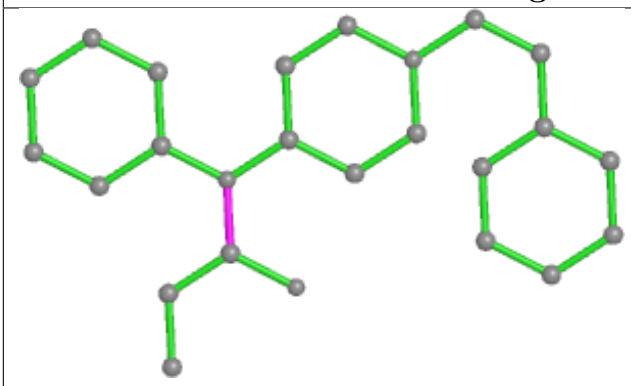


Torsions

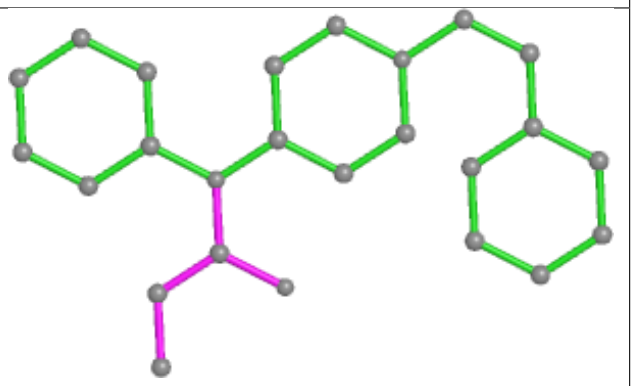


Rings

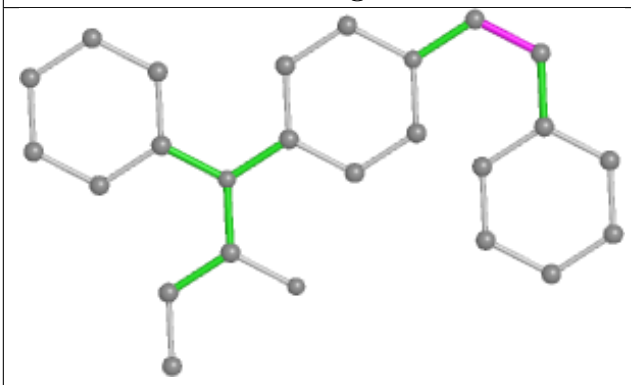
Ligand 7V7 G 301



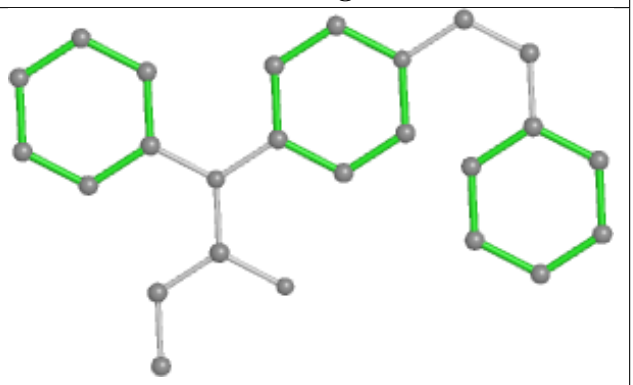
Bond lengths



Bond angles

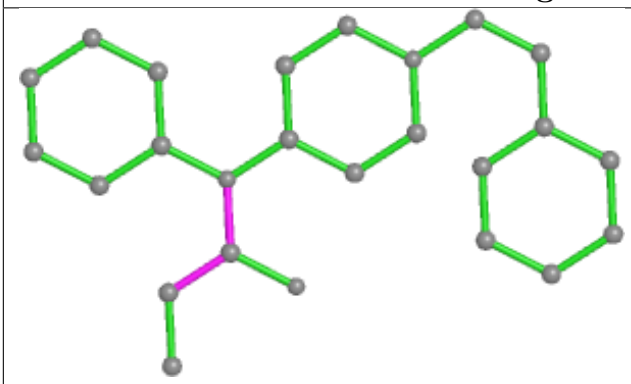


Torsions

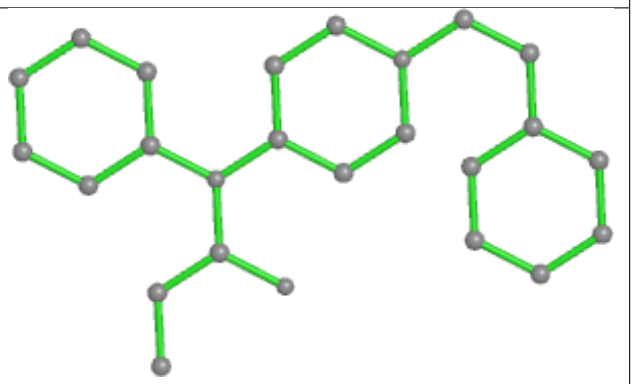


Rings

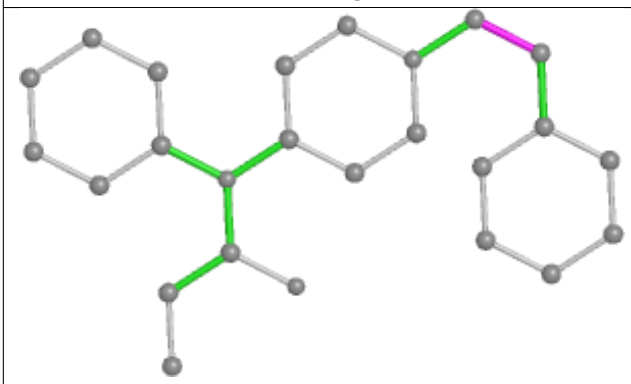
Ligand 7V7 I 301



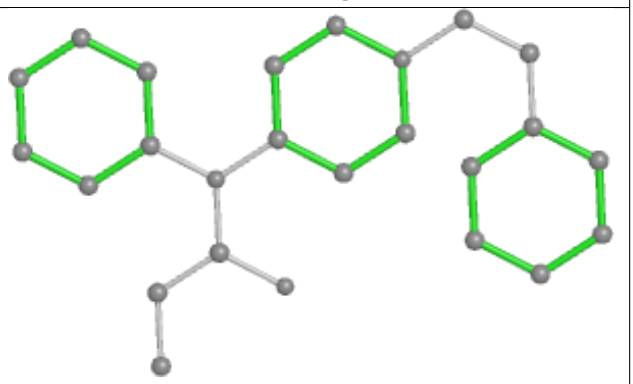
Bond lengths



Bond angles

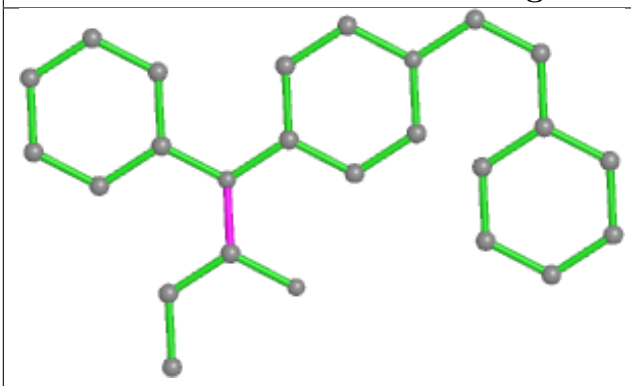


Torsions

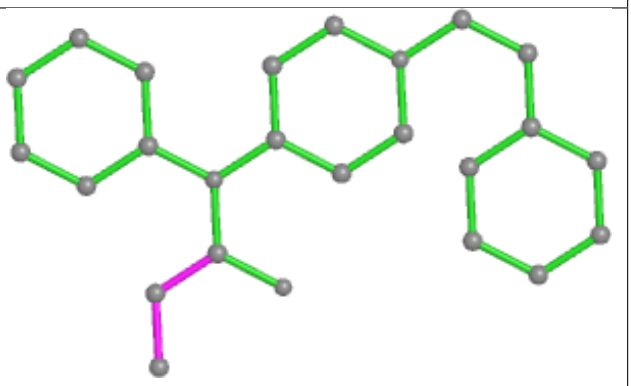


Rings

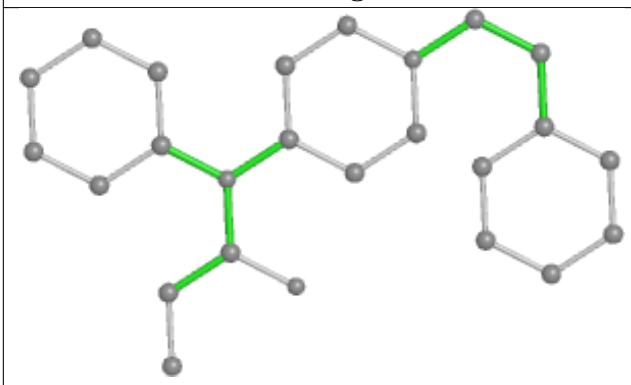
Ligand 7V7 M 301



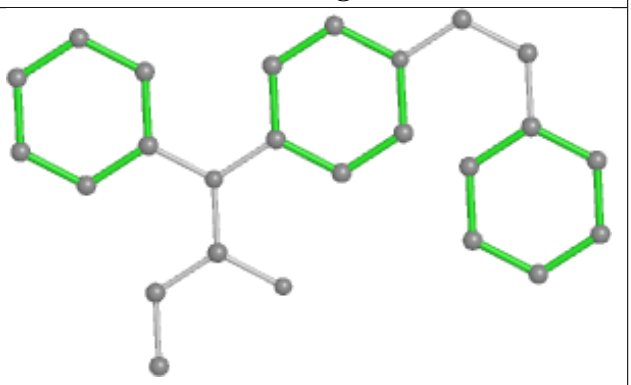
Bond lengths



Bond angles

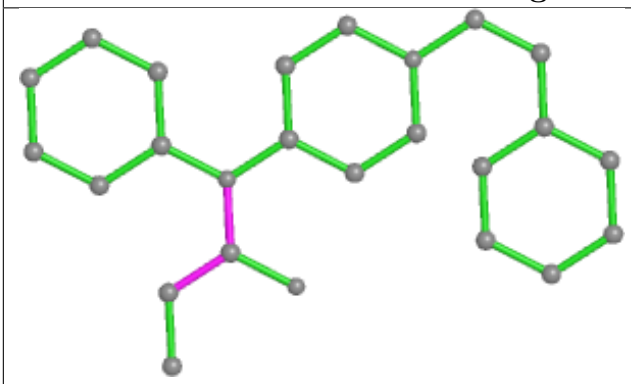


Torsions

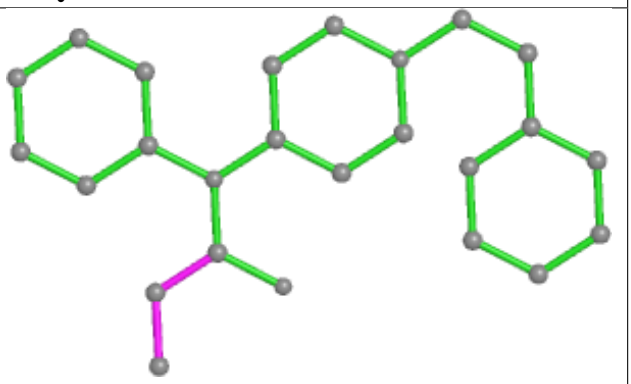


Rings

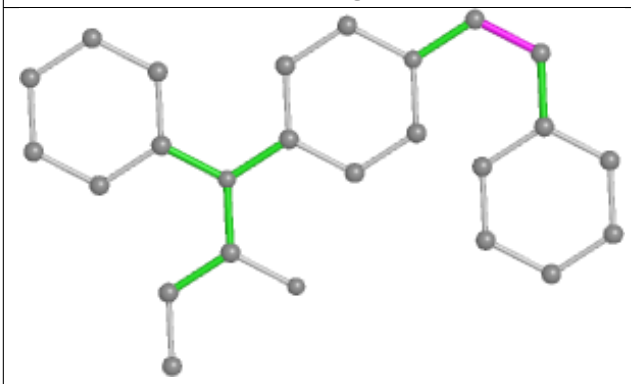
Ligand 7V7 Q 301



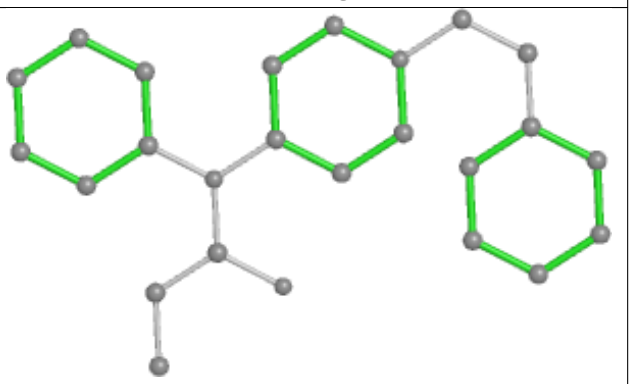
Bond lengths



Bond angles

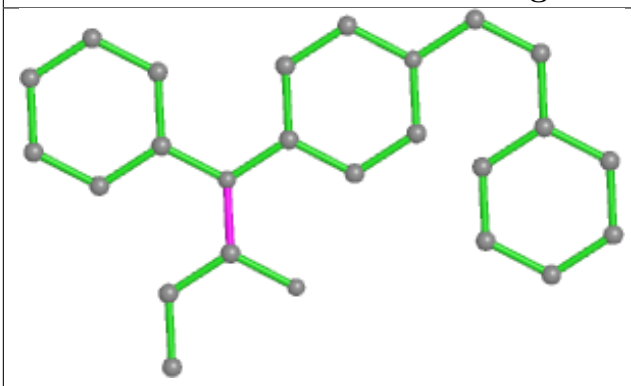


Torsions

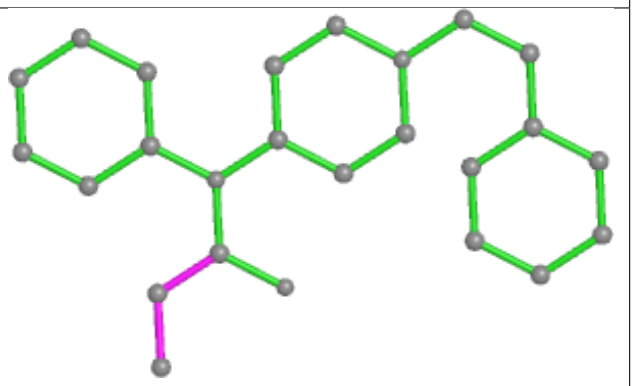


Rings

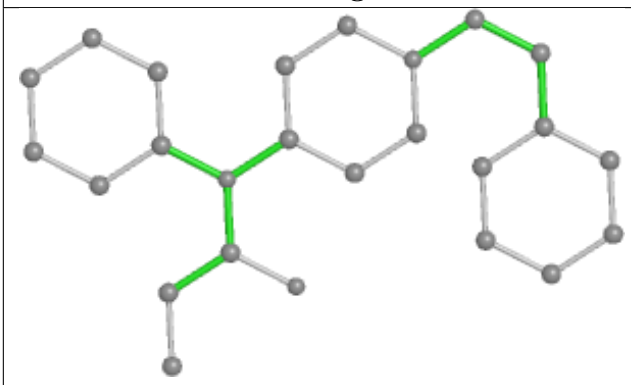
Ligand 7V7 C 301



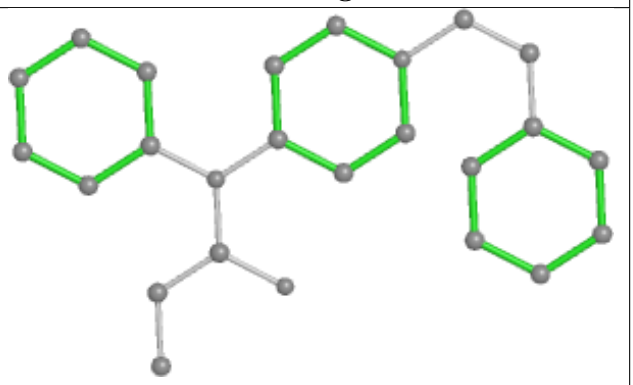
Bond lengths



Bond angles

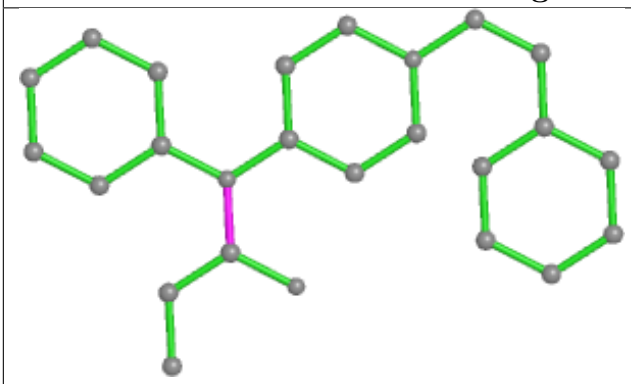


Torsions

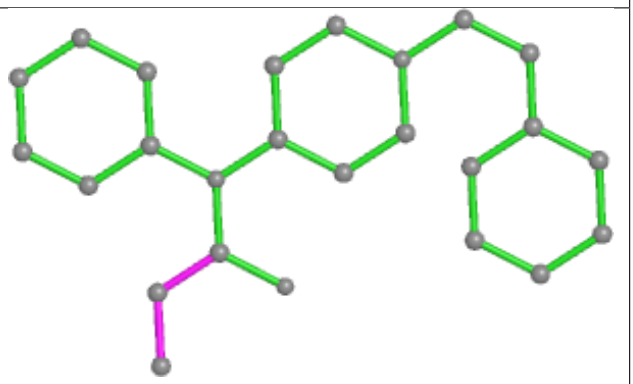


Rings

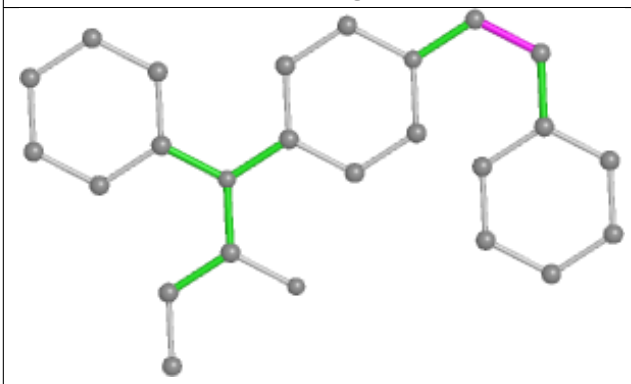
Ligand 7V7 E 301



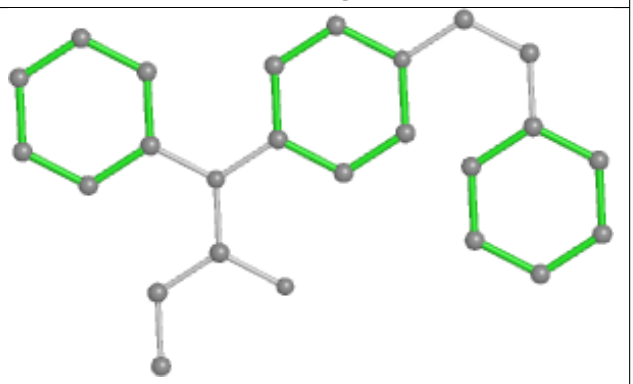
Bond lengths



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	222/226 (98%)	-0.35	1 (0%) 91 93	10, 17, 36, 57	0
1	C	222/226 (98%)	-0.22	7 (3%) 47 54	18, 27, 48, 74	0
1	E	222/226 (98%)	-0.32	1 (0%) 91 93	9, 17, 40, 64	0
1	G	222/226 (98%)	-0.04	13 (5%) 22 27	12, 21, 42, 72	0
1	I	222/226 (98%)	-0.38	2 (0%) 84 89	8, 15, 34, 56	0
1	K	222/226 (98%)	-0.27	4 (1%) 68 76	9, 17, 42, 68	0
1	M	222/226 (98%)	-0.11	9 (4%) 37 44	19, 28, 49, 73	0
1	O	222/226 (98%)	-0.33	1 (0%) 91 93	9, 18, 39, 68	0
1	Q	222/226 (98%)	-0.36	2 (0%) 84 89	9, 16, 36, 59	0
2	B	216/219 (98%)	-0.42	0 100 100	8, 19, 35, 45	1 (0%)
2	D	216/219 (98%)	-0.21	5 (2%) 60 67	17, 31, 52, 63	1 (0%)
2	F	216/219 (98%)	-0.38	0 100 100	8, 19, 36, 46	1 (0%)
2	H	216/219 (98%)	-0.01	11 (5%) 28 34	12, 25, 43, 56	1 (0%)
2	J	216/219 (98%)	-0.45	1 (0%) 91 93	9, 19, 34, 44	1 (0%)
2	L	216/219 (98%)	-0.42	0 100 100	9, 20, 37, 45	1 (0%)
2	N	216/219 (98%)	-0.12	7 (3%) 47 54	19, 33, 52, 61	1 (0%)
2	P	216/219 (98%)	-0.43	0 100 100	8, 20, 36, 45	1 (0%)
2	R	216/219 (98%)	-0.46	0 100 100	8, 18, 35, 43	1 (0%)
All	All	3942/4005 (98%)	-0.29	64 (1%) 72 79	8, 21, 43, 74	9 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	SER	5.2
1	O	1	GLU	5.1
1	M	215	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	G	215	SER	4.4
1	I	100	TYR	4.3
1	G	100	TYR	4.2
1	C	100	TYR	4.1
1	M	100	TYR	3.8
2	H	157	GLY	3.8
1	G	1	GLU	3.8
1	G	133	GLY	3.8
2	N	157	GLY	3.7
1	K	1	GLU	3.7
1	C	1	GLU	3.7
1	K	100	TYR	3.5
1	C	214	LYS	3.4
1	M	1	GLU	3.3
2	D	1	ASP	3.2
1	Q	1	GLU	3.1
1	G	96	TYR	3.0
2	H	9	PHE	3.0
1	G	128	SER	3.0
2	D	67	SER	2.9
1	M	214	LYS	2.9
2	N	1	ASP	2.9
2	H	67	SER	2.8
2	H	158	ASN	2.8
2	N	68	GLY	2.8
2	D	157	GLY	2.7
2	H	68	GLY	2.7
1	G	132	SER	2.7
1	E	215	SER	2.6
2	H	156	SER	2.6
1	C	160	THR	2.6
1	C	96	TYR	2.6
2	J	1	ASP	2.5
2	H	27(D)	HIS	2.5
2	N	158	ASN	2.5
1	G	134	GLY	2.5
2	H	154	LEU	2.4
1	M	96	TYR	2.4
1	G	131	THR	2.4
2	D	68	GLY	2.4
1	Q	100	TYR	2.4
1	M	128	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	29	GLY	2.3
2	H	27(E)	SER	2.3
2	N	67	SER	2.3
1	G	98	ASP	2.3
1	M	159	LEU	2.3
2	N	156	SER	2.3
1	M	133	GLY	2.3
2	N	154	LEU	2.3
1	K	161	SER	2.2
1	G	99	ASN	2.2
2	H	66	GLY	2.2
1	I	215	SER	2.1
1	M	207	VAL	2.1
1	K	215	SER	2.1
1	A	100	TYR	2.0
2	D	66	GLY	2.0
1	C	131	THR	2.0
1	G	160	THR	2.0
1	G	191	THR	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
4	ACT	B	306	4/4	0.69	0.14	41,51,52,56	0
4	ACT	H	309	4/4	0.88	0.12	30,37,39,44	0
3	7V7	G	301	25/25	0.89	0.16	19,28,57,60	0
4	ACT	A	303	4/4	0.89	0.18	34,36,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	Q	307	4/4	0.89	0.14	26,29,34,34	0
4	ACT	F	305	4/4	0.90	0.15	30,31,35,36	0
3	7V7	C	301	25/25	0.90	0.14	23,36,63,64	0
3	7V7	M	301	25/25	0.90	0.14	29,41,63,67	0
4	ACT	H	310	4/4	0.92	0.12	27,34,35,51	0
4	ACT	P	305	4/4	0.92	0.10	23,26,34,35	0
4	ACT	H	307	4/4	0.92	0.10	35,40,41,48	0
4	ACT	P	304	4/4	0.94	0.12	20,23,27,31	0
4	ACT	A	305	4/4	0.94	0.11	29,32,35,37	0
4	ACT	Q	305	4/4	0.94	0.11	25,33,33,38	0
4	ACT	O	302	4/4	0.94	0.09	19,24,32,34	0
4	ACT	R	306	4/4	0.94	0.12	25,27,29,33	0
4	ACT	M	303	4/4	0.95	0.14	19,36,42,42	0
4	ACT	B	305	4/4	0.95	0.06	25,28,32,35	0
4	ACT	B	304	4/4	0.95	0.09	26,32,37,41	0
4	ACT	H	308	4/4	0.95	0.10	32,34,40,40	0
4	ACT	P	307	4/4	0.95	0.09	26,30,41,42	0
4	ACT	C	302	4/4	0.95	0.12	29,33,39,41	0
4	ACT	F	303	4/4	0.95	0.07	24,33,35,35	0
4	ACT	L	304	4/4	0.95	0.08	26,29,32,33	0
4	ACT	J	305	4/4	0.96	0.07	27,28,37,43	0
4	ACT	K	303	4/4	0.96	0.14	22,22,22,26	0
4	ACT	P	306	4/4	0.96	0.17	22,25,32,38	0
4	ACT	A	306	4/4	0.96	0.15	27,28,32,51	0
4	ACT	G	302	4/4	0.96	0.12	23,23,32,35	0
3	7V7	K	301	25/25	0.96	0.09	14,19,40,45	0
4	ACT	R	305	4/4	0.96	0.12	23,27,35,36	0
4	ACT	O	303	4/4	0.96	0.10	18,21,23,23	0
5	NA	H	302	1/1	0.96	0.06	33,33,33,33	0
4	ACT	J	304	4/4	0.97	0.16	23,32,35,38	0
4	ACT	A	304	4/4	0.97	0.16	30,30,34,34	0
4	ACT	E	303	4/4	0.97	0.14	19,23,23,23	0
4	ACT	K	304	4/4	0.97	0.08	25,29,32,32	0
3	7V7	E	301	25/25	0.97	0.09	12,16,36,38	0
4	ACT	L	305	4/4	0.97	0.10	24,33,40,40	0
4	ACT	M	302	4/4	0.97	0.11	23,24,24,25	0
4	ACT	F	304	4/4	0.97	0.09	16,20,21,23	0
3	7V7	A	301	25/25	0.97	0.08	12,15,32,37	0
4	ACT	B	301	4/4	0.97	0.08	19,20,22,24	0
4	ACT	O	304	4/4	0.97	0.09	26,30,34,37	0
4	ACT	G	303	4/4	0.97	0.08	31,33,34,34	0
4	ACT	H	304	4/4	0.97	0.07	12,16,17,18	0

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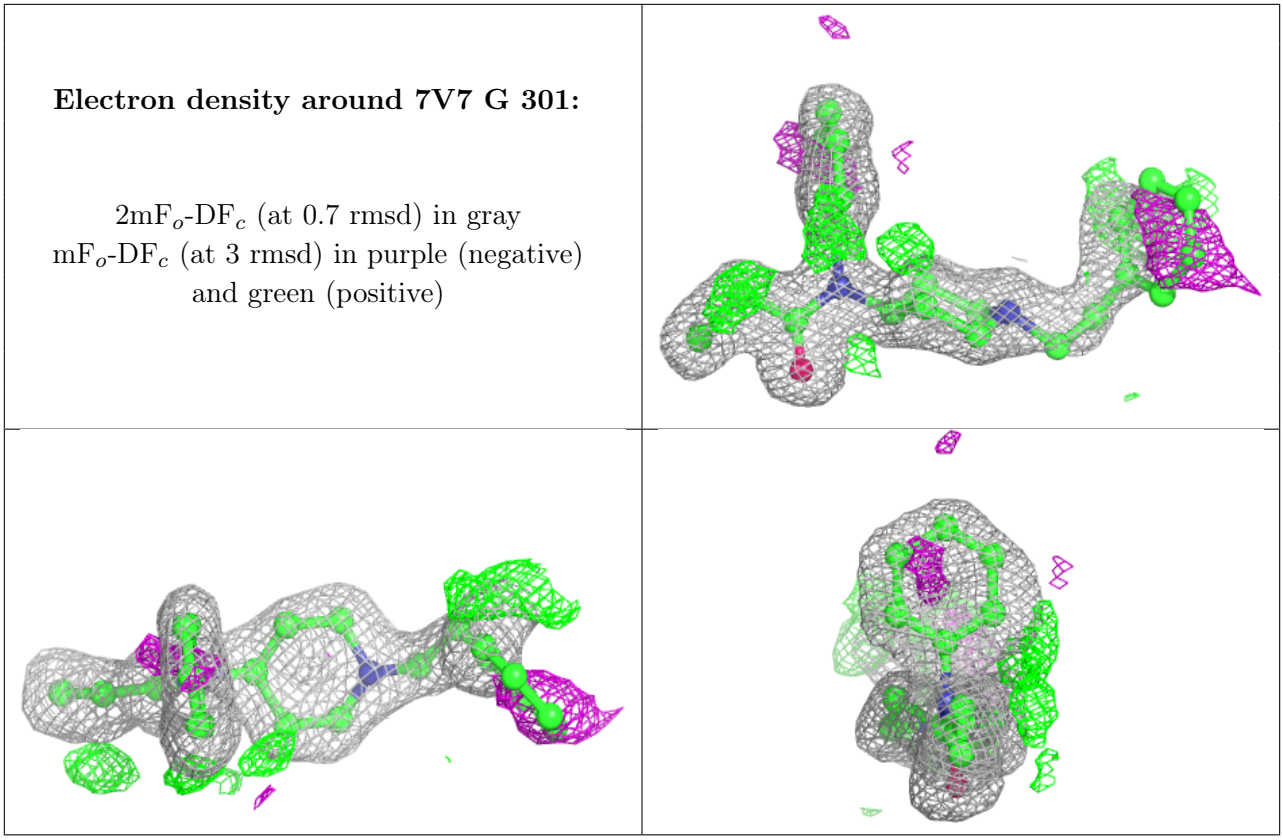
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ACT	H	306	4/4	0.97	0.06	27,28,37,41	0
4	ACT	B	303	4/4	0.97	0.07	27,29,34,35	0
4	ACT	Q	304	4/4	0.97	0.08	21,23,25,28	0
3	7V7	O	301	25/25	0.97	0.09	14,19,43,45	0
4	ACT	Q	306	4/4	0.97	0.15	28,33,34,37	0
3	7V7	Q	301	25/25	0.97	0.08	11,16,36,40	0
4	ACT	R	304	4/4	0.97	0.09	26,37,38,40	0
3	7V7	I	301	25/25	0.97	0.07	12,17,36,38	0
4	ACT	I	303	4/4	0.97	0.11	30,30,30,31	0
4	ACT	R	307	4/4	0.97	0.20	21,27,34,36	0
4	ACT	J	303	4/4	0.97	0.07	11,13,13,15	0
4	ACT	H	305	4/4	0.98	0.09	19,21,23,25	0
4	ACT	B	302	4/4	0.98	0.10	21,30,33,43	0
4	ACT	R	302	4/4	0.98	0.07	12,12,13,19	0
4	ACT	R	303	4/4	0.98	0.11	16,20,23,24	0
4	ACT	I	302	4/4	0.98	0.08	20,21,23,29	0
4	ACT	E	304	4/4	0.98	0.12	25,27,28,29	0
4	ACT	Q	303	4/4	0.98	0.07	11,12,12,14	0
4	ACT	L	303	4/4	0.98	0.10	21,24,25,33	0
4	ACT	F	302	4/4	0.98	0.07	11,13,14,15	0
5	NA	J	301	1/1	0.98	0.07	26,26,26,26	0
4	ACT	P	303	4/4	0.99	0.05	11,13,15,16	0
5	NA	D	301	1/1	0.99	0.05	21,21,21,21	0
5	NA	H	301	1/1	0.99	0.05	29,29,29,29	0
4	ACT	A	302	4/4	0.99	0.13	23,23,24,30	0
4	ACT	L	302	4/4	0.99	0.06	11,13,13,17	0
5	NA	K	302	1/1	0.99	0.05	20,20,20,20	0
5	NA	P	301	1/1	0.99	0.06	27,27,27,27	0
5	NA	E	302	1/1	1.00	0.05	20,20,20,20	0
5	NA	J	302	1/1	1.00	0.07	14,14,14,14	0
5	NA	F	301	1/1	1.00	0.08	11,11,11,11	0
5	NA	L	301	1/1	1.00	0.07	13,13,13,13	0
5	NA	H	303	1/1	1.00	0.05	15,15,15,15	0
5	NA	P	302	1/1	1.00	0.06	12,12,12,12	0
5	NA	Q	302	1/1	1.00	0.09	12,12,12,12	0
5	NA	R	301	1/1	1.00	0.08	13,13,13,13	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.

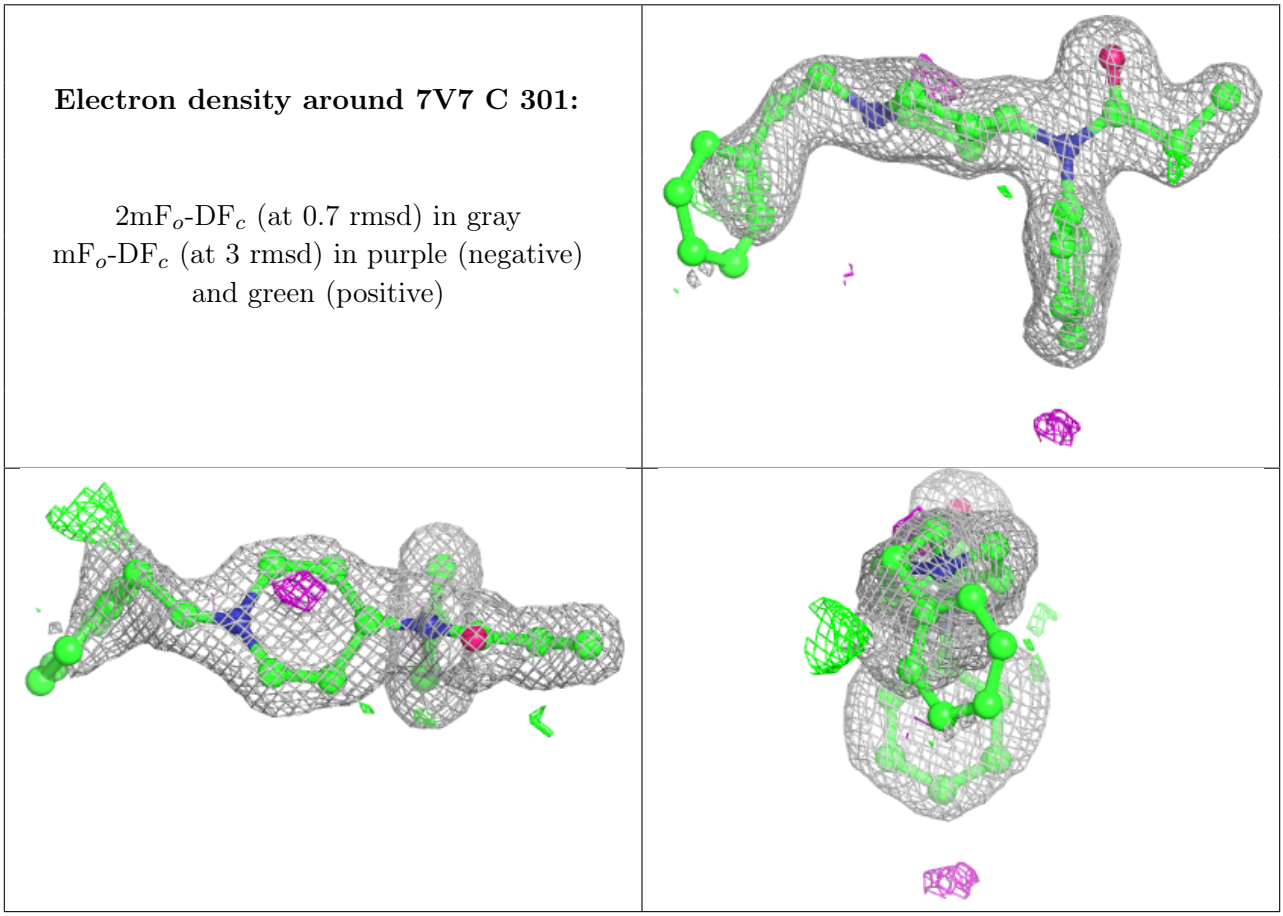
Electron density around 7V7 G 301:

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



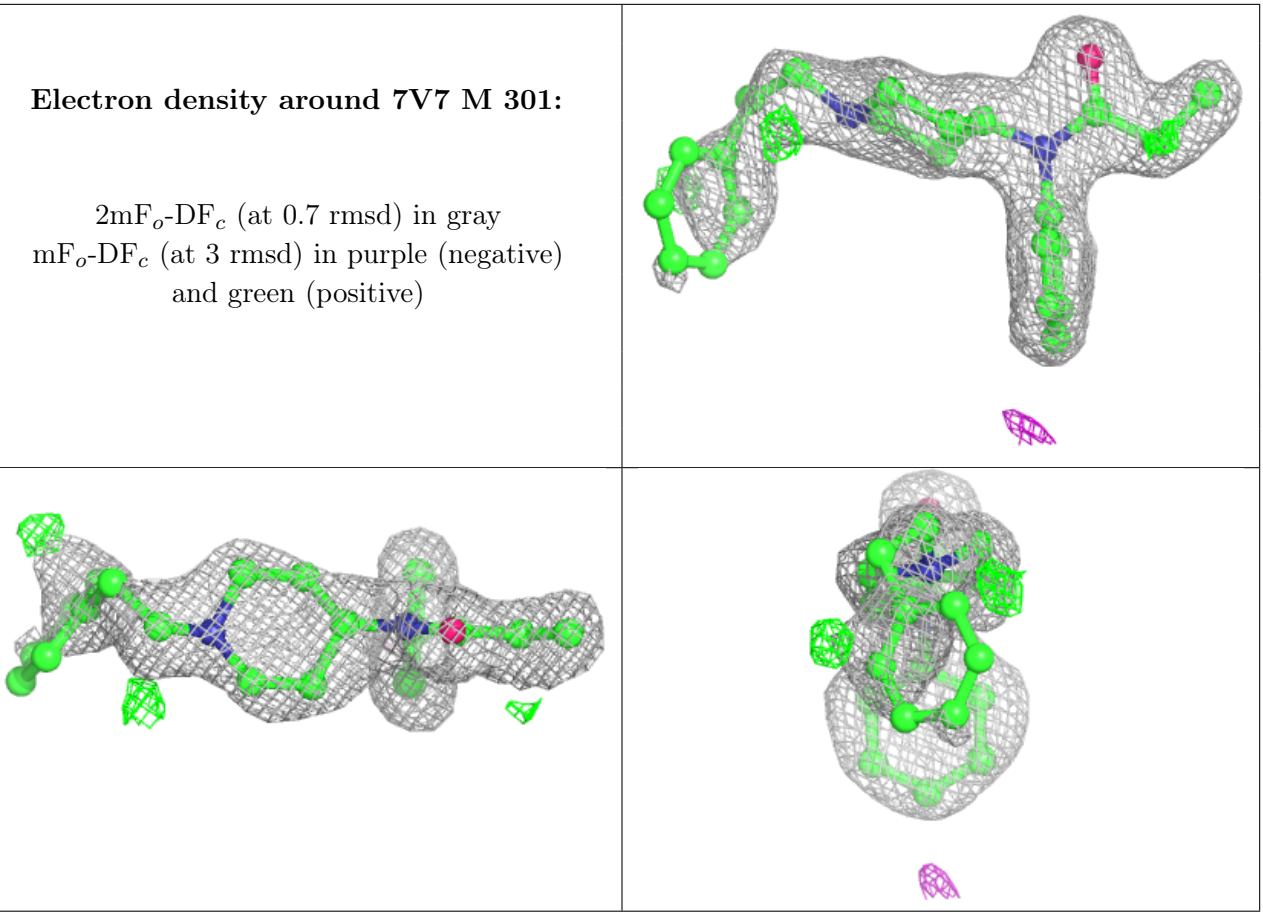
Electron density around 7V7 C 301:

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



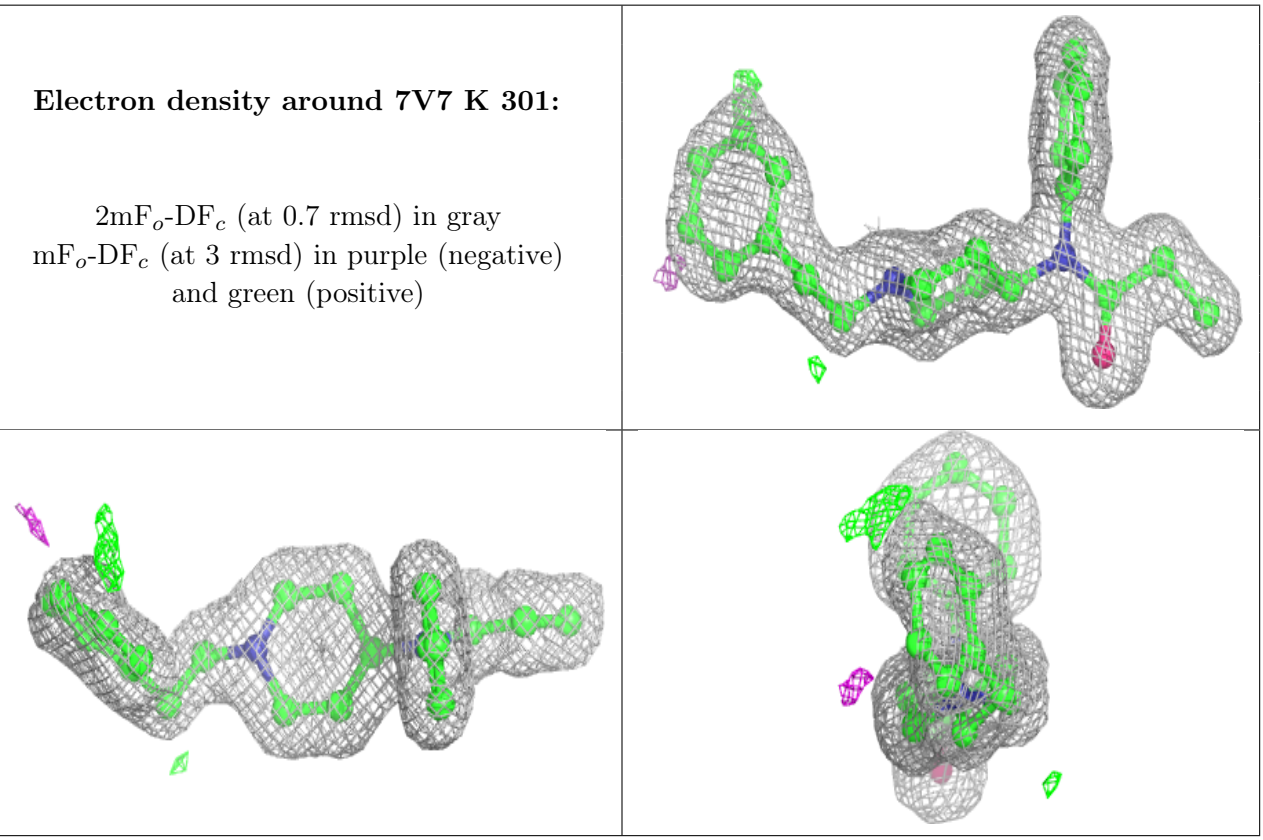
Electron density around 7V7 M 301:

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



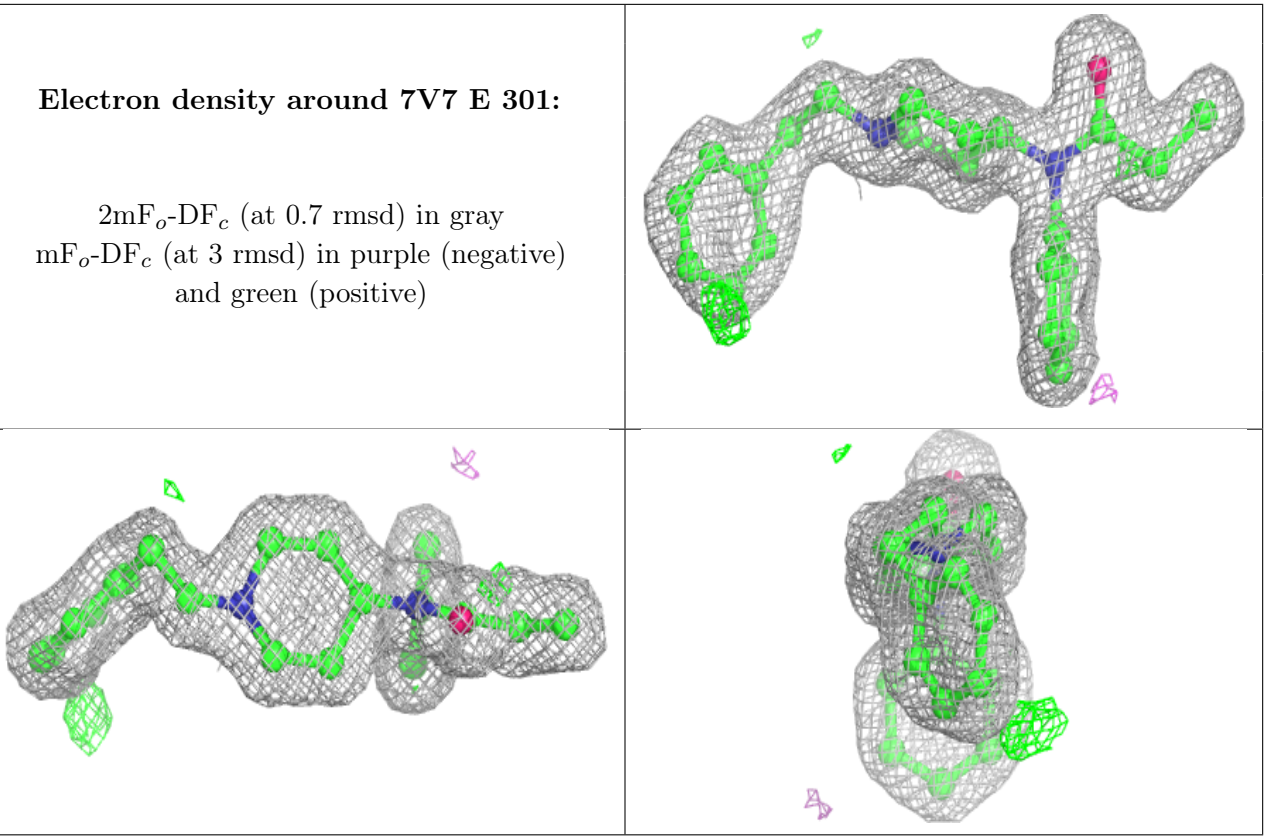
Electron density around 7V7 K 301:

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



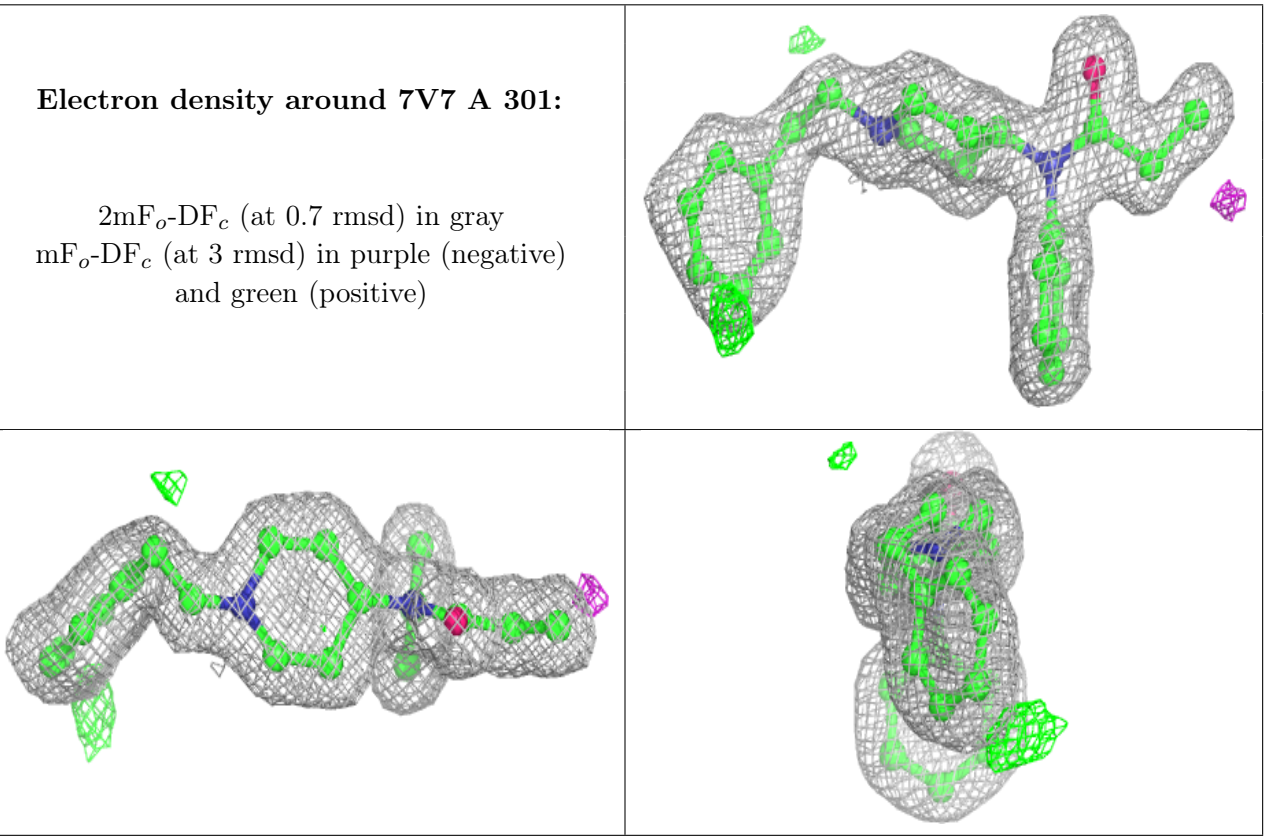
Electron density around 7V7 E 301:

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



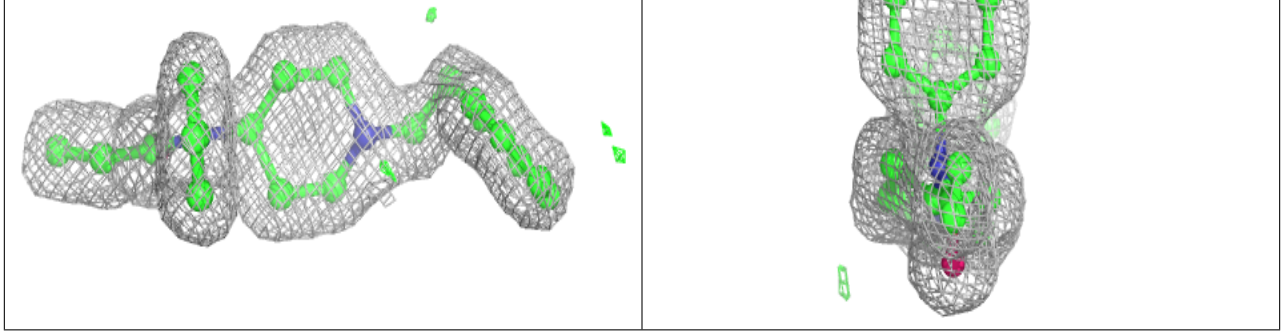
Electron density around 7V7 A 301:

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



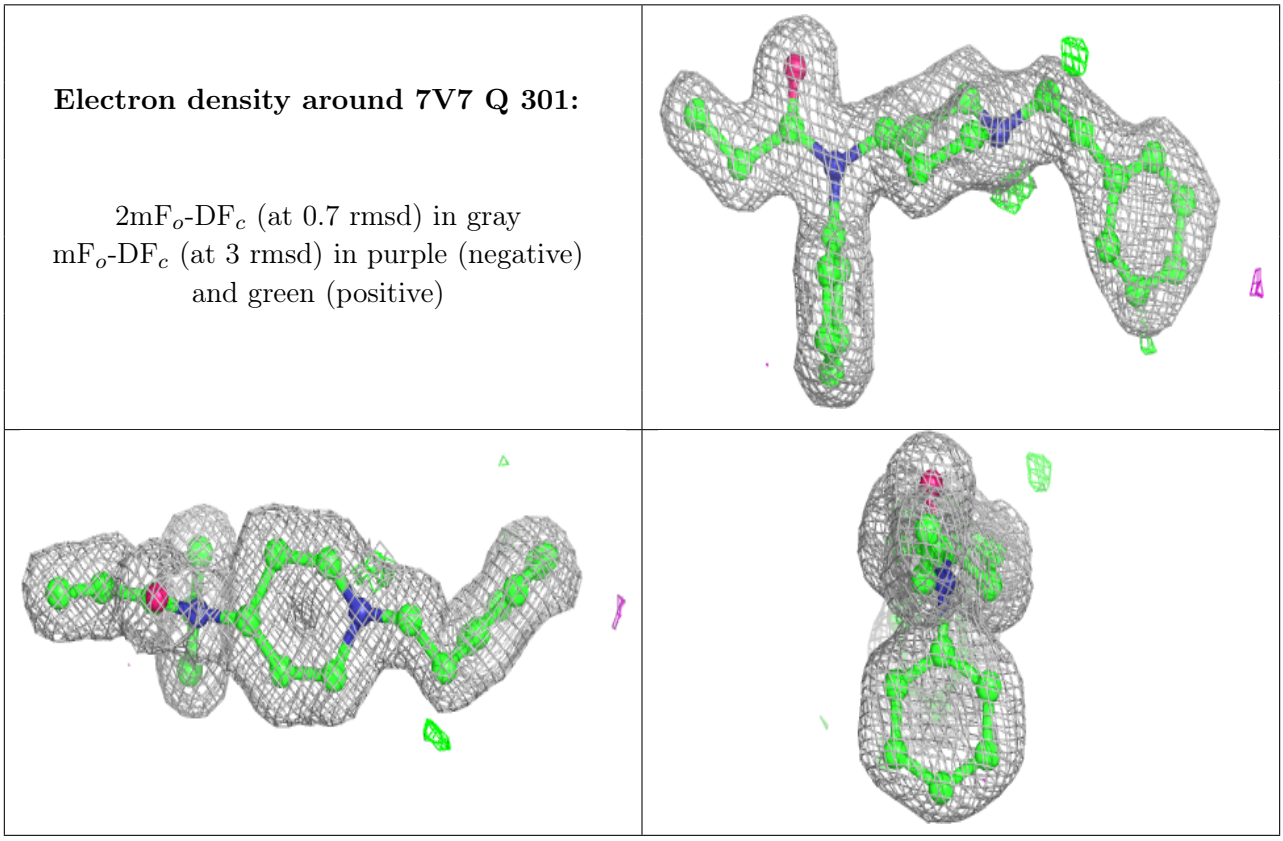
Electron density around 7V7 O 301:

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



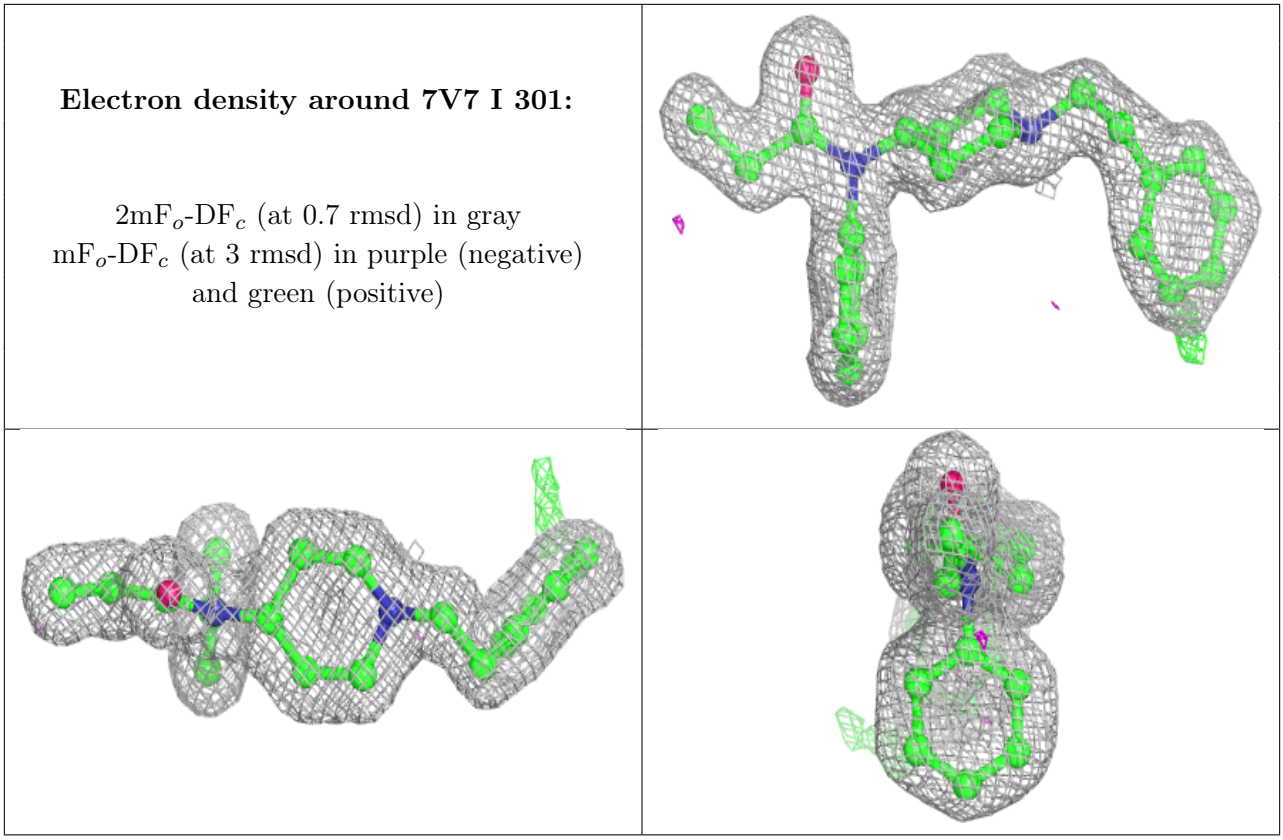
Electron density around 7V7 Q 301:

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



Electron density around 7V7 I 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.