



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 7U64 / pdb_00007u64
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

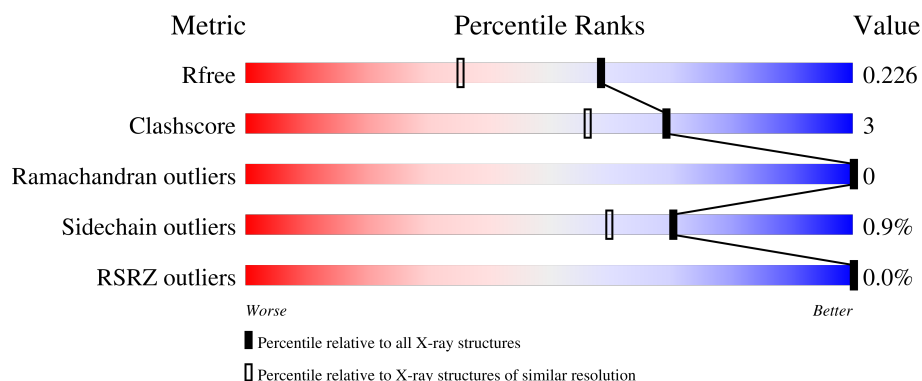
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



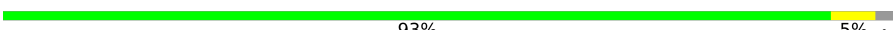
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	226	91% 7% .
1	C	226	88% 9% .
1	E	226	92% 6% ..
1	G	226	91% 8% .
1	I	226	92% 5% .

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Mol	Chain	Length	Quality of chain
1	K	226	 91% 7% .
1	M	226	 87% 11% .
1	O	226	 93% 5% .
1	Q	226	 92% 7% .
2	B	219	 90% 8% .
2	D	219	 88% 10% .
2	F	219	 90% 8% .
2	H	219	 91% 6% ..
2	J	219	 90% 8% .
2	L	219	 89% 10% .
2	N	219	 84% 14% .
2	P	219	 92% 7% .
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

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.

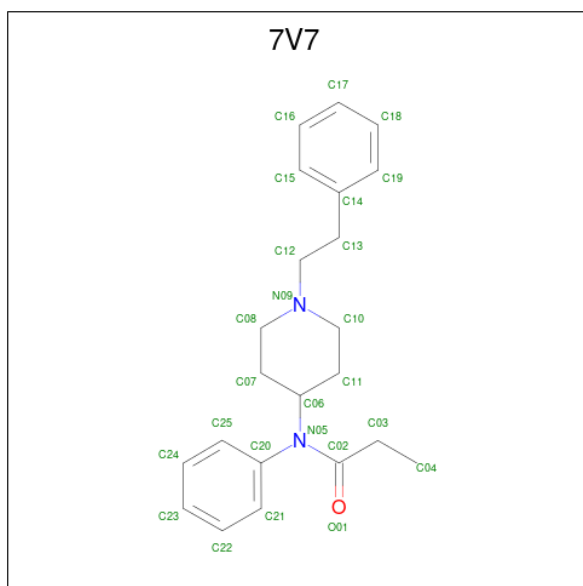
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	D	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	F	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	H	216	Total	C	N	O	S	0	0	0
			1667	1050	279	332	6			
2	J	216	Total	C	N	O	S	0	0	0
			1667	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 (CCD ID: 7V7) (formula: C₂₂H₂₈N₂O) (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	0	0
			25	22	2	1		
3	Q	1	Total	C	N	O	0	0
			25	22	2	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

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

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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	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	0	0
			4	2	2		
4	Q	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		
4	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total 192	O 192	0	0
6	B	157	Total 157	O 157	0	0
6	C	118	Total 118	O 118	0	0
6	D	113	Total 113	O 113	0	0
6	E	184	Total 184	O 184	0	0
6	F	154	Total 154	O 154	0	0
6	G	174	Total 174	O 174	0	0
6	H	124	Total 124	O 124	0	0
6	I	203	Total 203	O 203	0	0
6	J	149	Total 149	O 149	0	0
6	K	185	Total 185	O 185	0	0
6	L	148	Total 148	O 148	0	0
6	M	120	Total 120	O 120	0	0
6	N	122	Total 122	O 122	0	0
6	O	177	Total 177	O 177	0	0
6	P	161	Total 161	O 161	0	0
6	Q	182	Total 182	O 182	0	0
6	R	166	Total 166	O 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:  91% 7% .



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

Chain C:  88% 9% .



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

Chain E:  92% 6% ..



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

Chain G:  91% 8% .



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

Chain I:  92% 5% .



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

Chain K:  91% 7%



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

Chain M:  87% 11%



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

Chain O:  93% 5%



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

Chain Q:  92% 7%



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

Chain B:  90% 8%



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

Chain D:  88% 10%



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

Chain F:  90% 8%



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

Chain H:  91% 6% ..



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

Chain J:  90% 8% .



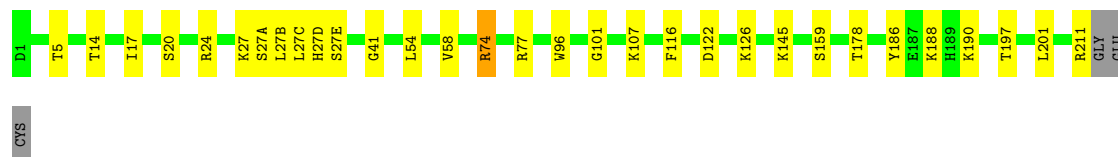
- Molecule 2: HY6-F9.6 Fab light chain

Chain L:  89% 10% .



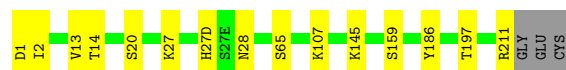
- Molecule 2: HY6-F9.6 Fab light chain

Chain N:  84% 14% .



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

Chain P:  92% 7% .



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

Chain R:  91% 7% .



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.225 0.198 , 0.226	Depositor DCC
R_{free} test set	23996 reflections (3.65%)	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 , 27.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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	0.98	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 7V7, ACT

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	0.29	0/1724	0.55	0/2353
1	C	0.23	0/1724	0.47	0/2353
1	E	0.30	0/1724	0.57	0/2353
1	G	0.27	0/1724	0.51	0/2353
1	I	0.31	0/1724	0.56	0/2353
1	K	0.29	0/1724	0.55	0/2353
1	M	0.22	0/1724	0.46	0/2353
1	O	0.29	0/1724	0.54	0/2353
1	Q	0.30	0/1724	0.56	0/2353
2	B	0.30	0/1703	0.55	0/2313
2	D	0.22	0/1703	0.45	0/2313
2	F	0.32	0/1703	0.55	0/2313
2	H	0.37	2/1703 (0.1%)	0.52	0/2313
2	J	0.29	0/1703	0.53	0/2313
2	L	0.30	0/1703	0.54	0/2313
2	N	0.22	0/1703	0.44	0/2313
2	P	0.28	0/1703	0.53	0/2313
2	R	0.31	0/1703	0.57	0/2313
All	All	0.29	2/30843 (0.0%)	0.53	0/41994

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	67	SER	N-CA	-7.58	1.41	1.46
2	H	67	SER	CA-C	6.94	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1681	0	1630	11	0
1	C	1681	0	1630	12	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	17	0
1	O	1681	0	1630	7	0
1	Q	1681	0	1630	10	0
2	B	1667	0	1633	16	0
2	D	1667	0	1633	15	0
2	F	1667	0	1633	15	0
2	H	1667	0	1633	9	0
2	J	1667	0	1633	11	0
2	L	1667	0	1633	15	0
2	N	1667	0	1633	19	0
2	P	1667	0	1633	10	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	210	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 (210) 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
2:N:188:LYS:NZ	6:N:312:HOH:O	2.32	0.62
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
1:C:28:SER:HG	1:C:30:THR:HG1	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:31:THR:HG21	2:J:51:MET:HE2	1.91	0.52
2:P:159:SER:O	6:P:401:HOH:O	2.19	0.52
2:F:1:ASP:CG	2:F:2:ILE:H	2.18	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
2:J:149:LYS:HZ3	2:J:154:LEU:HB2	1.75	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:51:MET:HE1	2:F:71:PHE:CD1	2.49	0.48
1:K:117:LYS:NZ	6:K:410:HOH:O	2.46	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
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:M:28:SER:HG	1:M:30:THR:HG1	1.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:67:SER:OG	2:D:68:GLY:N	2.47	0.45
2:B:167:ASP:CG	2:B:169:LYS:HZ2	2.25	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:R:14:THR:HG23	2:R:107:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:F:51:MET:HE1	2:F:71:PHE:HD1	1.85	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
2:L:51:MET:HE2	2:L:51:MET:HB3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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 ⓘ

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 ⓘ

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%)	192 (99%)	2 (1%)	68	56
1	C	194/198 (98%)	192 (99%)	2 (1%)	68	56
1	E	194/198 (98%)	192 (99%)	2 (1%)	68	56
1	G	194/198 (98%)	192 (99%)	2 (1%)	68	56
1	I	194/198 (98%)	193 (100%)	1 (0%)	81	75
1	K	194/198 (98%)	193 (100%)	1 (0%)	81	75
1	M	194/198 (98%)	193 (100%)	1 (0%)	81	75
1	O	194/198 (98%)	192 (99%)	2 (1%)	68	56
1	Q	194/198 (98%)	194 (100%)	0	100	100
2	B	190/192 (99%)	189 (100%)	1 (0%)	81	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	190/192 (99%)	188 (99%)	2 (1%)	65	52
2	F	190/192 (99%)	190 (100%)	0	100	100
2	H	190/192 (99%)	188 (99%)	2 (1%)	65	52
2	J	190/192 (99%)	190 (100%)	0	100	100
2	L	190/192 (99%)	189 (100%)	1 (0%)	81	75
2	N	190/192 (99%)	182 (96%)	8 (4%)	26	8
2	P	190/192 (99%)	189 (100%)	1 (0%)	81	75
2	R	190/192 (99%)	188 (99%)	2 (1%)	65	52
All	All	3456/3510 (98%)	3426 (99%)	30 (1%)	70	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	67	ILE
2	B	51	MET
1	C	105	GLN
1	C	209	LYS
2	D	1	ASP
2	D	74	ARG
1	E	2	VAL
1	E	18	LEU
1	G	2	VAL
1	G	215	SER
2	H	105	GLU
2	H	169	LYS
1	I	18	LEU
1	K	2	VAL
2	L	206	THR
1	M	18	LEU
2	N	27	LYS
2	N	27(A)	SER
2	N	27(B)	LEU
2	N	27(C)	LEU
2	N	27(D)	HIS
2	N	27(E)	SER
2	N	74	ARG
2	N	190	LYS
1	O	2	VAL

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Mol	Chain	Res	Type
1	O	18	LEU
2	P	65	SER
2	R	169	LYS
2	R	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	43	ASN
1	A	82(A)	ASN
2	B	11	ASN
2	B	210	ASN
1	C	192	GLN
2	D	210	ASN
1	E	3	GLN
1	E	82(A)	ASN
1	E	199	ASN
2	F	45	GLN
2	F	50	GLN
1	G	82(A)	ASN
2	H	11	ASN
2	H	53	ASN
2	H	147	GLN
1	I	5	GLN
1	I	82(A)	ASN
1	I	192	GLN
2	J	45	GLN
1	K	5	GLN
1	K	82(A)	ASN
1	K	199	ASN
2	L	45	GLN
2	L	158	ASN
2	L	210	ASN
1	M	82(A)	ASN
1	M	105	GLN
2	N	50	GLN
2	N	155	GLN
2	N	189	HIS
1	O	82(A)	ASN
1	O	199	ASN
2	P	11	ASN

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Mol	Chain	Res	Type
2	P	210	ASN
1	Q	82(A)	ASN
1	Q	105	GLN
2	R	11	ASN
2	R	38	GLN
2	R	45	GLN
2	R	155	GLN
2	R	199	GLN
2	R	210	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	I	303	-	3,3,3	1.44	1 (33%)	3,3,3	1.64	1 (33%)
4	ACT	Q	305	-	3,3,3	1.44	0	3,3,3	1.59	1 (33%)
4	ACT	P	303	5	3,3,3	1.61	1 (33%)	3,3,3	1.44	0
4	ACT	F	305	-	3,3,3	1.34	0	3,3,3	1.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	K	304	-	3,3,3	1.68	1 (33%)	3,3,3	1.55	0
4	ACT	R	304	-	3,3,3	1.43	1 (33%)	3,3,3	1.36	0
4	ACT	B	304	-	3,3,3	1.41	1 (33%)	3,3,3	1.44	0
4	ACT	F	303	-	3,3,3	1.32	0	3,3,3	1.33	0
4	ACT	Q	303	5	3,3,3	1.56	1 (33%)	3,3,3	1.15	0
3	7V7	I	301	-	27,27,27	1.17	2 (7%)	34,35,35	0.88	1 (2%)
4	ACT	C	302	-	3,3,3	1.35	0	3,3,3	1.63	0
4	ACT	Q	307	-	3,3,3	1.17	0	3,3,3	1.82	1 (33%)
4	ACT	R	303	-	3,3,3	1.51	1 (33%)	3,3,3	1.41	0
4	ACT	B	305	-	3,3,3	1.63	1 (33%)	3,3,3	1.48	0
4	ACT	B	306	-	3,3,3	1.44	1 (33%)	3,3,3	1.52	1 (33%)
4	ACT	B	303	-	3,3,3	1.64	1 (33%)	3,3,3	1.45	0
4	ACT	P	304	-	3,3,3	1.63	1 (33%)	3,3,3	1.47	0
4	ACT	P	306	-	3,3,3	1.59	1 (33%)	3,3,3	1.47	0
4	ACT	A	305	-	3,3,3	1.52	1 (33%)	3,3,3	1.59	0
4	ACT	G	302	-	3,3,3	1.15	0	3,3,3	1.54	1 (33%)
4	ACT	A	306	-	3,3,3	1.26	0	3,3,3	1.59	1 (33%)
4	ACT	H	308	-	3,3,3	1.48	0	3,3,3	1.43	0
4	ACT	M	302	-	3,3,3	1.47	1 (33%)	3,3,3	1.66	2 (66%)
3	7V7	C	301	-	27,27,27	0.80	1 (3%)	34,35,35	0.92	1 (2%)
3	7V7	O	301	-	27,27,27	0.93	1 (3%)	34,35,35	0.89	1 (2%)
4	ACT	J	304	-	3,3,3	1.50	1 (33%)	3,3,3	1.44	0
4	ACT	F	304	-	3,3,3	1.57	1 (33%)	3,3,3	1.55	1 (33%)
4	ACT	E	304	-	3,3,3	1.54	1 (33%)	3,3,3	1.39	0
4	ACT	I	302	-	3,3,3	1.48	1 (33%)	3,3,3	1.30	0
4	ACT	R	306	-	3,3,3	1.63	1 (33%)	3,3,3	1.55	1 (33%)
4	ACT	L	304	-	3,3,3	1.54	1 (33%)	3,3,3	1.47	0
3	7V7	G	301	-	27,27,27	0.78	1 (3%)	34,35,35	0.92	1 (2%)
4	ACT	A	302	-	3,3,3	1.34	0	3,3,3	1.69	2 (66%)
4	ACT	M	303	-	3,3,3	1.06	0	3,3,3	1.60	1 (33%)
4	ACT	H	306	-	3,3,3	1.57	1 (33%)	3,3,3	1.54	0
4	ACT	O	303	-	3,3,3	1.60	1 (33%)	3,3,3	1.40	0
4	ACT	E	303	-	3,3,3	1.34	0	3,3,3	1.60	1 (33%)
4	ACT	B	302	-	3,3,3	1.27	0	3,3,3	1.70	2 (66%)
4	ACT	H	310	-	3,3,3	1.17	0	3,3,3	1.62	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	H	304	5	3,3,3	1.36	0	3,3,3	1.29	0
3	7V7	A	301	-	27,27,27	0.88	2 (7%)	34,35,35	0.89	1 (2%)
4	ACT	G	303	-	3,3,3	1.43	1 (33%)	3,3,3	1.54	0
4	ACT	A	303	-	3,3,3	1.47	1 (33%)	3,3,3	1.65	1 (33%)
3	7V7	M	301	-	27,27,27	0.88	1 (3%)	34,35,35	0.95	1 (2%)
4	ACT	Q	306	-	3,3,3	1.59	1 (33%)	3,3,3	1.55	0
3	7V7	E	301	-	27,27,27	0.78	1 (3%)	34,35,35	0.89	1 (2%)
4	ACT	L	305	-	3,3,3	1.27	0	3,3,3	1.48	0
4	ACT	L	303	-	3,3,3	1.46	1 (33%)	3,3,3	1.43	0
4	ACT	R	302	5	3,3,3	1.84	1 (33%)	3,3,3	1.23	0
4	ACT	R	305	-	3,3,3	1.33	0	3,3,3	1.56	0
4	ACT	O	304	-	3,3,3	1.56	1 (33%)	3,3,3	1.43	0
4	ACT	P	307	-	3,3,3	1.61	1 (33%)	3,3,3	1.44	0
4	ACT	P	305	-	3,3,3	1.36	1 (33%)	3,3,3	1.59	1 (33%)
4	ACT	O	302	-	3,3,3	0.74	0	3,3,3	1.98	2 (66%)
4	ACT	H	309	-	3,3,3	1.28	0	3,3,3	1.48	1 (33%)
4	ACT	H	305	-	3,3,3	1.22	0	3,3,3	1.29	0
4	ACT	L	302	5	3,3,3	1.60	1 (33%)	3,3,3	1.26	0
3	7V7	K	301	-	27,27,27	1.00	2 (7%)	34,35,35	0.89	1 (2%)
4	ACT	H	307	-	3,3,3	1.55	1 (33%)	3,3,3	1.55	0
4	ACT	A	304	-	3,3,3	1.65	1 (33%)	3,3,3	1.51	0
4	ACT	Q	304	-	3,3,3	1.50	1 (33%)	3,3,3	1.15	0
4	ACT	K	303	-	3,3,3	1.46	1 (33%)	3,3,3	1.41	0
4	ACT	R	307	-	3,3,3	1.10	0	3,3,3	1.45	0
4	ACT	J	305	-	3,3,3	1.26	0	3,3,3	1.45	1 (33%)
4	ACT	F	302	5	3,3,3	1.67	1 (33%)	3,3,3	1.33	0
3	7V7	Q	301	-	27,27,27	0.97	2 (7%)	34,35,35	0.82	1 (2%)
4	ACT	J	303	5	3,3,3	1.70	1 (33%)	3,3,3	1.25	0
4	ACT	B	301	-	3,3,3	1.29	0	3,3,3	1.73	2 (66%)

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	C	301	-	-	0/19/29/29	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7V7	A	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	G	301	-	-	1/19/29/29	0/3/3/3
3	7V7	E	301	-	-	1/19/29/29	0/3/3/3
3	7V7	I	301	-	-	1/19/29/29	0/3/3/3
3	7V7	Q	301	-	-	1/19/29/29	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	7V7	C03-C02	3.96	1.57	1.51
3	O	301	7V7	C02-N05	3.13	1.41	1.36
3	K	301	7V7	C02-N05	3.01	1.41	1.36
3	I	301	7V7	C02-N05	3.00	1.41	1.36
3	M	301	7V7	C02-N05	2.89	1.41	1.36
3	Q	301	7V7	C02-N05	2.86	1.41	1.36
4	R	302	ACT	CH3-C	2.86	1.60	1.49
3	K	301	7V7	C03-C02	2.72	1.55	1.51
4	J	303	ACT	CH3-C	2.67	1.59	1.49
4	F	302	ACT	CH3-C	2.63	1.59	1.49
4	L	302	ACT	CH3-C	2.58	1.59	1.49
3	C	301	7V7	C02-N05	2.57	1.41	1.36
3	E	301	7V7	C02-N05	2.43	1.40	1.36
4	P	306	ACT	CH3-C	2.42	1.58	1.49
3	G	301	7V7	C02-N05	2.42	1.40	1.36
4	K	304	ACT	CH3-C	2.42	1.58	1.49
4	P	303	ACT	CH3-C	2.41	1.58	1.49
4	A	304	ACT	CH3-C	2.41	1.58	1.49
3	A	301	7V7	C02-N05	2.40	1.40	1.36
4	Q	303	ACT	CH3-C	2.37	1.58	1.49
3	Q	301	7V7	C03-C02	2.37	1.54	1.51
4	Q	306	ACT	CH3-C	2.30	1.58	1.49
4	O	304	ACT	CH3-C	2.30	1.58	1.49
4	R	303	ACT	CH3-C	2.25	1.58	1.49
4	H	306	ACT	CH3-C	2.24	1.57	1.49
4	P	304	ACT	CH3-C	2.24	1.57	1.49
4	H	307	ACT	CH3-C	2.24	1.57	1.49
4	B	303	ACT	CH3-C	2.22	1.57	1.49
4	A	305	ACT	CH3-C	2.22	1.57	1.49
4	E	304	ACT	CH3-C	2.22	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	306	ACT	CH3-C	2.21	1.57	1.49
4	B	305	ACT	CH3-C	2.21	1.57	1.49
4	Q	304	ACT	CH3-C	2.21	1.57	1.49
4	J	304	ACT	CH3-C	2.17	1.57	1.49
4	I	302	ACT	CH3-C	2.16	1.57	1.49
4	B	304	ACT	CH3-C	2.15	1.57	1.49
4	P	305	ACT	CH3-C	2.14	1.57	1.49
4	M	302	ACT	CH3-C	2.14	1.57	1.49
4	I	303	ACT	CH3-C	2.12	1.57	1.49
3	A	301	7V7	C03-C02	2.12	1.54	1.51
4	L	303	ACT	CH3-C	2.12	1.57	1.49
4	L	304	ACT	CH3-C	2.12	1.57	1.49
4	G	303	ACT	CH3-C	2.12	1.57	1.49
4	K	303	ACT	CH3-C	2.11	1.57	1.49
4	O	303	ACT	CH3-C	2.11	1.57	1.49
4	P	307	ACT	CH3-C	2.08	1.57	1.49
4	B	306	ACT	CH3-C	2.07	1.57	1.49
4	F	304	ACT	CH3-C	2.06	1.57	1.49
4	A	303	ACT	CH3-C	2.03	1.57	1.49
4	R	304	ACT	CH3-C	2.01	1.57	1.49

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	7V7	C04-C03-C02	-2.52	108.28	112.69
3	M	301	7V7	C04-C03-C02	-2.50	108.32	112.69
3	A	301	7V7	C04-C03-C02	-2.48	108.35	112.69
3	C	301	7V7	C04-C03-C02	-2.47	108.36	112.69
4	O	302	ACT	O-C-CH3	-2.46	112.44	122.53
4	Q	307	ACT	OXT-C-O	2.43	131.04	122.03
4	O	302	ACT	OXT-C-O	2.36	130.77	122.03
3	E	301	7V7	C04-C03-C02	-2.30	108.67	112.69
3	K	301	7V7	C04-C03-C02	-2.28	108.70	112.69
3	O	301	7V7	C04-C03-C02	-2.24	108.77	112.69
3	Q	301	7V7	C04-C03-C02	-2.23	108.79	112.69
4	G	302	ACT	OXT-C-O	2.18	130.11	122.03
4	B	301	ACT	O-C-CH3	-2.17	113.65	122.53
4	M	303	ACT	OXT-C-O	2.11	129.87	122.03
4	E	303	ACT	OXT-C-O	2.11	129.86	122.03
4	F	304	ACT	OXT-C-O	2.09	129.80	122.03
4	B	302	ACT	OXT-C-O	2.09	129.78	122.03
4	A	302	ACT	OXT-C-O	2.08	129.75	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	301	7V7	C04-C03-C02	-2.08	109.05	112.69
4	J	305	ACT	OXT-C-O	2.07	129.70	122.03
4	B	302	ACT	O-C-CH3	-2.06	114.08	122.53
4	A	303	ACT	OXT-C-O	2.06	129.66	122.03
4	P	305	ACT	O-C-CH3	-2.06	114.10	122.53
4	Q	305	ACT	OXT-C-O	2.05	129.65	122.03
4	A	302	ACT	O-C-CH3	-2.05	114.11	122.53
4	R	306	ACT	OXT-C-O	2.05	129.63	122.03
4	I	303	ACT	O-C-CH3	-2.05	114.13	122.53
4	H	309	ACT	OXT-C-O	2.04	129.59	122.03
4	M	302	ACT	O-C-CH3	-2.03	114.20	122.53
4	M	302	ACT	OXT-C-O	2.02	129.53	122.03
4	B	301	ACT	OXT-C-O	2.01	129.50	122.03
4	B	306	ACT	OXT-C-O	2.01	129.50	122.03
4	A	306	ACT	OXT-C-O	2.01	129.49	122.03
4	H	310	ACT	O-C-CH3	-2.00	114.31	122.53

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:

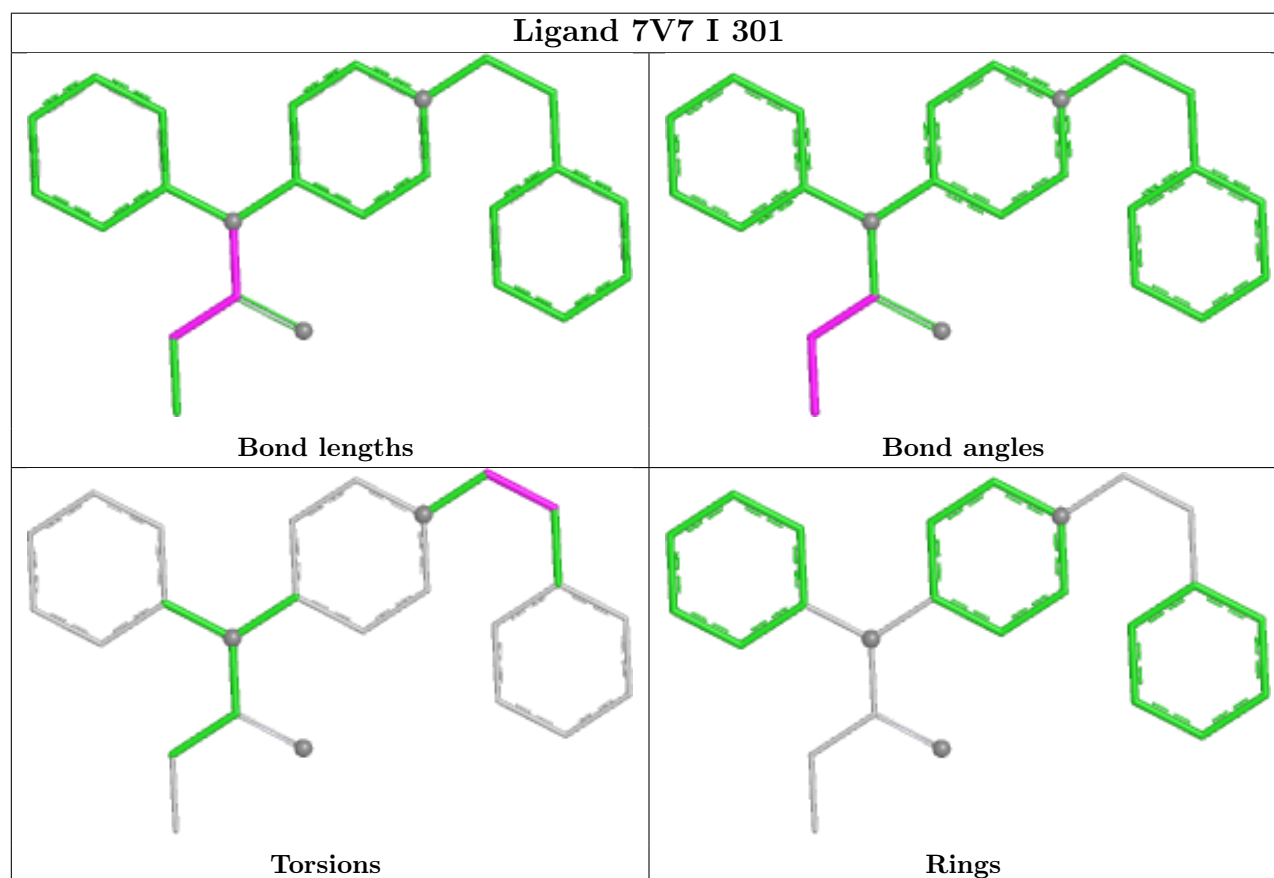
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	307	ACT	3	0
4	B	306	ACT	1	0
4	G	302	ACT	1	0
4	A	306	ACT	1	0
4	M	302	ACT	1	0
4	M	303	ACT	1	0
4	B	302	ACT	1	0
4	A	303	ACT	1	0

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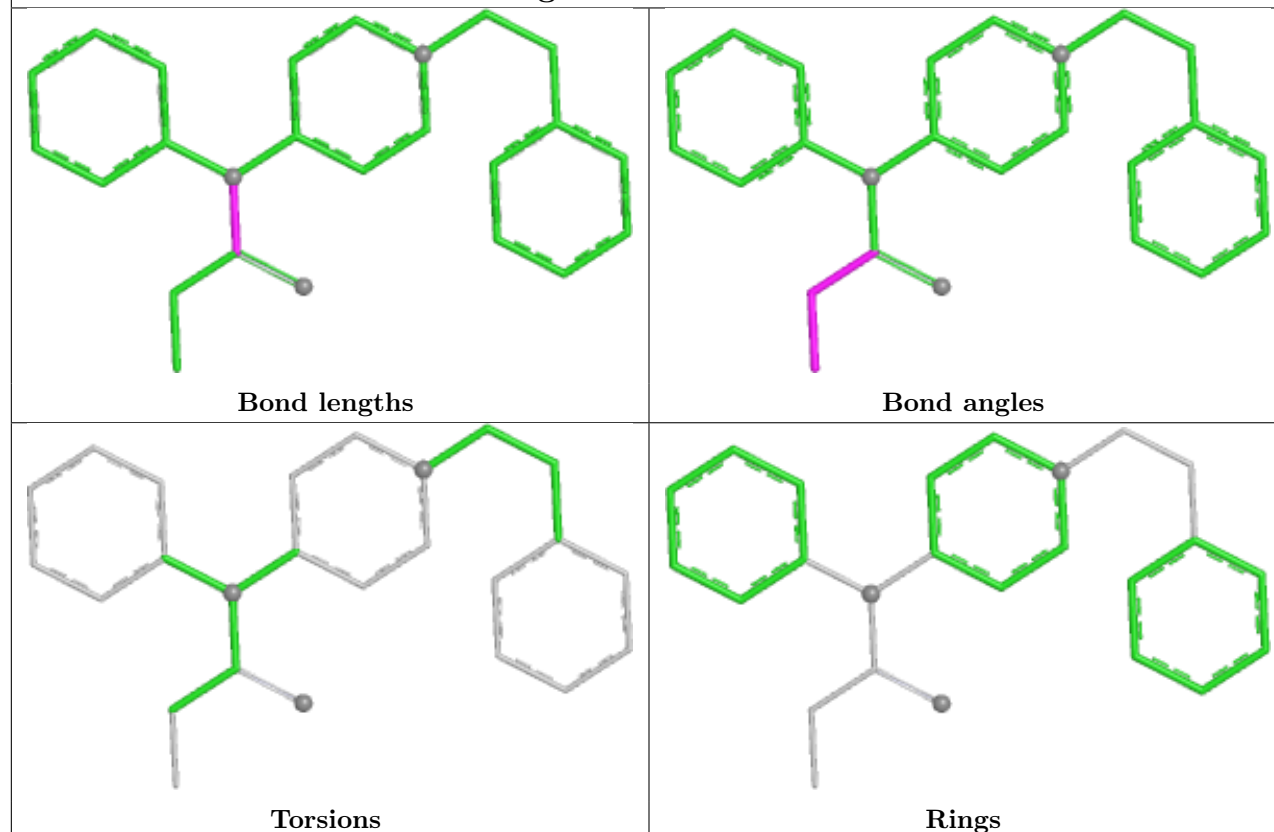
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	306	ACT	1	0
4	L	305	ACT	2	0
4	R	305	ACT	1	0
4	P	305	ACT	1	0
4	O	302	ACT	3	0
4	R	307	ACT	1	0
4	J	305	ACT	1	0

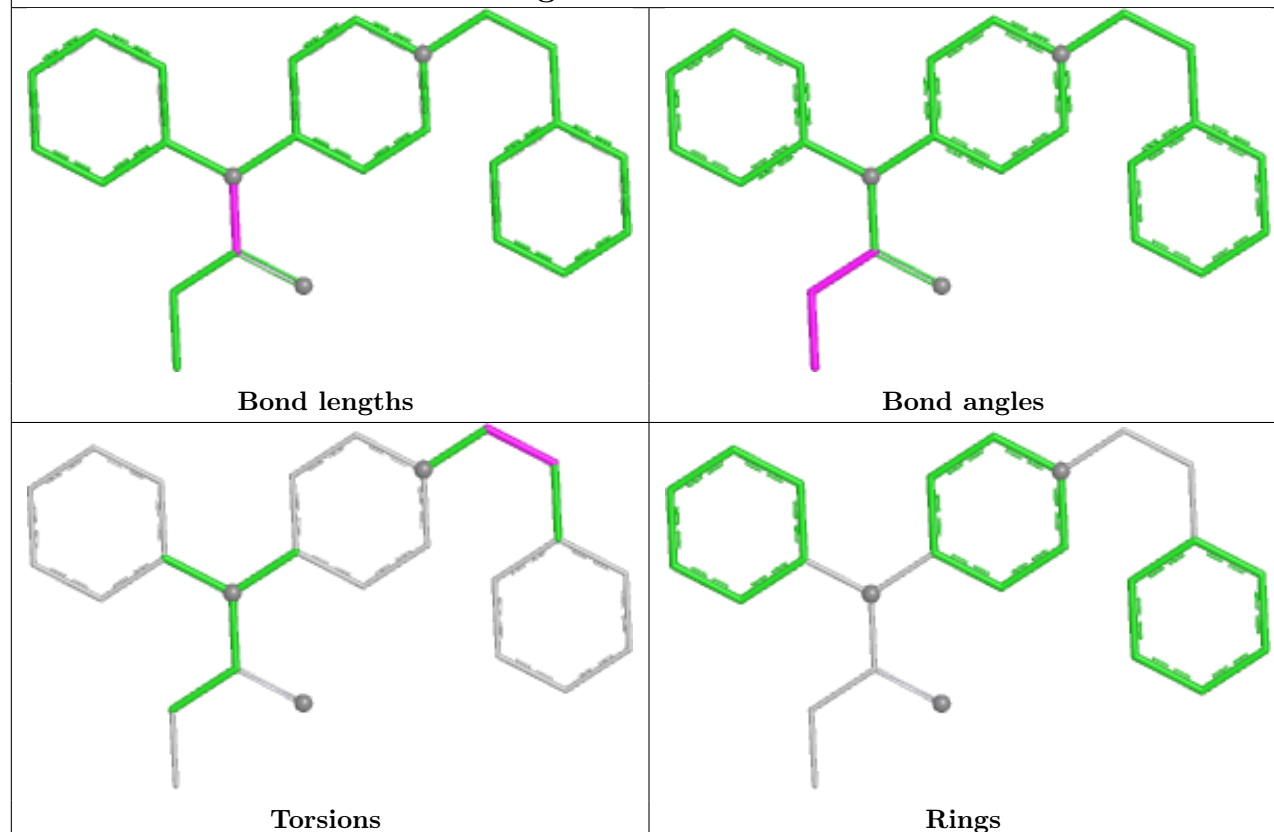
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



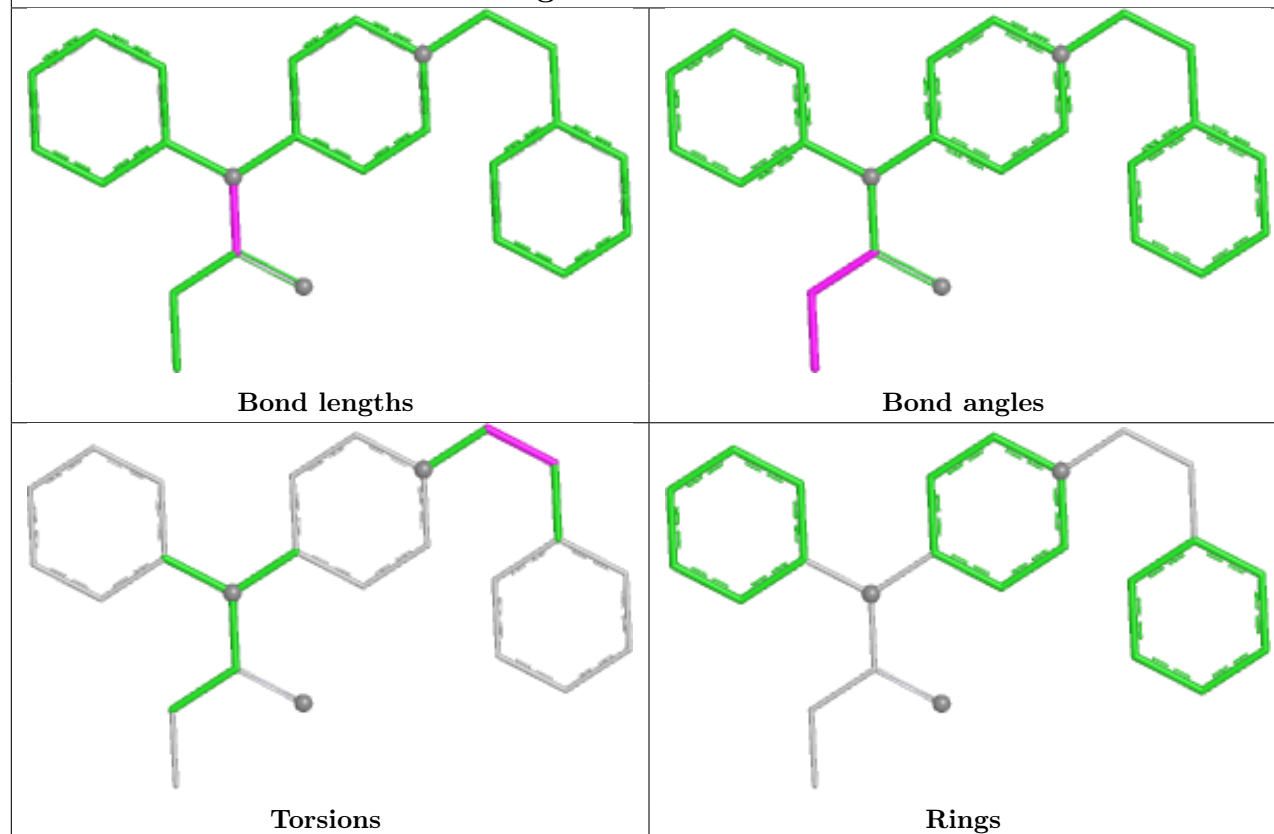
Ligand 7V7 C 301



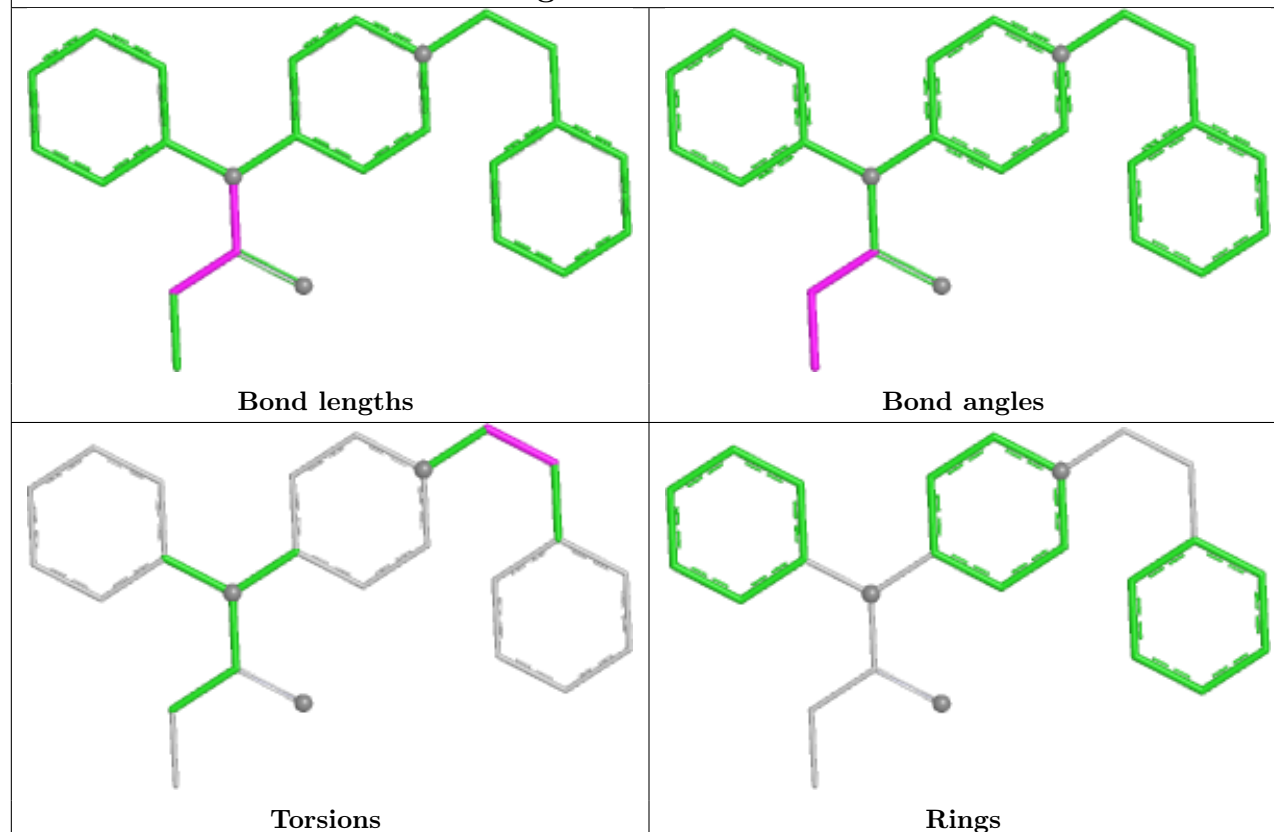
Ligand 7V7 O 301



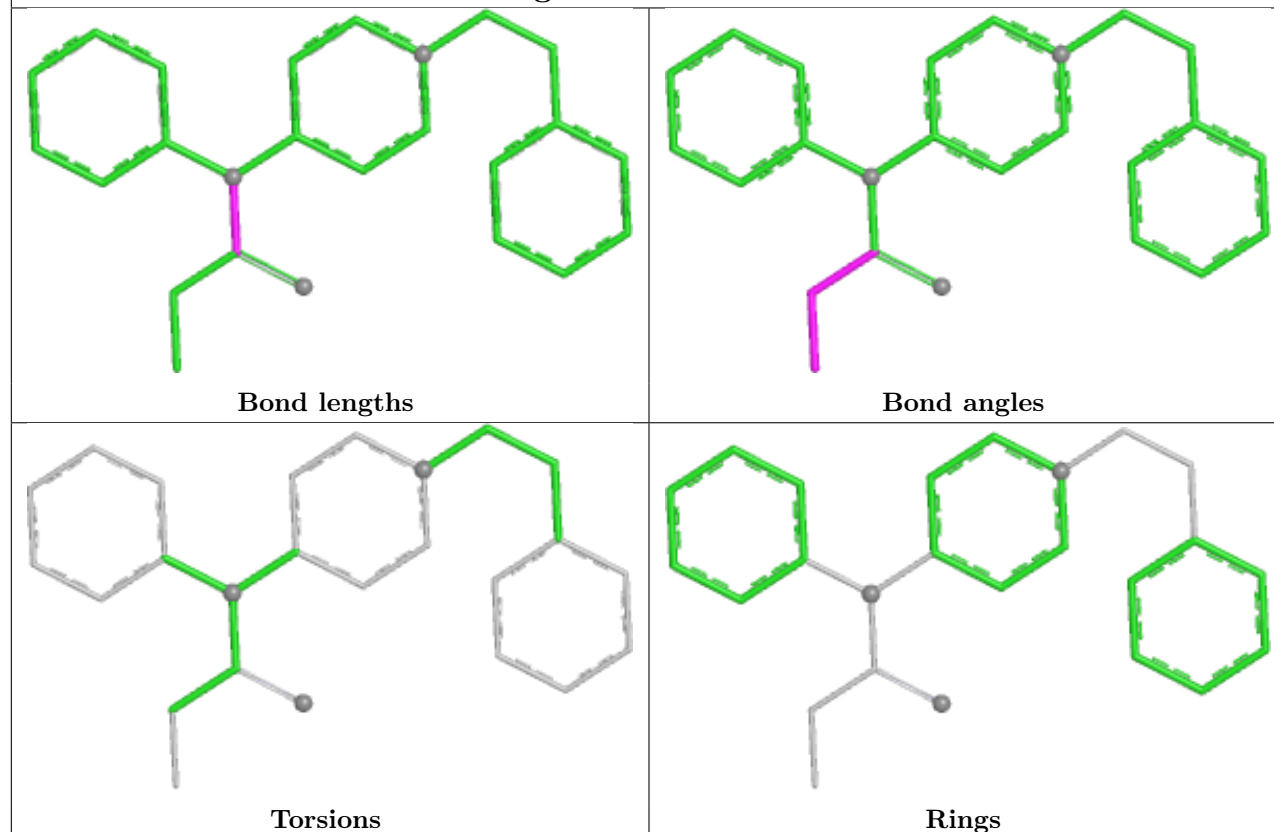
Ligand 7V7 G 301



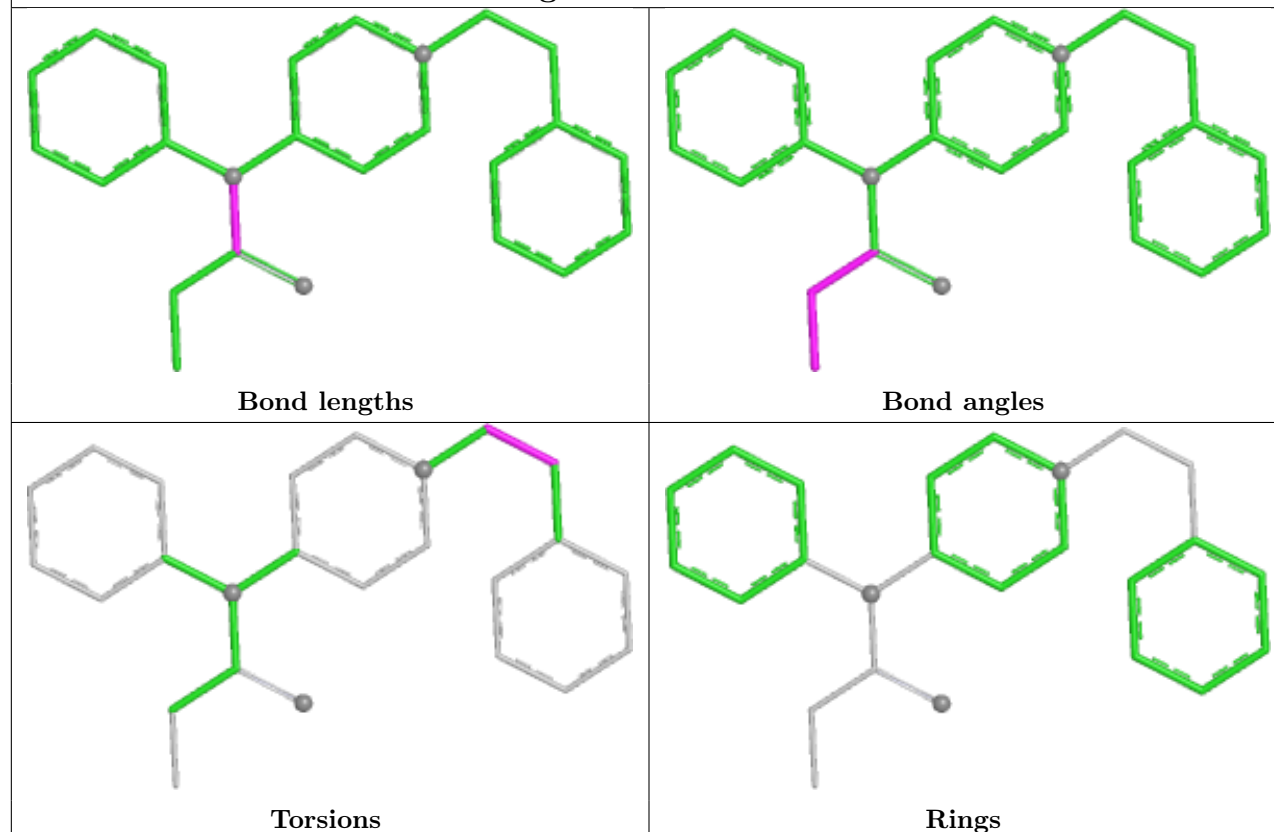
Ligand 7V7 A 301



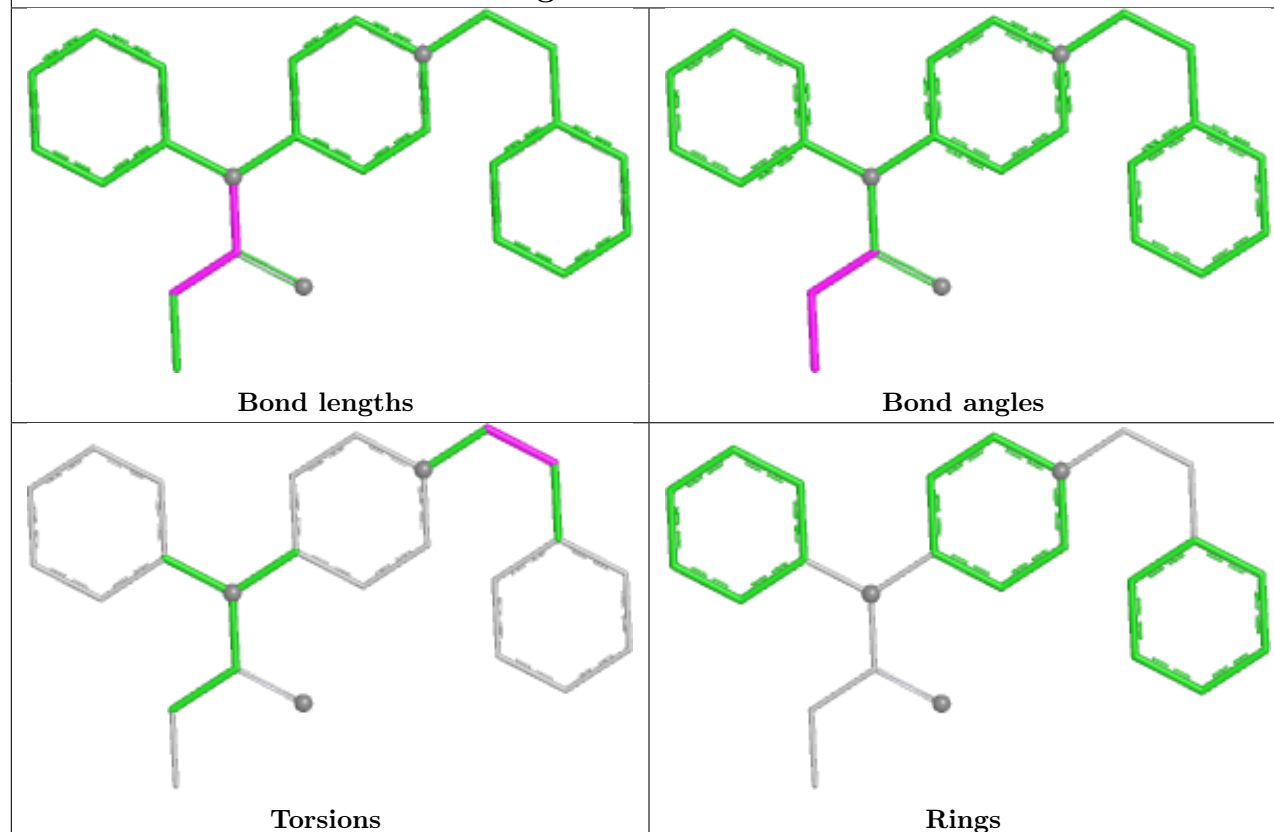
Ligand 7V7 M 301



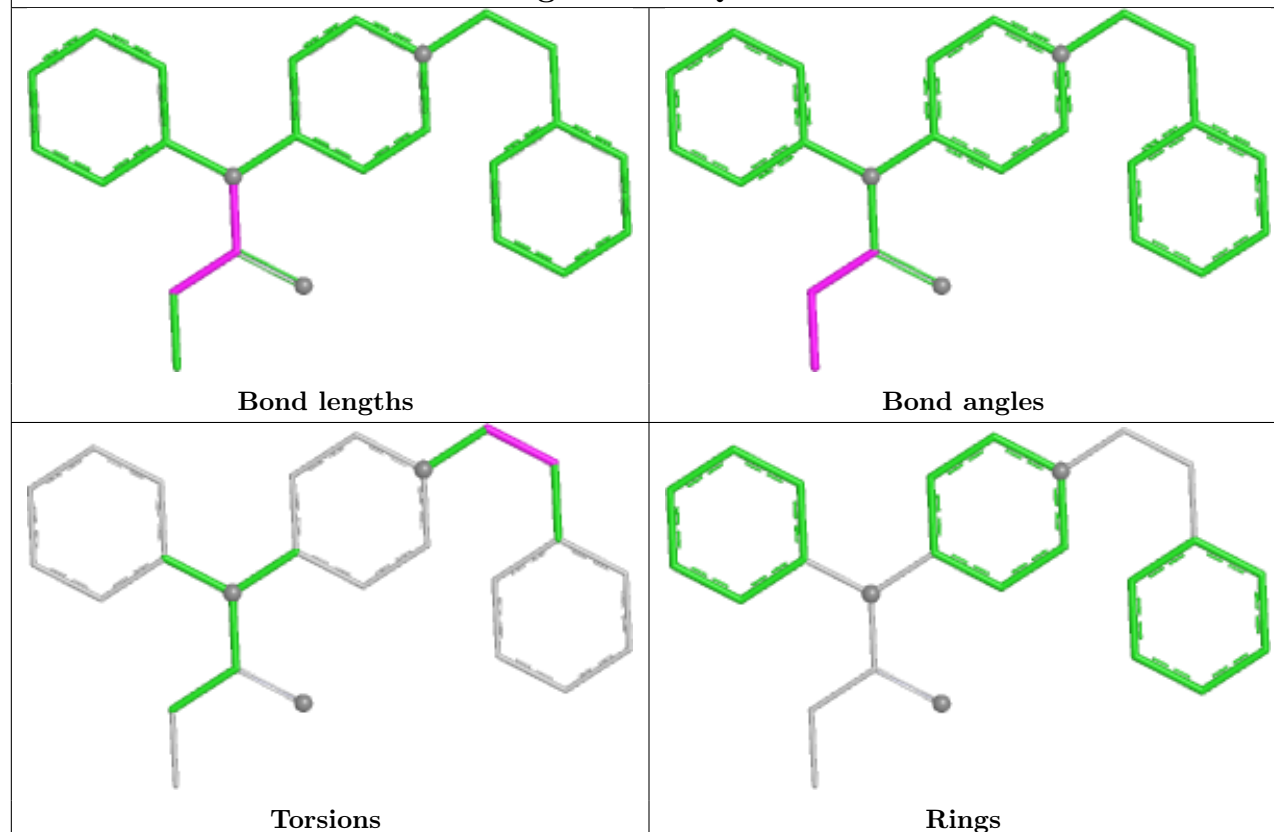
Ligand 7V7 E 301



Ligand 7V7 K 301



Ligand 7V7 Q 301



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/226 (98%)	-1.35	0 100 100	10, 17, 36, 57	0
1	C	222/226 (98%)	-1.12	0 100 100	18, 27, 48, 74	0
1	E	222/226 (98%)	-1.33	0 100 100	9, 17, 40, 64	0
1	G	222/226 (98%)	-0.90	1 (0%) 87 90	12, 21, 42, 72	0
1	I	222/226 (98%)	-1.37	0 100 100	8, 15, 34, 56	0
1	K	222/226 (98%)	-1.30	0 100 100	9, 17, 42, 68	0
1	M	222/226 (98%)	-1.03	0 100 100	19, 28, 49, 73	0
1	O	222/226 (98%)	-1.32	0 100 100	9, 18, 39, 68	0
1	Q	222/226 (98%)	-1.38	0 100 100	9, 16, 36, 59	0
2	B	216/219 (98%)	-1.36	0 100 100	8, 19, 35, 45	1 (0%)
2	D	216/219 (98%)	-1.06	0 100 100	17, 31, 52, 63	1 (0%)
2	F	216/219 (98%)	-1.33	0 100 100	8, 19, 36, 46	1 (0%)
2	H	216/219 (98%)	-0.85	0 100 100	12, 25, 43, 56	1 (0%)
2	J	216/219 (98%)	-1.35	0 100 100	9, 19, 34, 44	1 (0%)
2	L	216/219 (98%)	-1.32	0 100 100	9, 20, 37, 45	1 (0%)
2	N	216/219 (98%)	-0.98	0 100 100	19, 33, 52, 61	1 (0%)
2	P	216/219 (98%)	-1.34	0 100 100	8, 20, 36, 45	1 (0%)
2	R	216/219 (98%)	-1.37	0 100 100	8, 18, 35, 43	1 (0%)
All	All	3942/4005 (98%)	-1.23	1 (0%) 100 100	8, 21, 43, 74	9 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	215	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	A	303	4/4	0.98	0.06	34,36,40,43	0
4	ACT	A	304	4/4	0.98	0.05	30,30,34,34	0
4	ACT	B	304	4/4	0.98	0.06	26,32,37,41	0
4	ACT	F	303	4/4	0.98	0.05	24,33,35,35	0
4	ACT	K	304	4/4	0.98	0.04	25,29,32,32	0
4	ACT	L	304	4/4	0.98	0.04	26,29,32,33	0
4	ACT	O	303	4/4	0.98	0.07	18,21,23,23	0
4	ACT	O	304	4/4	0.98	0.05	26,30,34,37	0
4	ACT	P	305	4/4	0.98	0.05	23,26,34,35	0
4	ACT	P	307	4/4	0.98	0.07	26,30,41,42	0
3	7V7	M	301	25/25	0.99	0.05	29,41,63,67	0
4	ACT	B	305	4/4	0.99	0.04	25,28,32,35	0
4	ACT	B	306	4/4	0.99	0.05	41,51,52,56	0
4	ACT	C	302	4/4	0.99	0.05	29,33,39,41	0
4	ACT	E	303	4/4	0.99	0.06	19,23,23,23	0
4	ACT	E	304	4/4	0.99	0.06	25,27,28,29	0
3	7V7	C	301	25/25	0.99	0.04	23,36,63,64	0
4	ACT	F	304	4/4	0.99	0.05	16,20,21,23	0
4	ACT	F	305	4/4	0.99	0.06	30,31,35,36	0
4	ACT	G	302	4/4	0.99	0.05	23,23,32,35	0
4	ACT	G	303	4/4	0.99	0.04	31,33,34,34	0
4	ACT	H	305	4/4	0.99	0.03	19,21,23,25	0
4	ACT	H	306	4/4	0.99	0.04	27,28,37,41	0
4	ACT	H	307	4/4	0.99	0.05	35,40,41,48	0
4	ACT	H	308	4/4	0.99	0.05	32,34,40,40	0
4	ACT	H	309	4/4	0.99	0.05	30,37,39,44	0
4	ACT	H	310	4/4	0.99	0.05	27,34,35,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACT	I	303	4/4	0.99	0.05	30,30,30,31	0
4	ACT	J	304	4/4	0.99	0.05	23,32,35,38	0
4	ACT	J	305	4/4	0.99	0.04	27,28,37,43	0
3	7V7	G	301	25/25	0.99	0.06	19,28,57,60	0
4	ACT	L	302	4/4	0.99	0.03	11,13,13,17	0
4	ACT	L	303	4/4	0.99	0.05	21,24,25,33	0
4	ACT	A	305	4/4	0.99	0.05	29,32,35,37	0
4	ACT	L	305	4/4	0.99	0.04	24,33,40,40	0
4	ACT	M	302	4/4	0.99	0.06	23,24,24,25	0
4	ACT	M	303	4/4	0.99	0.05	19,36,42,42	0
4	ACT	O	302	4/4	0.99	0.04	19,24,32,34	0
4	ACT	A	306	4/4	0.99	0.07	27,28,32,51	0
4	ACT	B	301	4/4	0.99	0.04	19,20,22,24	0
4	ACT	P	304	4/4	0.99	0.06	20,23,27,31	0
4	ACT	B	302	4/4	0.99	0.04	21,30,33,43	0
4	ACT	P	306	4/4	0.99	0.09	22,25,32,38	0
4	ACT	B	303	4/4	0.99	0.04	27,29,34,35	0
4	ACT	Q	303	4/4	0.99	0.02	11,12,12,14	0
4	ACT	Q	305	4/4	0.99	0.06	25,33,33,38	0
4	ACT	Q	306	4/4	0.99	0.05	28,33,34,37	0
4	ACT	Q	307	4/4	0.99	0.05	26,29,34,34	0
4	ACT	R	303	4/4	0.99	0.06	16,20,23,24	0
4	ACT	R	304	4/4	0.99	0.04	26,37,38,40	0
4	ACT	R	305	4/4	0.99	0.06	23,27,35,36	0
4	ACT	R	306	4/4	0.99	0.03	25,27,29,33	0
4	ACT	R	307	4/4	0.99	0.08	21,27,34,36	0
5	NA	H	301	1/1	0.99	0.03	29,29,29,29	0
5	NA	H	302	1/1	0.99	0.05	33,33,33,33	0
5	NA	P	301	1/1	0.99	0.02	27,27,27,27	0
3	7V7	Q	301	25/25	1.00	0.03	11,16,36,40	0
4	ACT	F	302	4/4	1.00	0.02	11,13,14,15	0
4	ACT	Q	304	4/4	1.00	0.02	21,23,25,28	0
4	ACT	A	302	4/4	1.00	0.04	23,23,24,30	0
3	7V7	A	301	25/25	1.00	0.03	12,15,32,37	0
3	7V7	I	301	25/25	1.00	0.02	12,17,36,38	0
4	ACT	R	302	4/4	1.00	0.03	12,12,13,19	0
4	ACT	I	302	4/4	1.00	0.03	20,21,23,29	0
3	7V7	K	301	25/25	1.00	0.03	14,19,40,45	0
4	ACT	J	303	4/4	1.00	0.02	11,13,13,15	0
3	7V7	E	301	25/25	1.00	0.03	12,16,36,38	0
4	ACT	P	303	4/4	1.00	0.02	11,13,15,16	0
5	NA	D	301	1/1	1.00	0.01	21,21,21,21	0

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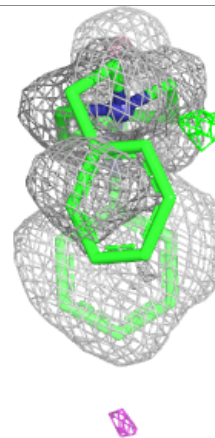
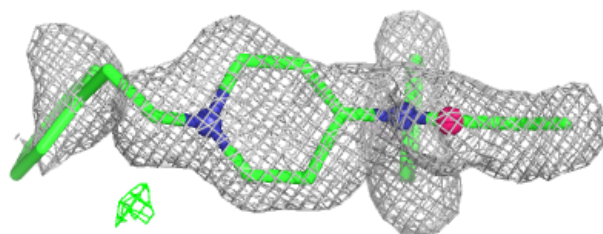
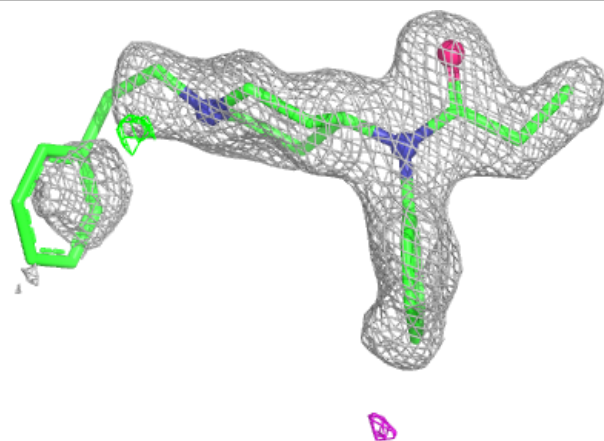
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	E	302	1/1	1.00	0.02	20,20,20,20	0
5	NA	F	301	1/1	1.00	0.01	11,11,11,11	0
4	ACT	H	304	4/4	1.00	0.03	12,16,17,18	0
4	ACT	K	303	4/4	1.00	0.05	22,22,22,26	0
5	NA	H	303	1/1	1.00	0.03	15,15,15,15	0
5	NA	J	301	1/1	1.00	0.01	26,26,26,26	0
5	NA	J	302	1/1	1.00	0.01	14,14,14,14	0
5	NA	K	302	1/1	1.00	0.03	20,20,20,20	0
5	NA	L	301	1/1	1.00	0.01	13,13,13,13	0
3	7V7	O	301	25/25	1.00	0.03	14,19,43,45	0
5	NA	P	302	1/1	1.00	0.01	12,12,12,12	0
5	NA	Q	302	1/1	1.00	0.01	12,12,12,12	0
5	NA	R	301	1/1	1.00	0.01	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.

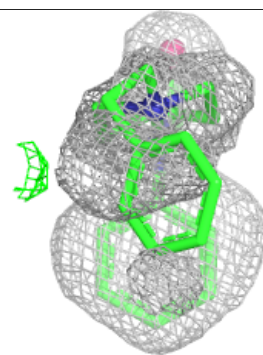
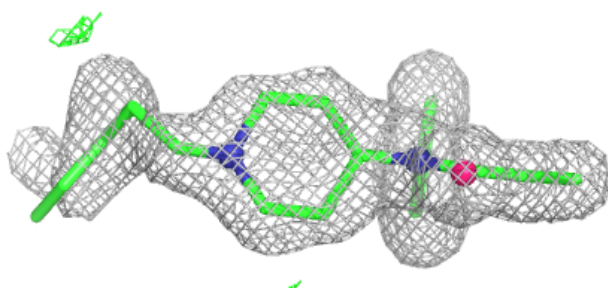
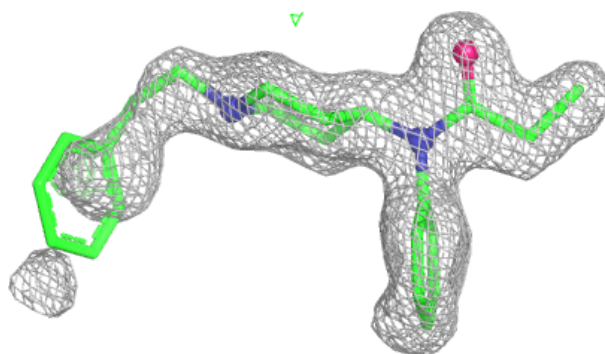
Electron density around 7V7 M 301:

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

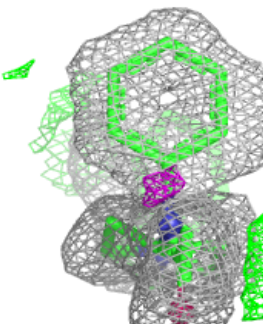
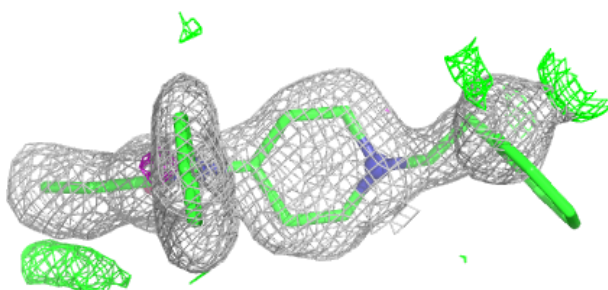
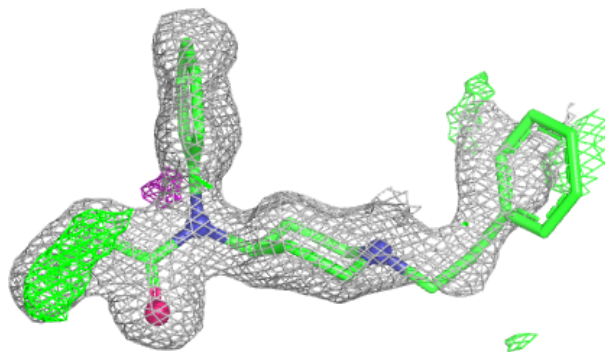


Electron density around 7V7 C 301:

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

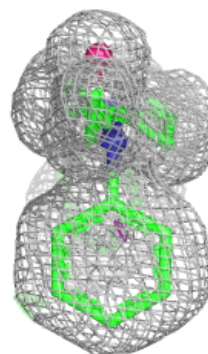
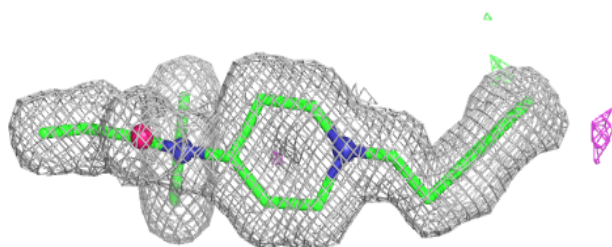
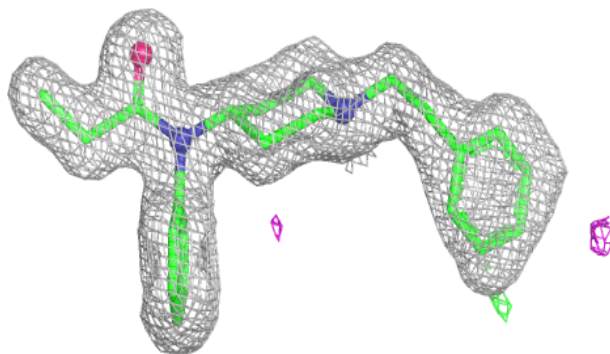
**Electron density around 7V7 G 301:**

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and green (positive)

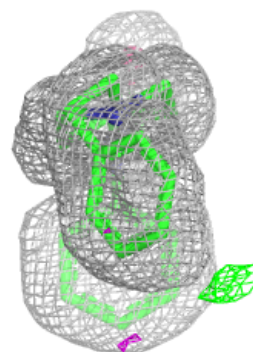
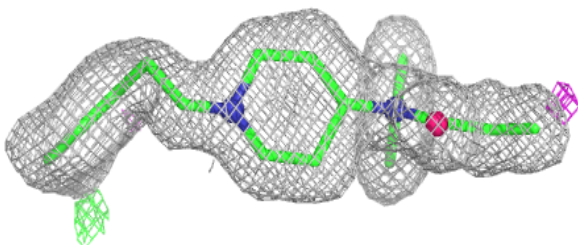
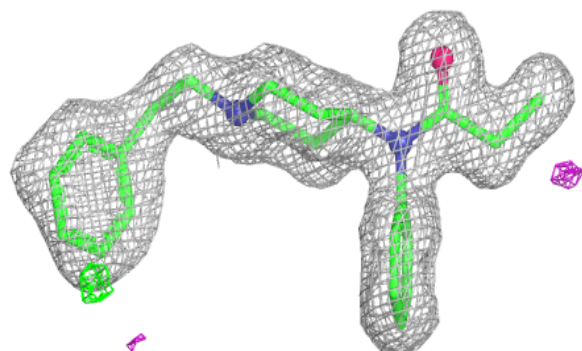


Electron density around 7V7 Q 301:

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

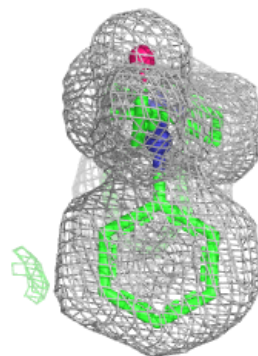
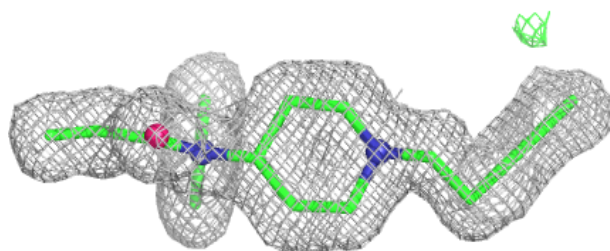
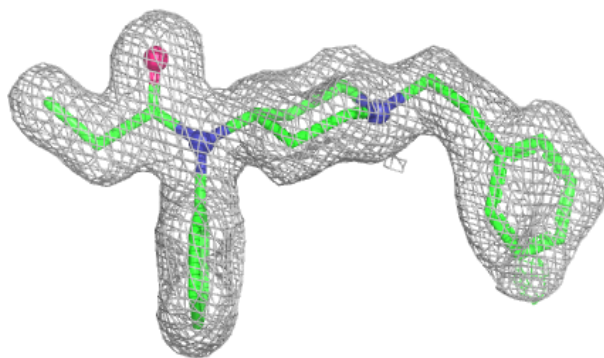
**Electron density around 7V7 A 301:**

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

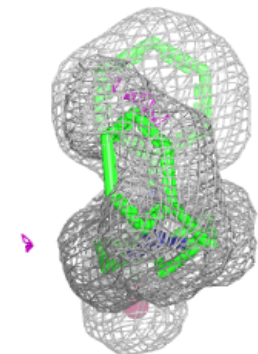
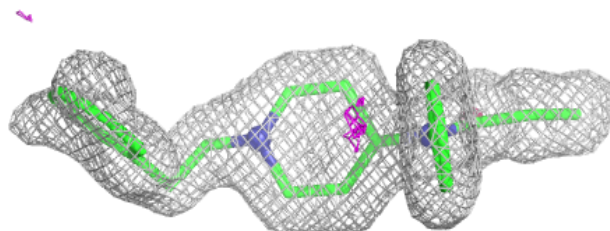
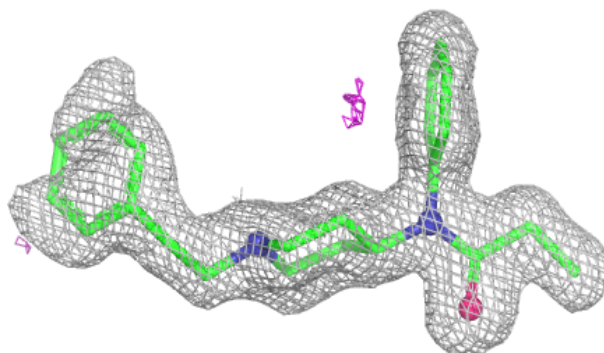


Electron density around 7V7 I 301:

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

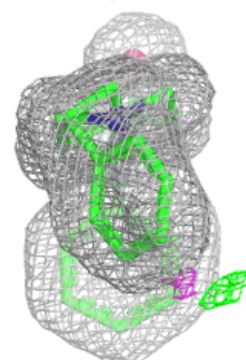
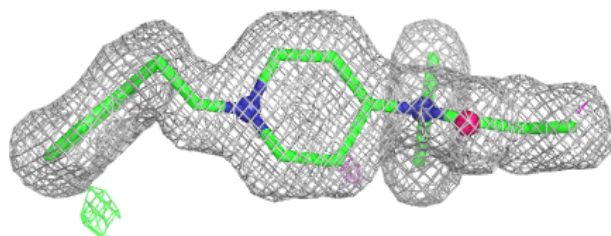
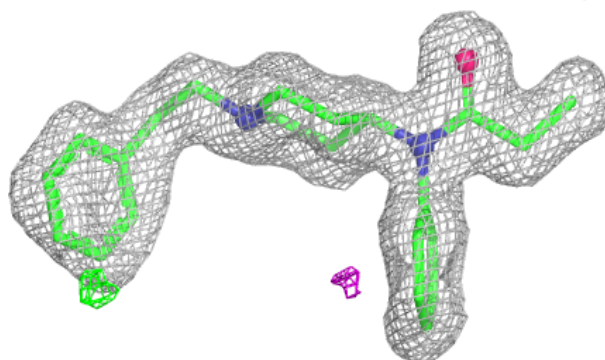
**Electron density around 7V7 K 301:**

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and green (positive)

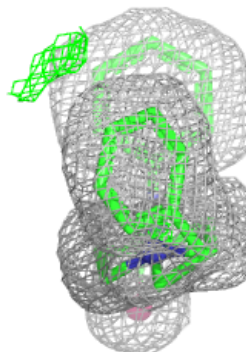
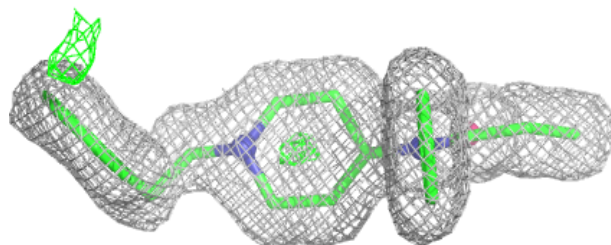
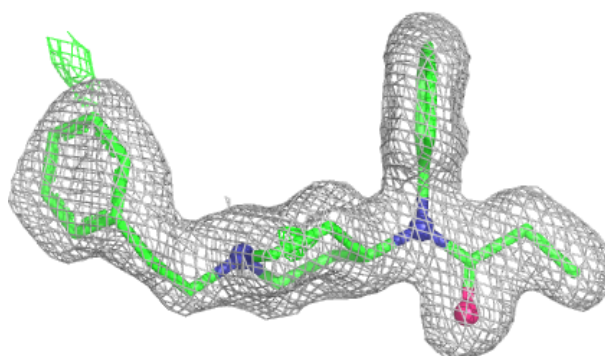


Electron density around 7V7 E 301:

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

**Electron density around 7V7 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.