Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2020 – 09:08 PM BST

PDB ID	:	6TBI
Title	:	Structure of a beta galactosidase with inhibitor
Authors	:	Offen, W.; Davies, G.
Deposited on	:	2019-11-01
Resolution	:	1.46 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 following versions of software and data (see references ①) were used in the production of this report:

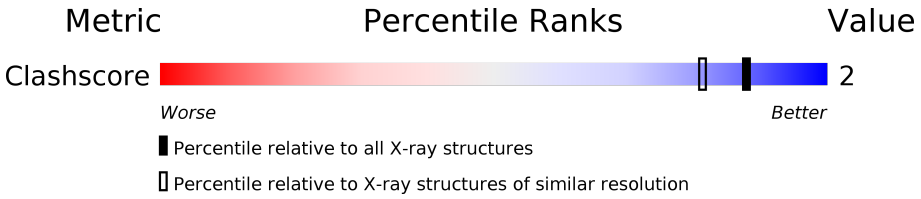
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.3.dev2

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 1.46 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))
Clashscore	141614	1202 (1.46-1.46)

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 on 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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	550	93% 5%
1	B	550	93% 5%
1	C	550	94%
1	D	550	94%
1	E	550	94%
1	F	550	93%
1	G	550	94%
1	H	550	93% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40015 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 Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	8	0
			4289	2745	725	803	16			
1	B	534	Total	C	N	O	S	0	9	0
			4266	2729	725	795	17			
1	C	536	Total	C	N	O	S	0	10	0
			4313	2757	741	799	16			
1	D	539	Total	C	N	O	S	0	11	0
			4317	2761	730	810	16			
1	E	538	Total	C	N	O	S	0	9	0
			4305	2758	727	803	17			
1	F	539	Total	C	N	O	S	0	20	0
			4406	2814	754	822	16			
1	G	540	Total	C	N	O	S	0	17	0
			4382	2800	745	820	17			
1	H	538	Total	C	N	O	S	0	16	0
			4356	2785	742	812	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	5	Total Na 5 5	0	0
2	D	6	Total Na 6 6	0	0
2	E	6	Total Na 6 6	0	0
2	H	5	Total Na 5 5	0	0
2	B	4	Total Na 4 4	0	0
2	C	4	Total Na 4 4	0	0
2	A	4	Total Na 4 4	0	0

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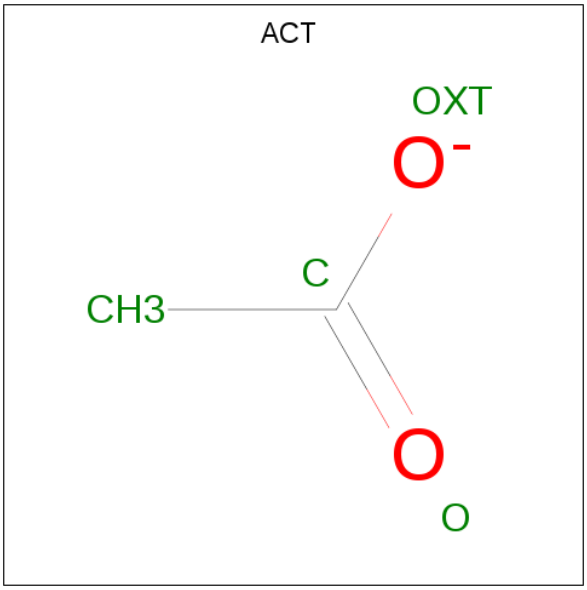
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	4	Total Na 4 4	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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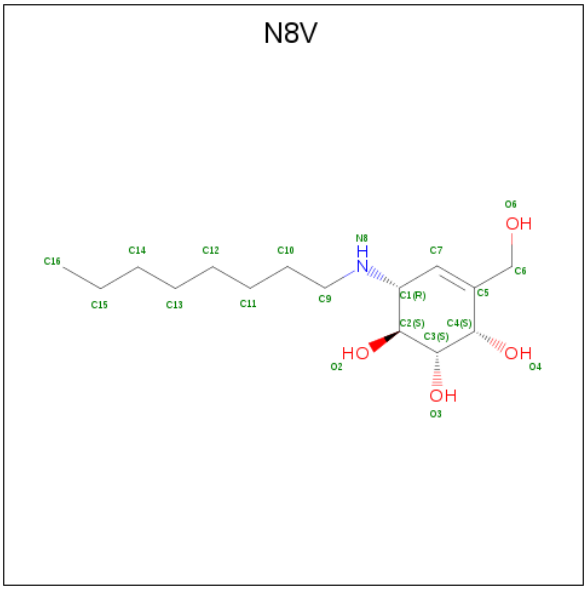
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is (1S,2S,3S,6R)-4-(hydroxymethyl)-6-(octylamino)cyclohex-4-ene-1,2,3-triol (three-letter code: N8V) (formula: $C_{15}H_{29}NO_4$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 20 15 1 4	0	0
4	B	1	Total C N O 20 15 1 4	0	0
4	C	1	Total C N O 16 11 1 4	0	0
4	D	1	Total C N O 20 15 1 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C N O 14 9 1 4	0	0
4	F	1	Total C N O 20 15 1 4	0	0
4	G	1	Total C N O 20 15 1 4	0	0
4	H	1	Total C N O 20 15 1 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	504	Total O 505 505	0	1
5	B	590	Total O 590 590	0	0
5	C	606	Total O 608 608	0	2
5	D	709	Total O 713 713	0	4
5	E	715	Total O 720 720	0	5
5	F	669	Total O 672 672	0	3
5	G	719	Total O 721 721	0	2
5	H	595	Total O 596 596	0	1

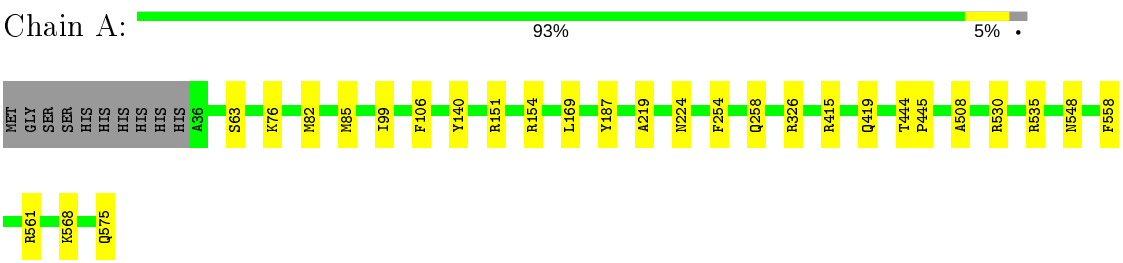
3 Residue-property plots

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. 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. 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.

Note EDS failed to run properly.

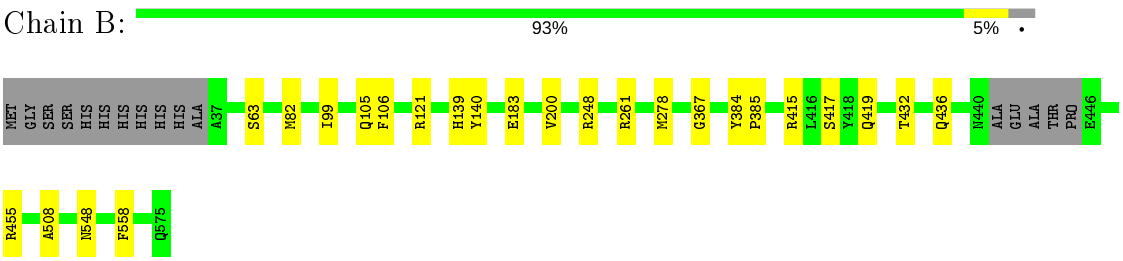
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain A:



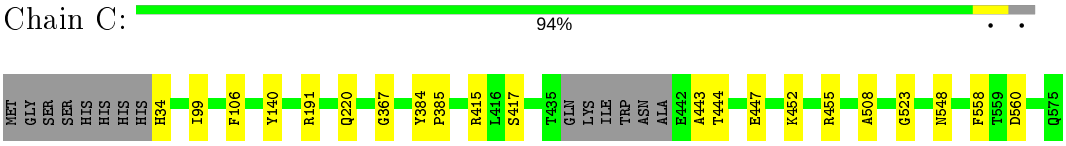
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain B:



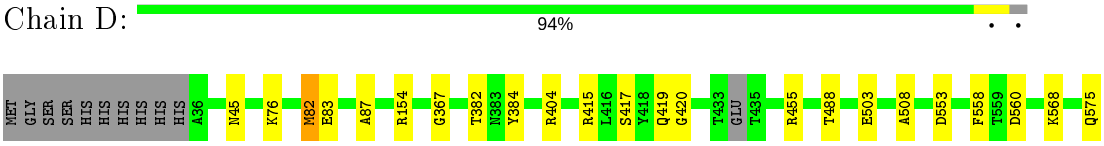
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain C:



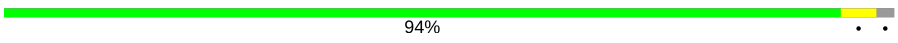
- Molecule 1: Beta-galactosidase, putative, bgl35A

Chain D:



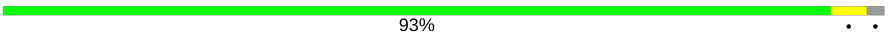
- Molecule 1: Beta-galactosidase, putative, bgl35A

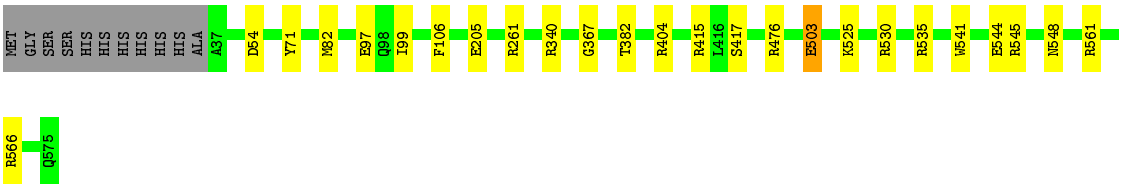
Chain E:



• Molecule 1: Beta-galactosidase, putative, bgl35A

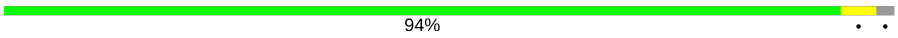
Chain F:

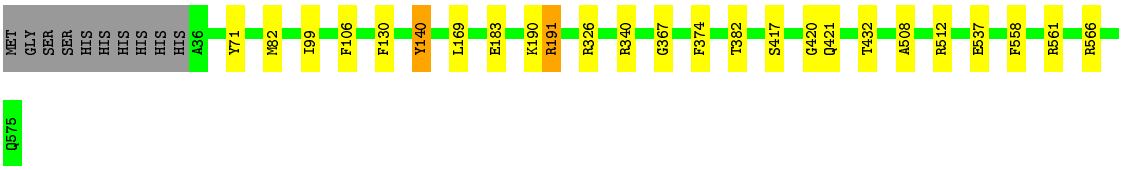




• Molecule 1: Beta-galactosidase, putative, bgl35A

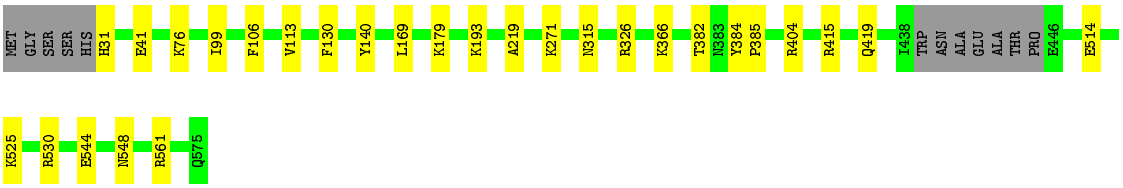
Chain G:





• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.12Å 115.91Å 116.10Å 90.20° 89.96° 90.08°	Depositor
Resolution (Å)	116.10 – 1.46	Depositor
% Data completeness (in resolution range)	96.3 (116.10-1.46)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.126 , 0.172	Depositor
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.219	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-l,k 0.000 for h,l,-k 0.000 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l 0.000 for -h,-l,-k 0.000 for -h,l,k	Xtriage
Total number of atoms	40015	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NA, N8V, 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	0.88	2/4403 (0.0%)	1.01	8/6002 (0.1%)
1	B	0.88	2/4378 (0.0%)	1.01	3/5965 (0.1%)
1	C	0.86	2/4428 (0.0%)	1.00	1/6026 (0.0%)
1	D	0.91	2/4433 (0.0%)	1.06	7/6039 (0.1%)
1	E	0.93	1/4418 (0.0%)	1.09	5/6014 (0.1%)
1	F	0.91	5/4523 (0.1%)	1.08	13/6153 (0.2%)
1	G	0.91	2/4495 (0.0%)	1.09	13/6116 (0.2%)
1	H	0.91	4/4475 (0.1%)	0.99	4/6094 (0.1%)
All	All	0.90	20/35553 (0.1%)	1.04	54/48409 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	544	GLU	CD-OE2	-7.13	1.17	1.25
1	F	525	LYS	CG-CD	-6.68	1.29	1.52
1	F	97	GLU	CD-OE2	-6.52	1.18	1.25
1	G	183	GLU	CD-OE2	-6.46	1.18	1.25
1	F	544	GLU	CD-OE2	-6.24	1.18	1.25
1	F	503	GLU	CD-OE1	6.20	1.32	1.25
1	C	523	GLY	C-O	6.04	1.33	1.23
1	H	326	ARG	C-O	5.80	1.34	1.23
1	H	41	GLU	CD-OE2	5.71	1.31	1.25
1	B	63	SER	CB-OG	-5.67	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	560	ASP	CG-OD1	-5.50	1.12	1.25
1	G	537	GLU	CD-OE2	5.35	1.31	1.25
1	E	397	GLU	CD-OE1	5.31	1.31	1.25
1	B	183	GLU	CD-OE2	-5.29	1.19	1.25
1	A	326	ARG	C-O	5.23	1.33	1.23
1	A	575	GLN	C-O	5.22	1.33	1.23
1	F	205	GLU	CD-OE1	5.13	1.31	1.25
1	D	560	ASP	CG-OD2	-5.10	1.13	1.25
1	D	503	GLU	CD-OE2	5.09	1.31	1.25
1	H	514	GLU	CD-OE1	5.03	1.31	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	512	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	H	404	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	E	561	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	G	561	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	530	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	E	561	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	G	326	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	E	530[A]	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	E	530[B]	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	D	82	MET	CG-SD-CE	-6.90	89.16	100.20
1	D	455	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	F	561	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	121	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	F	525	LYS	CB-CG-CD	6.57	128.69	111.60
1	G	130	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	F	404	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	455	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	F	476	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	G	340	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	F	561	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	G	561	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	G	326	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	H	561	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	561	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	535	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	154	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	H	130	PHE	CB-CG-CD1	5.94	124.96	120.80
1	C	191	ARG	NE-CZ-NH2	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	415	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	F	261	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	F	535	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	H	530	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	G	566	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	E	285	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	82	MET	CG-SD-CE	-5.65	91.16	100.20
1	D	154	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	553	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	384	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	151	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	F	340	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	G	140	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	F	545	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	404	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	561	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	F	82	MET	CG-SD-CE	-5.25	91.80	100.20
1	F	530[A]	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	F	530[B]	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	F	545	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	566	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	187	TYR	CB-CG-CD1	-5.06	117.97	121.00
1	G	130	PHE	CB-CG-CD1	5.05	124.33	120.80
1	G	71	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	B	261	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	G	191	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	71	TYR	Sidechain

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	4289	0	4100	15	0
1	B	4266	0	4088	19	0
1	C	4313	0	4151	15	0
1	D	4317	0	4139	18	0
1	E	4305	0	4150	14	0
1	F	4406	0	4232	11	0
1	G	4382	0	4206	18	0
1	H	4356	0	4161	28	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	6	0	0	0	0
2	E	6	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	4	0	3	0	0
3	B	8	0	6	1	0
3	C	4	0	3	0	0
3	D	8	0	6	0	0
3	E	16	0	12	0	0
3	F	8	0	6	0	0
3	G	16	0	12	1	0
3	H	4	0	3	0	0
4	A	20	0	29	0	0
4	B	20	0	29	0	0
4	C	16	0	18	0	0
4	D	20	0	29	1	0
4	E	14	0	14	0	0
4	F	20	0	29	0	0
4	G	20	0	29	1	0
4	H	20	0	29	0	0
5	A	505	0	0	3	0
5	B	590	0	0	10	0
5	C	608	0	0	6	0
5	D	713	0	0	17	0
5	E	720	0	0	9	0
5	F	672	0	0	5	0
5	G	721	0	0	10	0
5	H	596	0	0	21	0
All	All	40015	0	33484	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:503:GLU:OE2	1:F:566[A]:ARG:HD3	1.46	1.10
1:G:421:GLN:HA	5:G:703:HOH:O	1.52	1.09
1:B:248:ARG:HD2	5:B:1135:HOH:O	1.52	1.08
1:C:452:LYS:HE2	5:C:1086:HOH:O	1.56	1.06
1:G:421:GLN:HG2	5:G:703:HOH:O	1.60	0.99
1:H:31:HIS:ND1	5:H:702:HOH:O	2.03	0.92
1:H:415[B]:ARG:NH2	5:H:701:HOH:O	1.74	0.89
1:B:105:GLN:HG3	5:B:1230:HOH:O	1.77	0.85
1:F:503:GLU:OE2	1:F:566[A]:ARG:CD	2.25	0.84
1:E:76:LYS:HE2	5:E:940:HOH:O	1.78	0.84
1:B:419[B]:GLN:CG	5:B:717:HOH:O	2.24	0.83
1:D:76:LYS:HE2	5:D:936:HOH:O	1.80	0.80
3:B:603:ACT:OXT	5:B:701:HOH:O	1.99	0.79
1:H:179:LYS:CD	5:H:824:HOH:O	2.33	0.76
1:F:382[B]:THR:HG22	5:F:899:HOH:O	1.86	0.75
1:B:419[B]:GLN:HG2	5:B:717:HOH:O	1.87	0.74
1:D:420:GLY:N	5:D:701:HOH:O	2.22	0.71
1:B:82[B]:MET:HG2	5:B:789:HOH:O	1.90	0.71
1:D:419[A]:GLN:C	5:D:701:HOH:O	2.29	0.70
4:D:609:N8V:H18	5:D:1017:HOH:O	1.92	0.70
1:E:415:ARG:CZ	5:E:702:HOH:O	2.39	0.70
1:E:415:ARG:NH1	5:E:702:HOH:O	2.24	0.69
1:H:193:LYS:HD2	5:H:702:HOH:O	1.92	0.69
1:C:220:GLN:HG3	5:C:1018:HOH:O	1.93	0.69
1:D:420:GLY:CA	5:D:701:HOH:O	2.40	0.69
1:H:525[A]:LYS:CE	5:H:714:HOH:O	2.40	0.68
1:C:220:GLN:CG	5:C:1018:HOH:O	2.41	0.68
1:H:76:LYS:CE	5:H:956:HOH:O	2.41	0.68
1:D:575:GLN:OE1	1:D:575:GLN:HA	1.93	0.67
1:D:382[B]:THR:HG22	5:D:1067:HOH:O	1.94	0.67
1:D:488[B]:THR:HG23	5:D:1255:HOH:O	1.95	0.66
1:H:415[A]:ARG:NH1	5:H:706:HOH:O	2.30	0.65
1:A:76:LYS:CE	5:A:886:HOH:O	2.45	0.65
1:A:224:ASN:HB3	5:A:1100:HOH:O	1.97	0.64
1:D:76:LYS:NZ	5:D:704:HOH:O	2.30	0.64
1:C:34:HIS:HB3	5:D:869:HOH:O	1.99	0.62
1:H:415[A]:ARG:CZ	5:H:706:HOH:O	2.47	0.61
1:H:366:LYS:CE	5:H:703:HOH:O	2.49	0.61
1:G:382[A]:THR:HG22	5:G:1081:HOH:O	2.01	0.60
1:D:415:ARG:CZ	5:D:707:HOH:O	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:THR:HG23	1:B:436:GLN:HB2	1.86	0.56
1:A:415:ARG:HD2	1:A:419:GLN:CD	2.26	0.56
1:C:444:THR:CB	1:C:447:GLU:HG3	2.35	0.56
1:E:63[A]:SER:OG	1:E:82[A]:MET:SD	2.65	0.55
1:E:525[B]:LYS:HD3	1:E:574:VAL:HG11	1.89	0.54
1:G:421:GLN:CG	5:G:703:HOH:O	2.36	0.54
1:H:193:LYS:HE2	5:H:961:HOH:O	2.06	0.54
1:H:99:ILE:O	1:H:106:PHE:HA	2.08	0.54
1:F:382[B]:THR:CG2	5:F:899:HOH:O	2.47	0.53
1:D:419[B]:GLN:C	5:D:701:HOH:O	2.45	0.53
1:H:193:LYS:CD	5:H:702:HOH:O	2.54	0.52
1:D:415:ARG:NE	5:D:707:HOH:O	2.41	0.52
1:H:525[A]:LYS:HE3	5:H:714:HOH:O	2.07	0.52
1:H:382[B]:THR:HG22	5:H:1057:HOH:O	2.09	0.51
1:H:366:LYS:NZ	5:H:703:HOH:O	2.24	0.51
1:H:415[B]:ARG:HD3	5:H:701:HOH:O	2.11	0.51
1:H:193:LYS:CE	5:H:961:HOH:O	2.58	0.51
1:A:99:ILE:O	1:A:106:PHE:HA	2.11	0.51
1:G:420:GLY:N	5:G:709:HOH:O	2.44	0.50
1:A:415:ARG:HD2	1:A:419:GLN:NE2	2.26	0.50
1:E:419:GLN:C	5:E:706:HOH:O	2.49	0.49
1:E:83:GLU:OE1	5:E:701:HOH:O	2.19	0.49
1:G:420:GLY:CA	5:G:709:HOH:O	2.59	0.49
1:G:421:GLN:CA	5:G:703:HOH:O	2.28	0.48
1:C:415[A]:ARG:CZ	5:C:710:HOH:O	2.62	0.48
1:F:415[A]:ARG:CZ	5:F:729:HOH:O	2.62	0.47
1:E:444:THR:OG1	1:E:447:GLU:HG3	2.13	0.47
1:A:444:THR:HB	1:A:445:PRO:HD2	1.95	0.47
1:D:45:ASN:ND2	5:D:711:HOH:O	2.47	0.47
1:C:415[A]:ARG:NH2	5:C:710:HOH:O	2.48	0.47
1:C:443:ALA:HB1	1:C:447:GLU:HB2	1.96	0.47
1:E:420:GLY:N	5:E:706:HOH:O	2.48	0.47
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.50	0.47
1:G:420:GLY:O	5:G:703:HOH:O	2.20	0.47
1:G:432:THR:OG1	3:G:604:ACT:O	2.26	0.47
1:H:31:HIS:CE1	5:H:702:HOH:O	2.60	0.47
1:B:432:THR:CG2	1:B:436:GLN:HB2	2.45	0.46
1:C:99:ILE:O	1:C:106:PHE:HA	2.16	0.46
1:H:366:LYS:CD	5:H:703:HOH:O	2.63	0.46
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.50	0.46
1:B:248:ARG:CD	5:B:1135:HOH:O	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:TYR:CD1	1:B:385:PRO:HA	2.51	0.46
1:A:415:ARG:HD2	1:A:419:GLN:OE1	2.16	0.46
1:B:455:ARG:NH1	5:B:707:HOH:O	2.44	0.45
1:B:248:ARG:CG	5:B:1135:HOH:O	2.61	0.45
1:H:193:LYS:HD2	5:H:961:HOH:O	2.17	0.45
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.52	0.45
1:G:99:ILE:O	1:G:106:PHE:HA	2.17	0.45
1:F:541:TRP:CB	1:F:566[A]:ARG:HH21	2.29	0.45
1:A:169:LEU:HD13	1:A:219:ALA:HA	1.97	0.44
1:E:329:LYS:HD3	5:E:1327:HOH:O	2.16	0.44
1:G:374:PHE:CE1	4:G:610:N8V:H9	2.53	0.44
1:E:415:ARG:NE	5:E:702:HOH:O	2.50	0.44
1:D:82:MET:HG2	1:D:87:ALA:HB3	1.99	0.43
1:F:548:ASN:HB3	1:G:140:TYR:CZ	2.53	0.43
1:A:415:ARG:CD	1:A:419:GLN:CD	2.86	0.43
1:G:169:LEU:HD23	1:G:169:LEU:HA	1.91	0.43
1:B:548:ASN:HB3	1:H:140:TYR:CZ	2.54	0.43
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.53	0.43
1:B:99:ILE:O	1:B:106:PHE:HA	2.18	0.43
1:D:415:ARG:NH2	5:D:707:HOH:O	2.50	0.43
1:F:415[A]:ARG:NH1	5:F:702[A]:HOH:O	2.03	0.43
1:C:384:TYR:CG	1:C:385:PRO:HA	2.53	0.43
1:C:367:GLY:HA2	1:C:417[A]:SER:OG	2.19	0.43
1:A:63[A]:SER:HB3	1:A:85:MET:SD	2.58	0.42
1:H:384:TYR:CD1	1:H:385:PRO:HA	2.54	0.42
1:F:367:GLY:HA2	1:F:417[A]:SER:OG	2.19	0.42
1:G:367:GLY:HA2	1:G:417[A]:SER:OG	2.19	0.42
1:G:190:LYS:HG3	1:G:191:ARG:HG2	2.00	0.42
1:G:382[A]:THR:CG2	5:G:1081:HOH:O	2.64	0.42
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.55	0.42
1:H:169:LEU:HD12	1:H:219:ALA:HA	2.02	0.42
1:H:271:LYS:HE3	1:H:315:ASN:O	2.20	0.42
1:B:367:GLY:HA2	1:B:417[A]:SER:OG	2.19	0.42
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.55	0.41
1:D:508:ALA:HB3	1:D:558:PHE:CD1	2.54	0.41
1:E:382[B]:THR:HG22	5:E:1163:HOH:O	2.19	0.41
1:F:99:ILE:O	1:F:106:PHE:HA	2.21	0.41
1:G:82[B]:MET:HG2	5:G:786:HOH:O	2.20	0.41
1:H:415[A]:ARG:O	1:H:419:GLN:HG3	2.19	0.41
1:H:113[B]:VAL:HG12	5:H:1111:HOH:O	2.19	0.41
1:B:432:THR:HG23	1:B:436:GLN:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:ASP:OD1	5:F:703:HOH:O	2.21	0.41
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.55	0.41
1:A:254:PHE:O	1:A:258:GLN:HG2	2.20	0.41
1:D:568:LYS:HE3	5:D:1223:HOH:O	2.19	0.41
1:D:367:GLY:HA2	1:D:417[A]:SER:OG	2.20	0.40
1:A:140:TYR:CZ	1:C:548:ASN:HB3	2.57	0.40
1:B:139:HIS:HB2	5:B:1038:HOH:O	2.21	0.40
1:B:200:VAL:O	1:B:278:MET:HA	2.22	0.40
1:D:83:GLU:HG3	5:D:1234:HOH:O	2.22	0.40
5:D:728:HOH:O	1:E:527:MET:CE	2.69	0.40
1:A:568:LYS:HE2	5:A:756:HOH:O	2.21	0.40
1:C:455[A]:ARG:NH1	5:C:707:HOH:O	2.46	0.40
1:H:193:LYS:CD	5:H:961:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 38 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
3	ACT	A	602	-	1,3,3	5.23	1 (100%)	0,3,3	0.00	-
3	ACT	B	602	-	1,3,3	1.57	0	0,3,3	0.00	-
3	ACT	G	603	-	1,3,3	4.36	1 (100%)	0,3,3	0.00	-
3	ACT	F	604	-	1,3,3	5.44	1 (100%)	0,3,3	0.00	-
3	ACT	D	604	-	1,3,3	5.54	1 (100%)	0,3,3	0.00	-
4	N8V	H	607	-	20,20,20	1.48	5 (25%)	17,25,25	1.11	2 (11%)
3	ACT	E	606	-	1,3,3	2.04	1 (100%)	0,3,3	0.00	-
3	ACT	E	604	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
3	ACT	E	607	-	1,3,3	4.90	1 (100%)	0,3,3	0.00	-
3	ACT	B	603	-	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
4	N8V	C	606	-	16,16,20	1.68	3 (18%)	13,21,25	1.11	1 (7%)
3	ACT	D	605	-	1,3,3	3.21	1 (100%)	0,3,3	0.00	-
3	ACT	E	605	-	1,3,3	3.29	1 (100%)	0,3,3	0.00	-
4	N8V	F	607	-	20,20,20	2.09	4 (20%)	17,25,25	1.51	2 (11%)
3	ACT	F	605	-	1,3,3	2.14	1 (100%)	0,3,3	0.00	-
4	N8V	A	606	-	20,20,20	1.33	3 (15%)	17,25,25	1.15	0
4	N8V	E	611	-	14,14,20	2.29	3 (21%)	11,19,25	1.38	2 (18%)
4	N8V	B	607	-	20,20,20	1.83	6 (30%)	17,25,25	1.23	1 (5%)
4	N8V	D	609	-	20,20,20	1.83	4 (20%)	17,25,25	1.02	2 (11%)
4	N8V	G	610	-	20,20,20	1.67	4 (20%)	17,25,25	1.37	3 (17%)
3	ACT	C	603	-	1,3,3	4.43	1 (100%)	0,3,3	0.00	-
3	ACT	H	602	-	1,3,3	6.89	1 (100%)	0,3,3	0.00	-
3	ACT	G	604	-	1,3,3	1.54	0	0,3,3	0.00	-
3	ACT	G	606	-	1,3,3	2.89	1 (100%)	0,3,3	0.00	-
3	ACT	G	605	-	1,3,3	6.31	1 (100%)	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	N8V	F	607	-	-	2/11/31/31	0/1/1/1
4	N8V	D	609	-	-	0/11/31/31	0/1/1/1
4	N8V	C	606	-	-	0/7/27/31	0/1/1/1
4	N8V	G	610	-	-	3/11/31/31	0/1/1/1
4	N8V	A	606	-	-	1/11/31/31	0/1/1/1
4	N8V	E	611	-	-	0/5/25/31	0/1/1/1
4	N8V	H	607	-	-	1/11/31/31	0/1/1/1
4	N8V	B	607	-	-	1/11/31/31	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	607	N8V	C4-C5	-7.67	1.45	1.51
3	H	602	ACT	CH3-C	6.89	1.57	1.48
3	G	605	ACT	CH3-C	6.31	1.56	1.48
4	E	611	N8V	C4-C5	-5.78	1.46	1.51
4	D	609	N8V	C4-C5	-5.73	1.46	1.51
3	D	604	ACT	CH3-C	5.54	1.55	1.48
3	F	604	ACT	CH3-C	5.44	1.55	1.48
3	A	602	ACT	CH3-C	5.23	1.55	1.48
3	E	607	ACT	CH3-C	4.90	1.55	1.48
4	B	607	N8V	C4-C5	-4.82	1.47	1.51
4	C	606	N8V	C2-C1	4.55	1.58	1.52
3	C	603	ACT	CH3-C	4.43	1.54	1.48
3	G	603	ACT	CH3-C	4.36	1.54	1.48
4	E	611	N8V	C2-C1	4.19	1.58	1.52
4	G	610	N8V	C1-N8	3.74	1.55	1.47
4	E	611	N8V	C1-N8	3.39	1.54	1.47
3	B	603	ACT	CH3-C	3.38	1.53	1.48
4	G	610	N8V	C10-C9	3.32	1.64	1.51
3	E	605	ACT	CH3-C	3.29	1.52	1.48
4	F	607	N8V	O4-C4	3.27	1.48	1.42
3	D	605	ACT	CH3-C	3.21	1.52	1.48
4	D	609	N8V	C1-N8	3.19	1.54	1.47
4	A	606	N8V	C1-C7	-3.17	1.45	1.50
4	H	607	N8V	C2-C1	3.06	1.56	1.52
3	G	606	ACT	CH3-C	2.89	1.52	1.48
4	H	607	N8V	O2-C2	2.84	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	607	N8V	O4-C4	2.84	1.47	1.42
4	D	609	N8V	C2-C1	2.80	1.56	1.52
4	B	607	N8V	C1-C7	2.68	1.54	1.50
4	A	606	N8V	C7-C5	2.68	1.36	1.32
4	C	606	N8V	C6-C5	2.67	1.56	1.50
4	F	607	N8V	O2-C2	2.64	1.49	1.43
4	B	607	N8V	C2-C1	2.61	1.56	1.52
3	E	604	ACT	CH3-C	2.54	1.52	1.48
4	H	607	N8V	C4-C5	-2.52	1.49	1.51
4	A	606	N8V	C4-C5	-2.49	1.49	1.51
4	B	607	N8V	C1-N8	2.46	1.52	1.47
4	B	607	N8V	C6-C5	2.37	1.56	1.50
4	D	609	N8V	C1-C7	-2.21	1.47	1.50
4	C	606	N8V	C7-C5	-2.20	1.29	1.32
4	G	610	N8V	C6-C5	2.19	1.55	1.50
4	H	607	N8V	C7-C5	2.17	1.35	1.32
4	H	607	N8V	O4-C4	2.14	1.46	1.42
3	F	605	ACT	CH3-C	2.14	1.51	1.48
4	G	610	N8V	C2-C1	2.09	1.55	1.52
3	E	606	ACT	CH3-C	2.04	1.51	1.48
4	F	607	N8V	C2-C1	2.01	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	607	N8V	C7-C1-N8	-4.18	104.63	110.72
4	E	611	N8V	C7-C1-N8	-3.62	105.46	110.72
4	G	610	N8V	C7-C1-N8	-3.17	106.11	110.72
4	B	607	N8V	C7-C1-N8	-2.85	106.57	110.72
4	C	606	N8V	C7-C1-N8	-2.74	106.72	110.72
4	H	607	N8V	O4-C4-C3	-2.44	105.49	110.53
4	G	610	N8V	O3-C3-C4	-2.29	105.31	109.68
4	D	609	N8V	O2-C2-C1	2.15	113.44	109.12
4	G	610	N8V	O6-C6-C5	2.13	117.59	112.50
4	H	607	N8V	O4-C4-C5	2.09	114.85	110.82
4	E	611	N8V	O4-C4-C3	-2.09	106.22	110.53
4	D	609	N8V	O4-C4-C3	-2.07	106.25	110.53
4	F	607	N8V	C14-C13-C12	-2.01	104.23	114.42

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	607	N8V	C11-C10-C9-N8
4	G	610	N8V	C11-C10-C9-N8
4	A	606	N8V	C11-C12-C13-C14
4	G	610	N8V	C9-C10-C11-C12
4	F	607	N8V	C9-C10-C11-C12
4	B	607	N8V	C9-C10-C11-C12
4	H	607	N8V	C9-C10-C11-C12
4	G	610	N8V	C13-C14-C15-C16

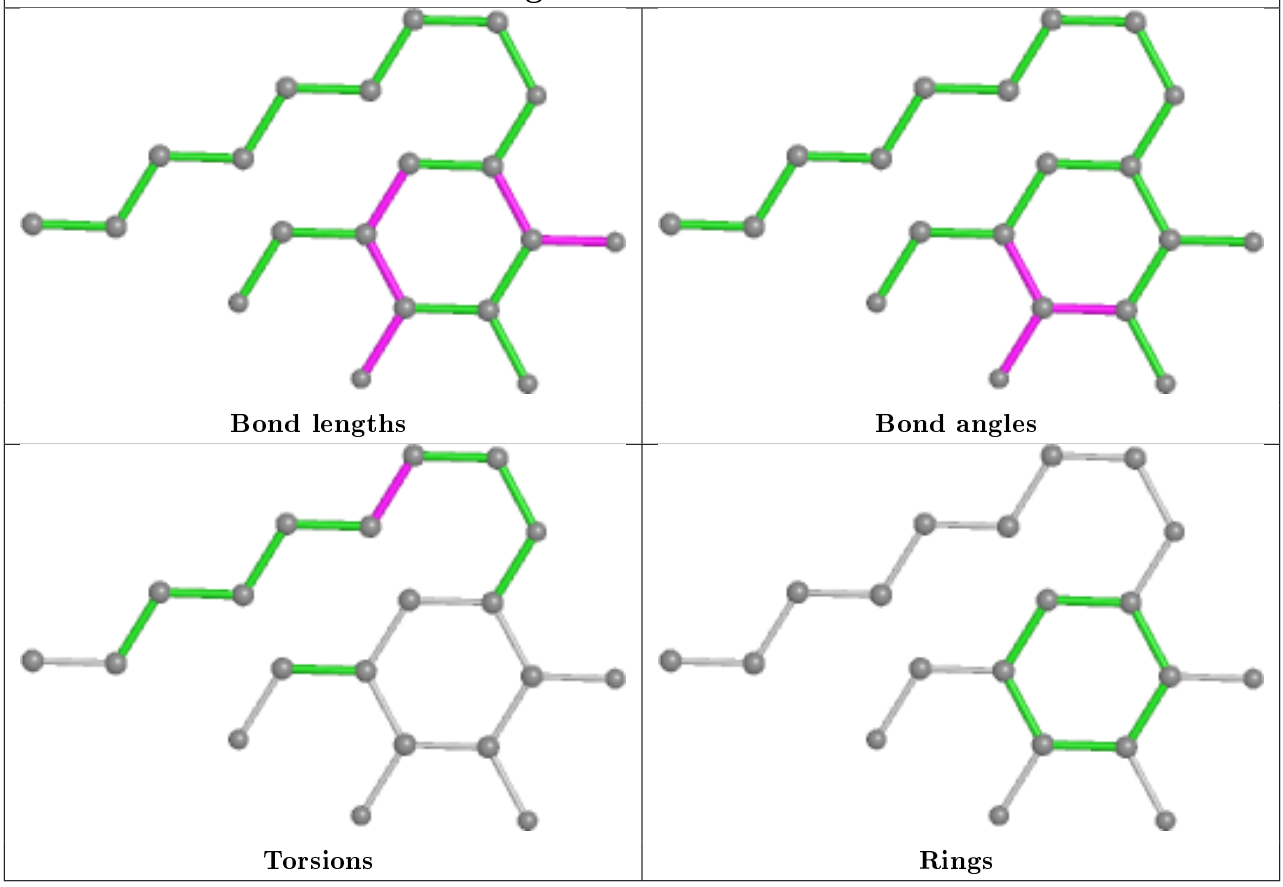
There are no ring outliers.

4 monomers are involved in 4 short contacts:

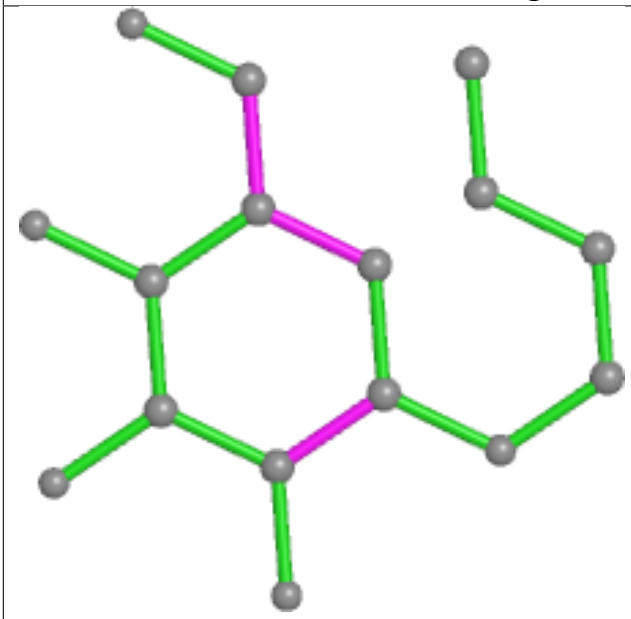
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	ACT	1	0
4	D	609	N8V	1	0
4	G	610	N8V	1	0
3	G	604	ACT	1	0

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.

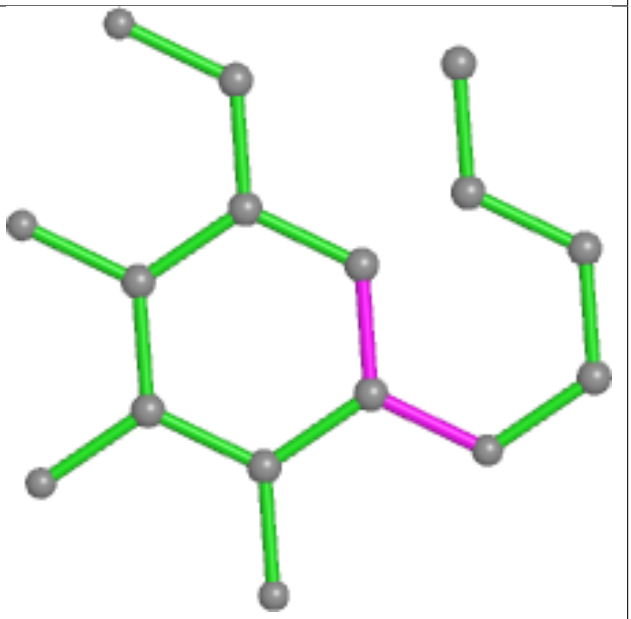
Ligand N8V H 607



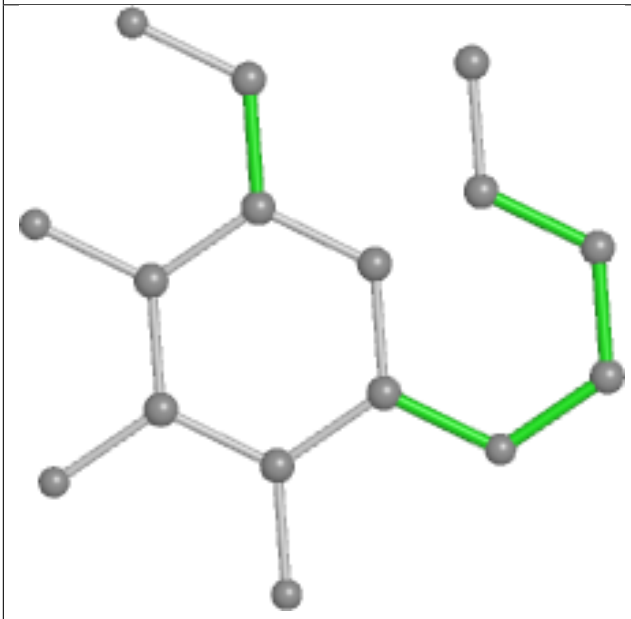
Ligand N8V C 606



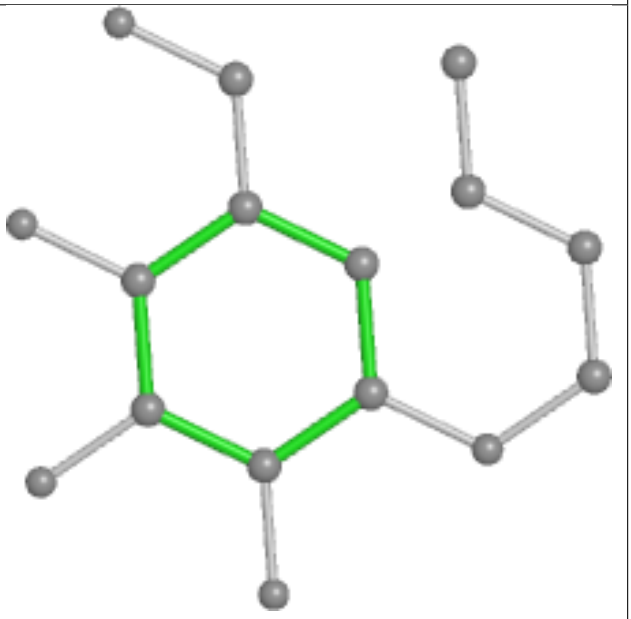
Bond lengths



Bond angles

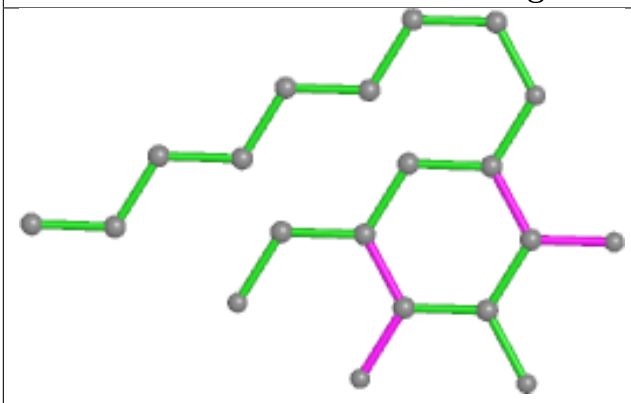


Torsions

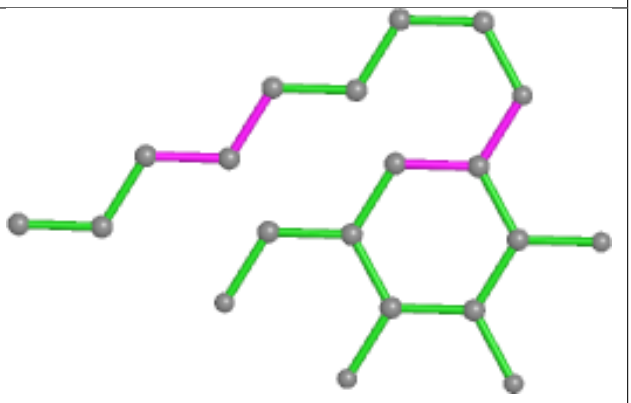


Rings

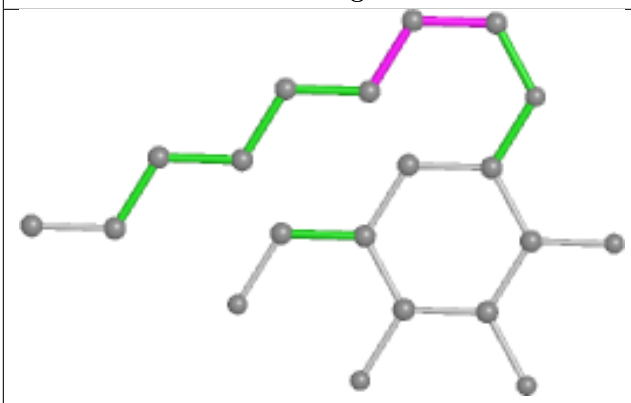
Ligand N8V F 607



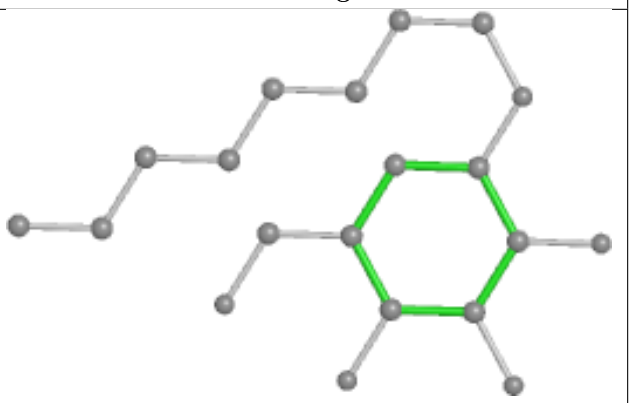
Bond lengths



Bond angles

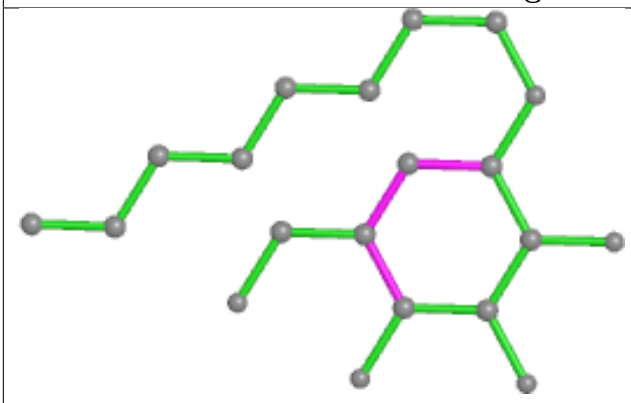


Torsions

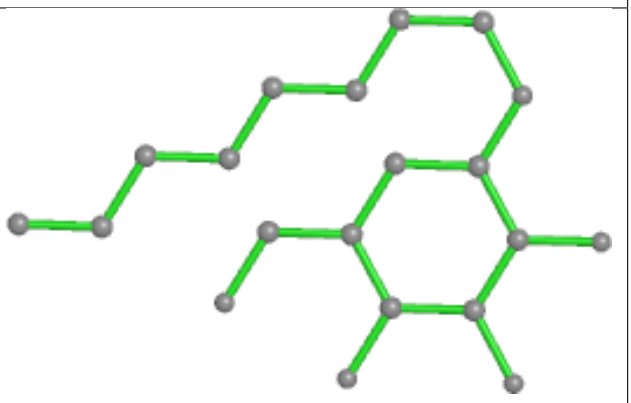


Rings

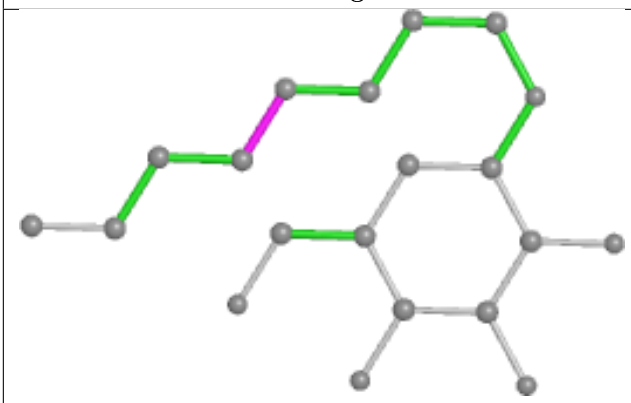
Ligand N8V A 606



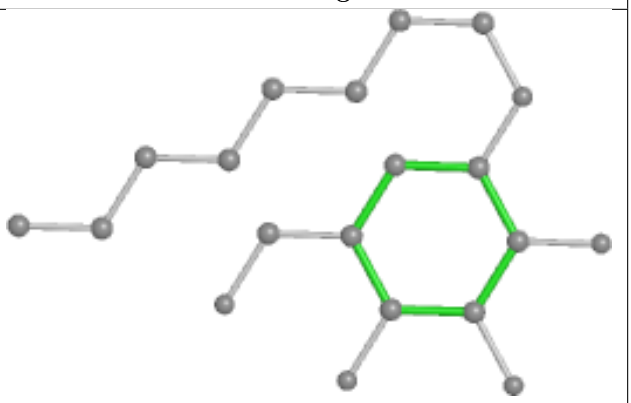
Bond lengths



Bond angles

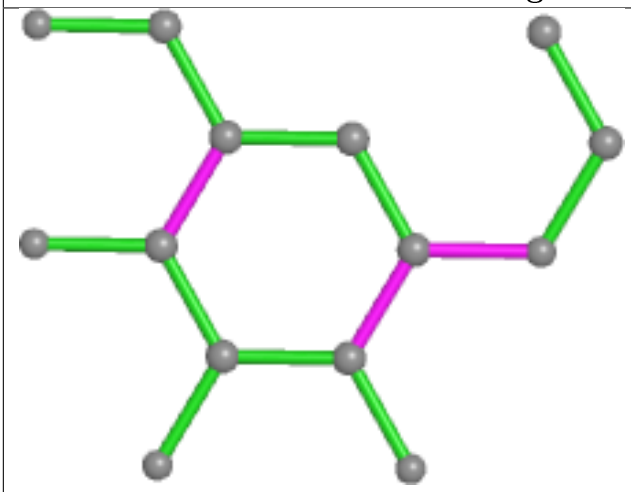


Torsions

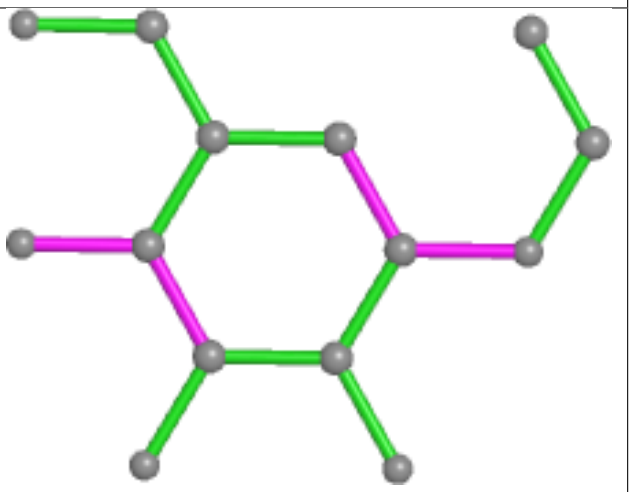


Rings

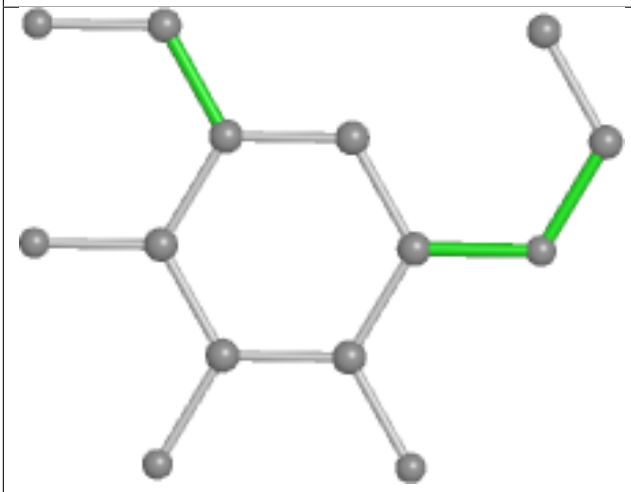
Ligand N8V E 611



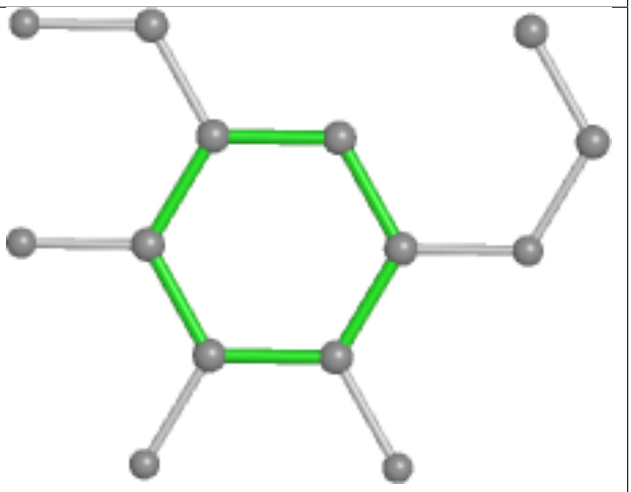
Bond lengths



Bond angles

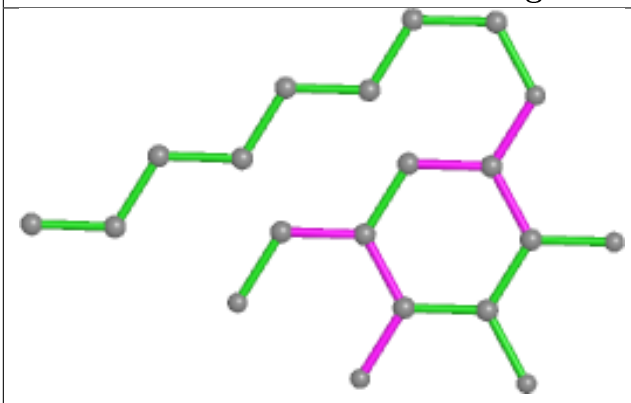


Torsions

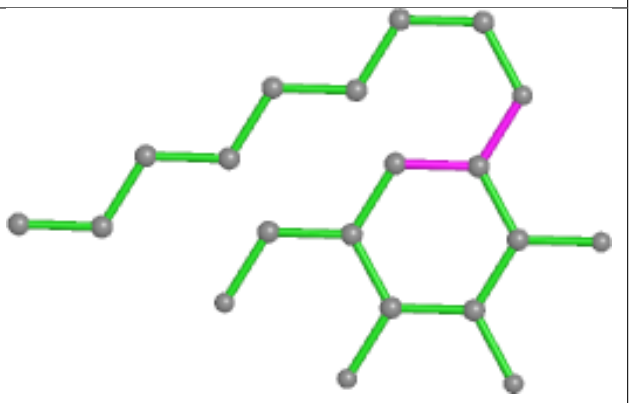


Rings

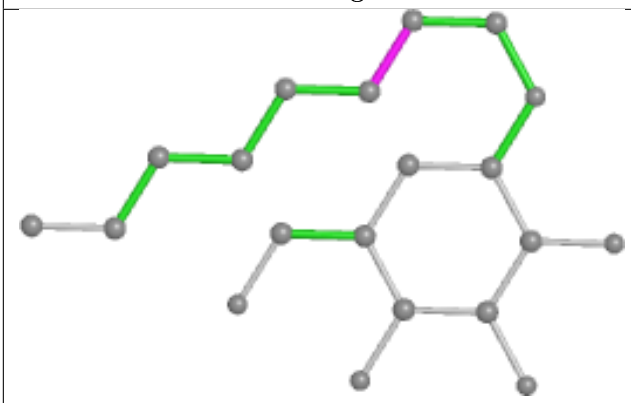
Ligand N8V B 607



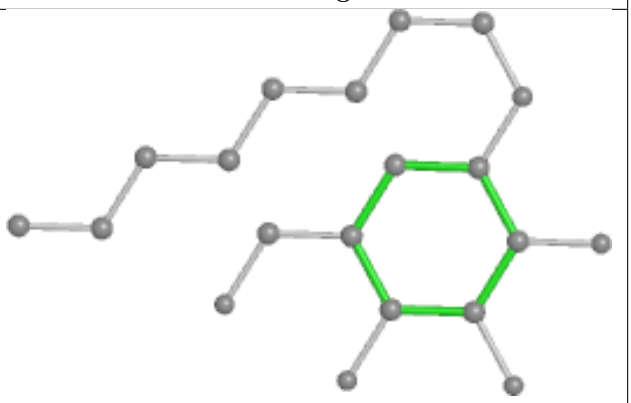
Bond lengths



Bond angles

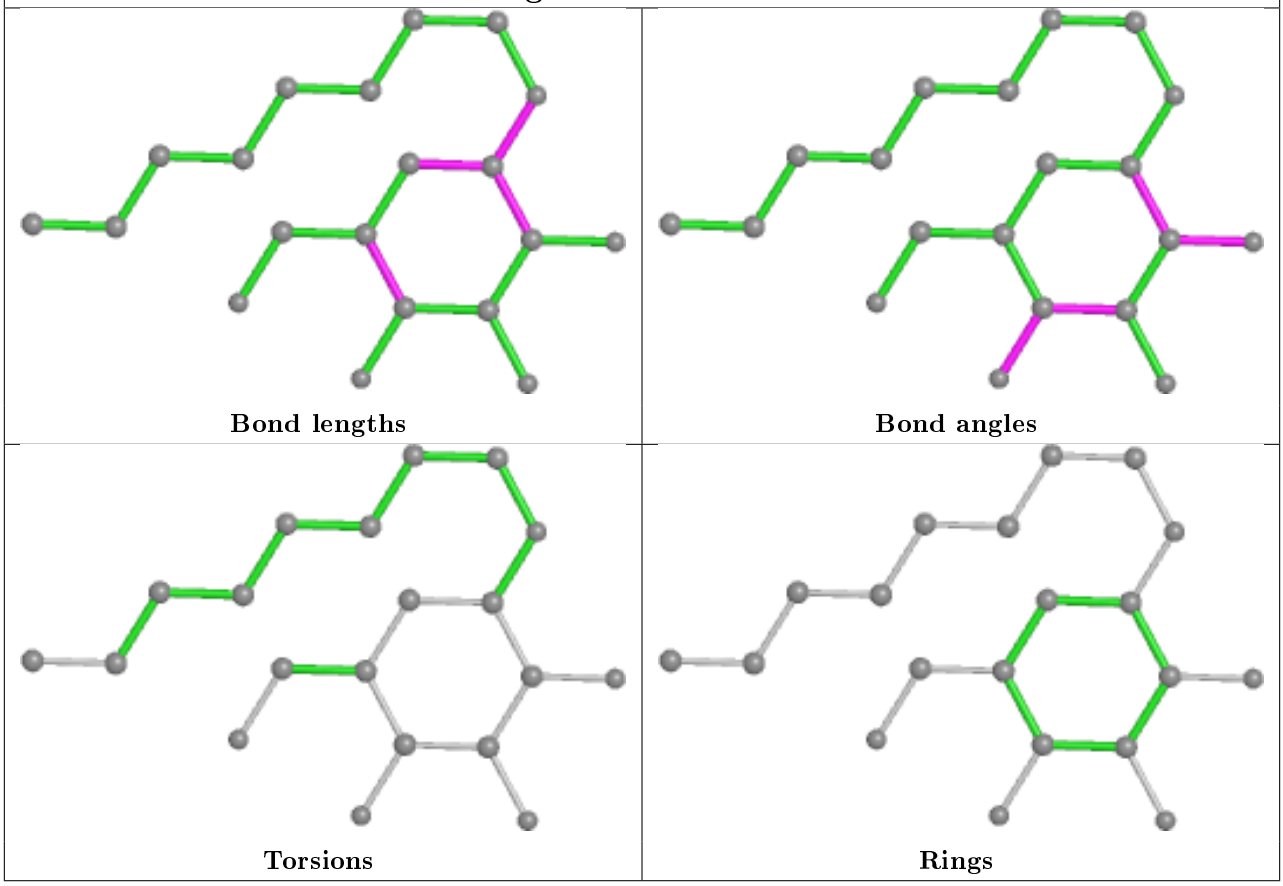


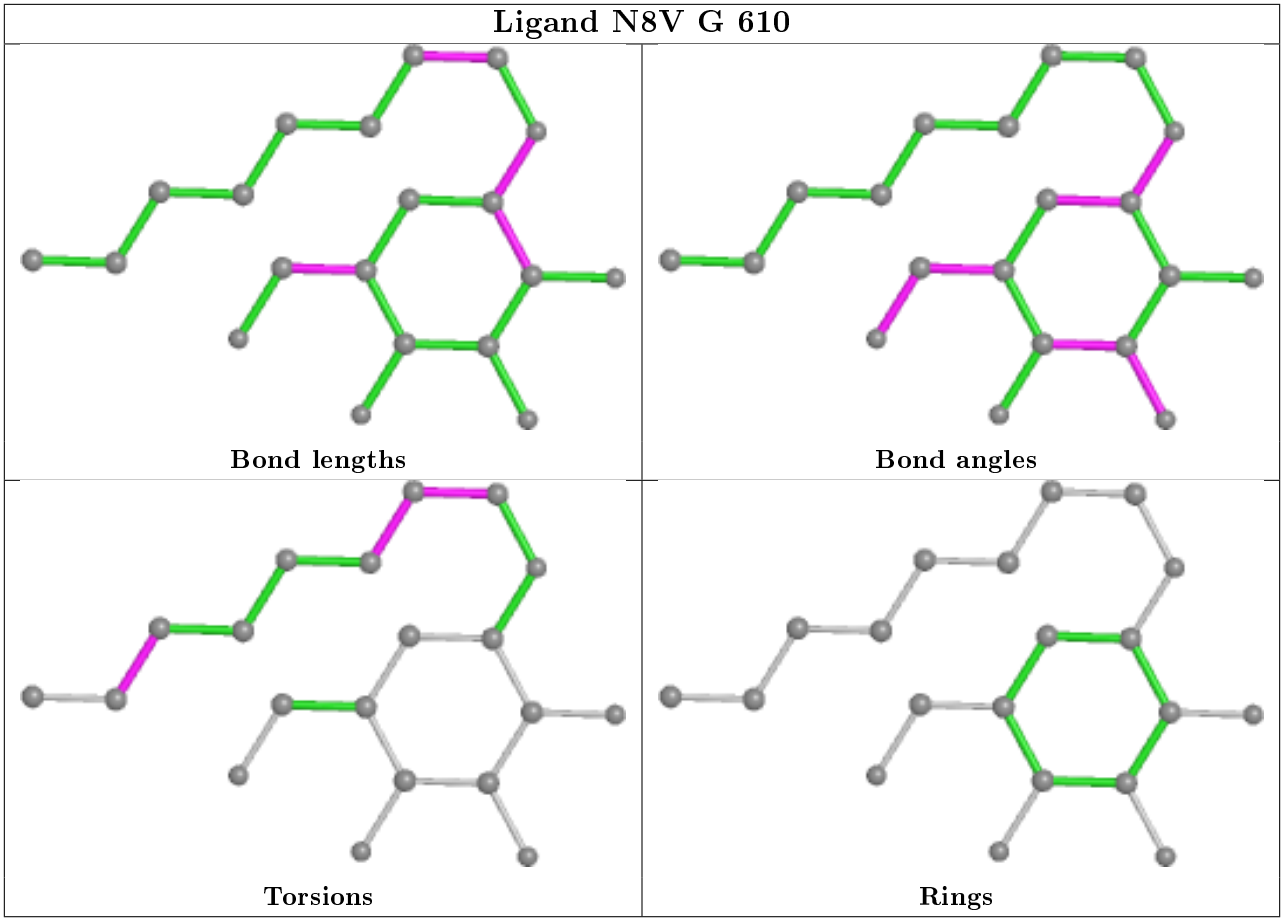
Torsions



Rings

Ligand N8V D 609





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

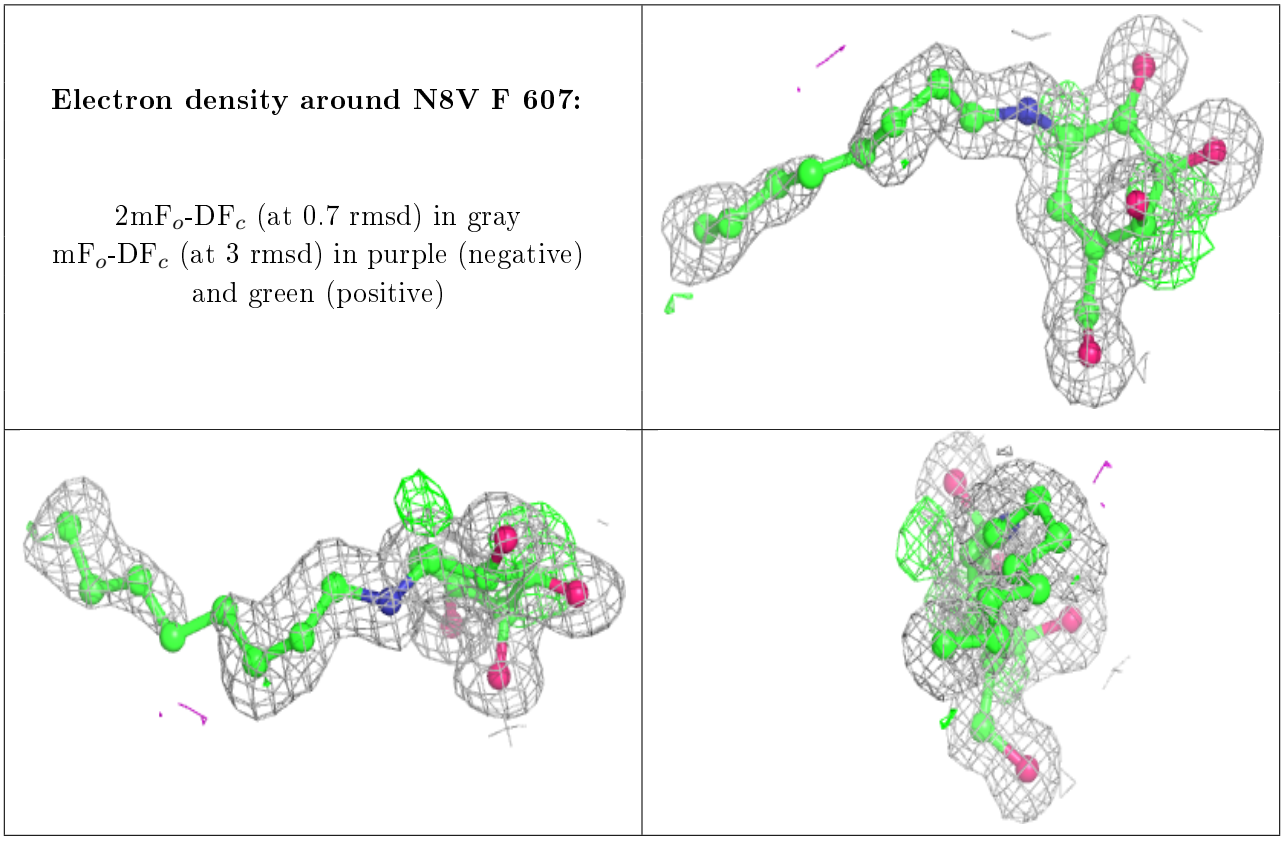
6.4 Ligands

EDS failed to run properly - this section is therefore empty.

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.

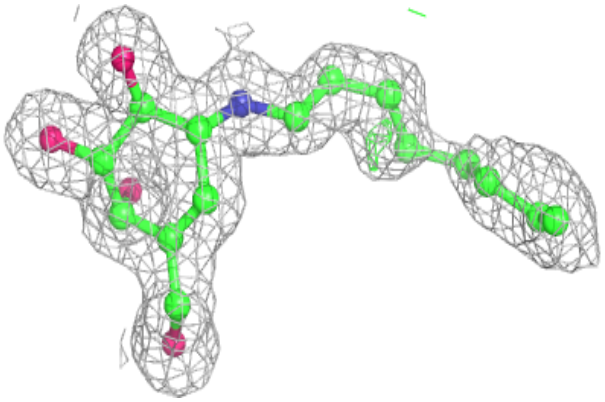
Electron density around N8V F 607:

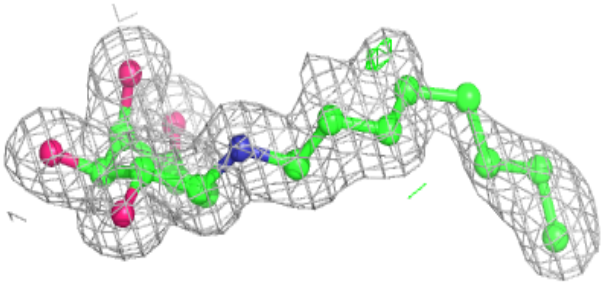
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

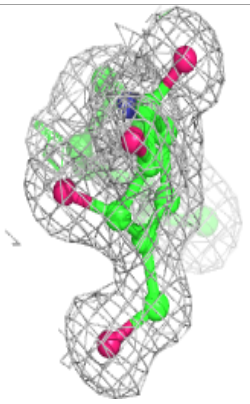


Electron density around N8V H 607:

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

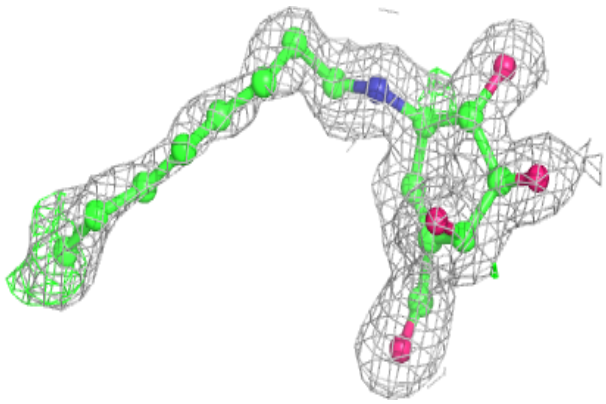


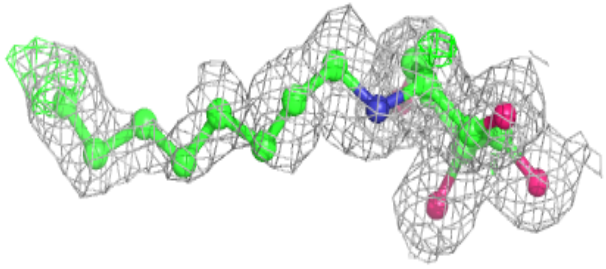


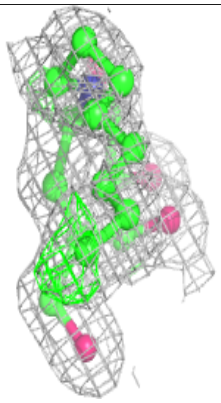


Electron density around N8V D 609:

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

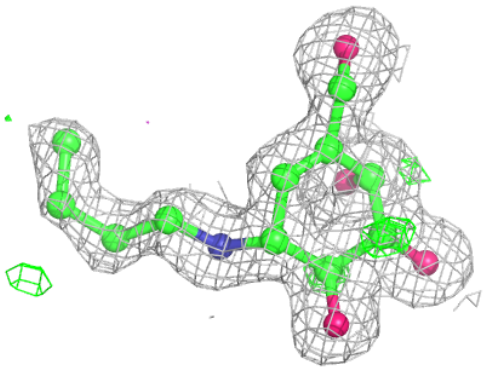


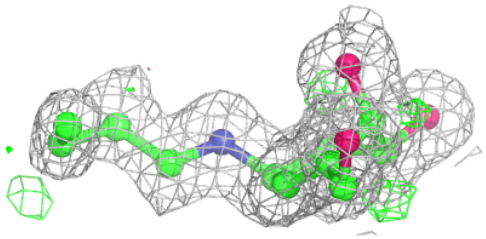


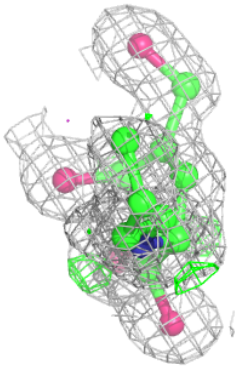


Electron density around N8V C 606:

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

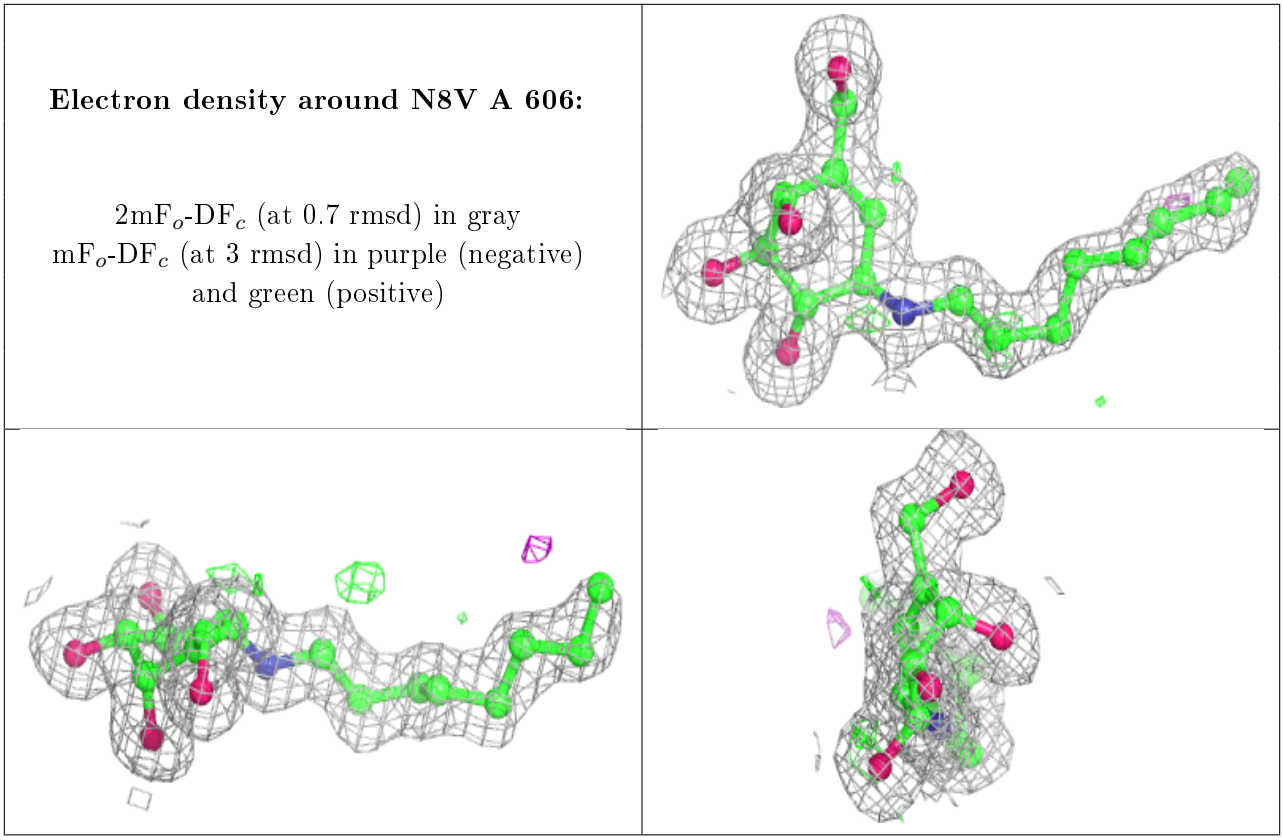






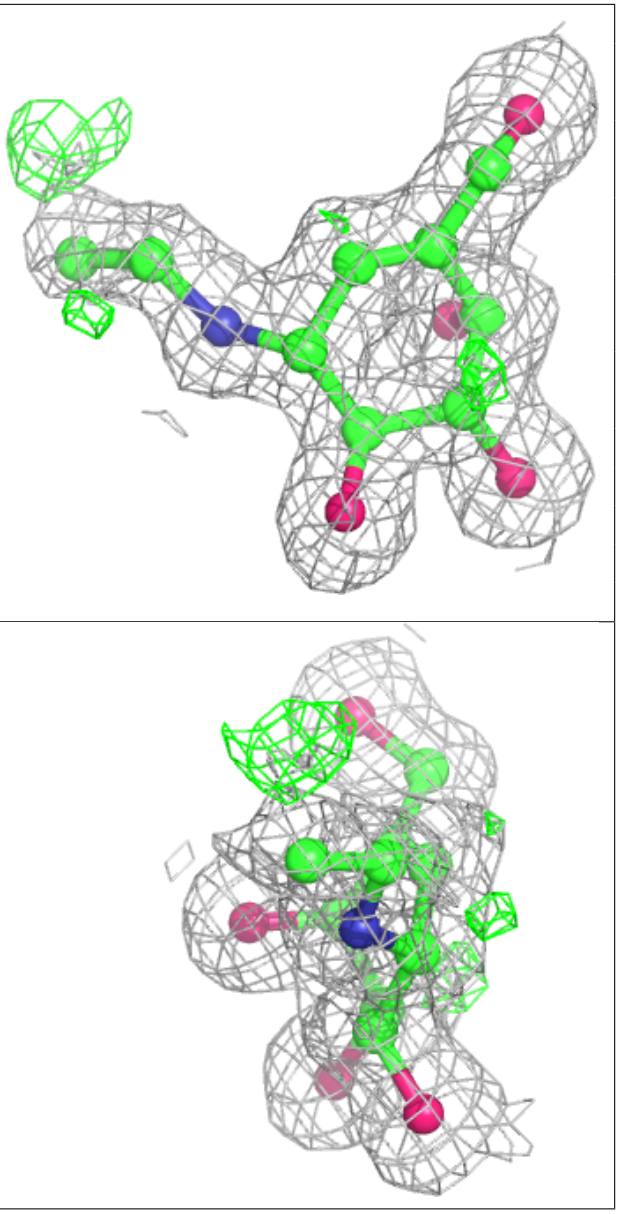
Electron density around N8V A 606:

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



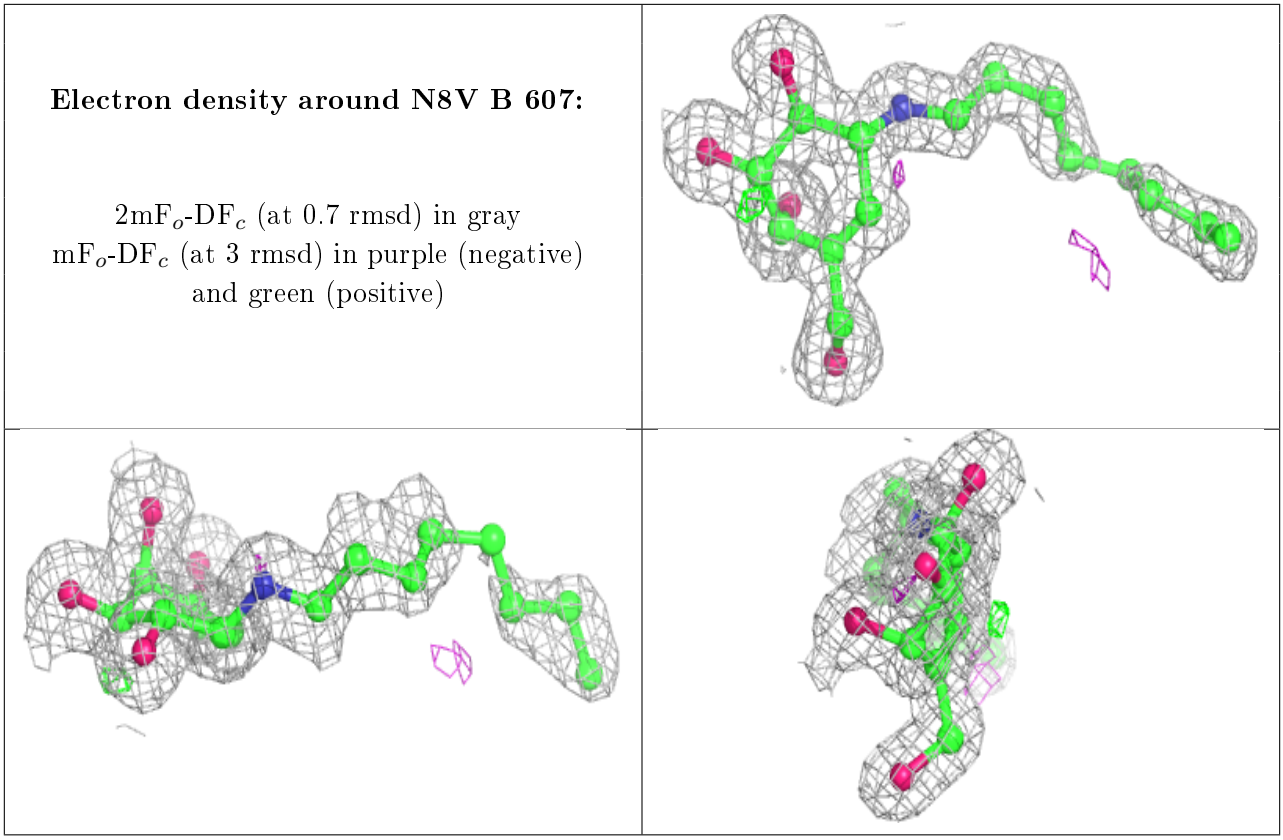
Electron density around N8V E 611:

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



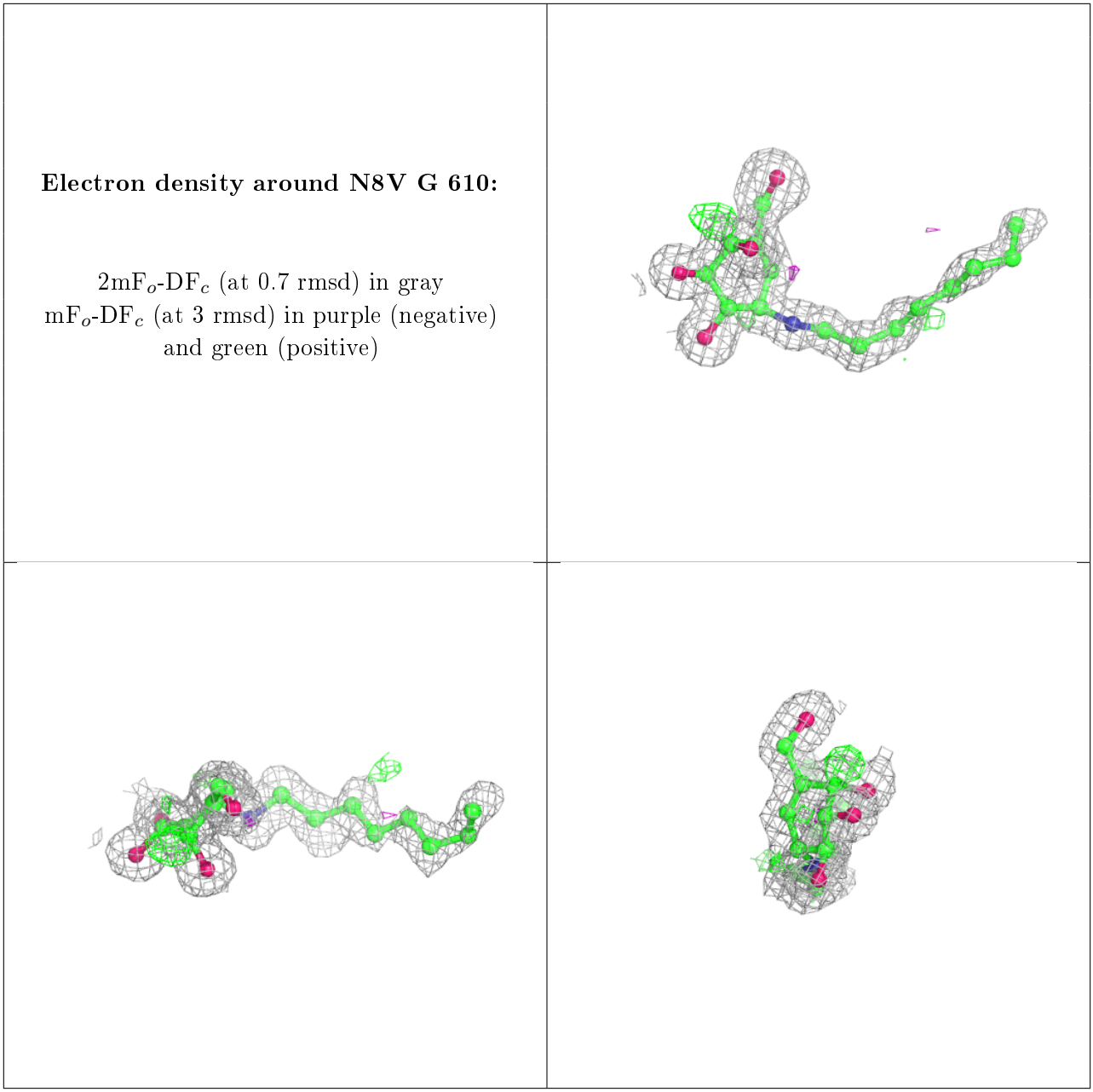
Electron density around N8V B 607:

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



Electron density around N8V G 610:

$2mF_o$-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

EDS failed to run properly - this section is therefore empty.