



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:15 AM UTC

PDB ID : 6TBI / pdb_00006tbi
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 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

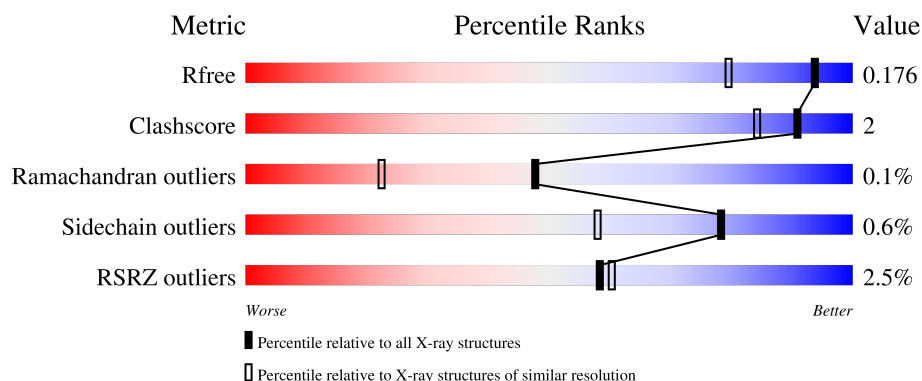
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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))
R_{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (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 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	550	
1	B	550	
1	C	550	
1	D	550	
1	E	550	

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Mol	Chain	Length	Quality of chain
1	F	550	2% 92% 5%
1	G	550	3% 91% 7%
1	H	550	3% 90% 8%

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 (CCD ID: NA) (formula: Na).

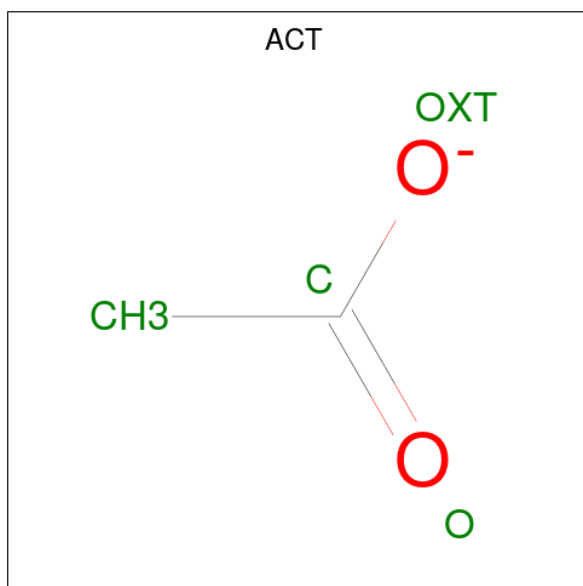
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Na 4 4	0	0
2	B	4	Total Na 4 4	0	0
2	C	4	Total Na 4 4	0	0
2	D	6	Total Na 6 6	0	0
2	E	6	Total Na 6 6	0	0
2	F	4	Total Na 4 4	0	0
2	G	5	Total Na 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	5	Total	Na	0	0
			5	5		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



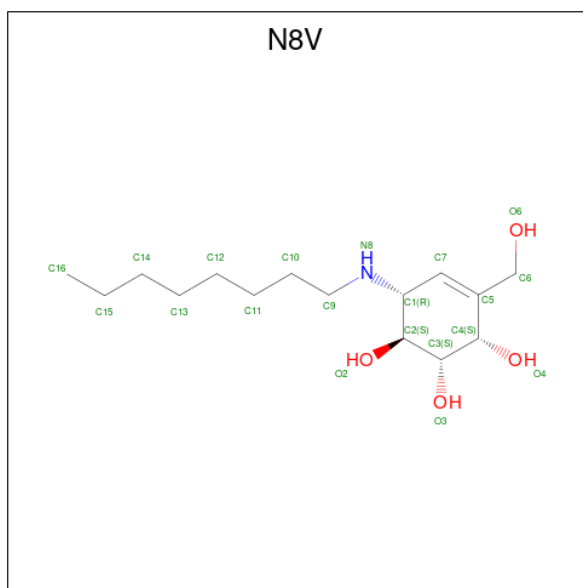
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total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

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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 (CCD ID: N8V) (formula: C₁₅H₂₉NO₄) (labeled as "Ligand of Interest" by depositor).



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	0	0
			14	9	1	4		
4	F	1	Total	C	N	O	0	0
			20	15	1	4		
4	G	1	Total	C	N	O	0	0
			20	15	1	4		
4	H	1	Total	C	N	O	0	0
			20	15	1	4		

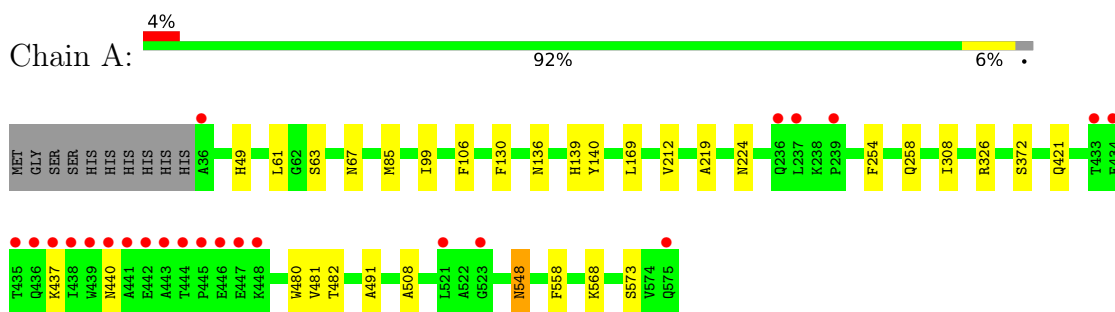
- Molecule 5 is water.

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

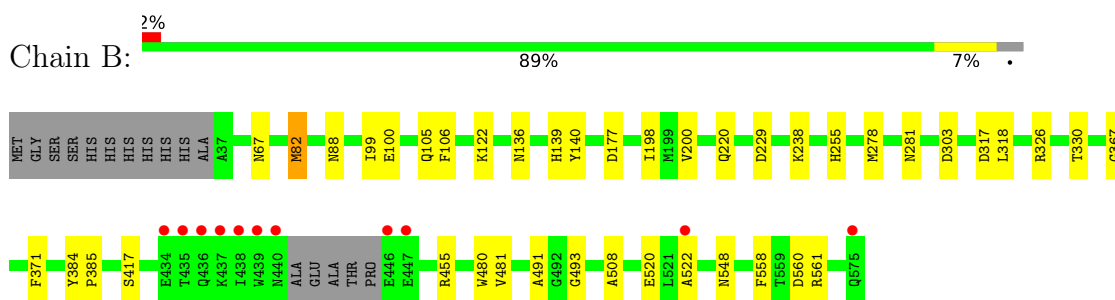
3 Residue-property plots

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 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.

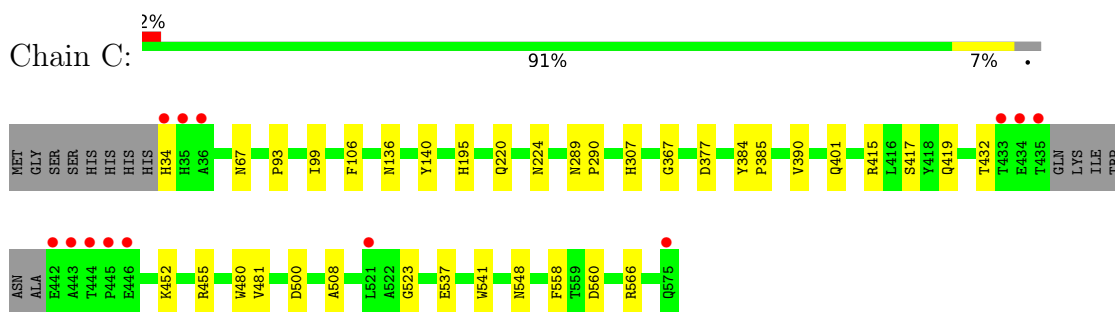
- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



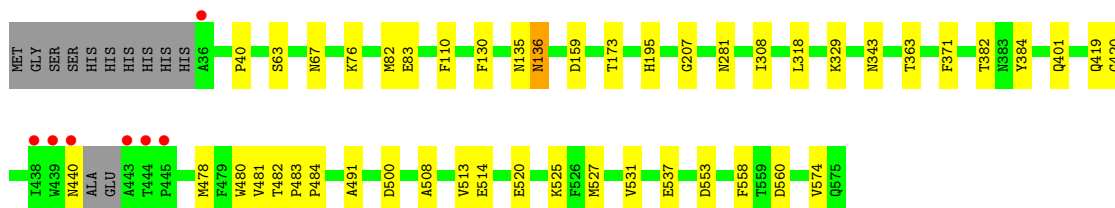
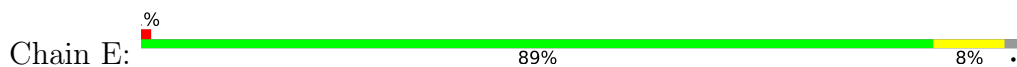
- Molecule 1: Beta-galactosidase, putative, bgl35A



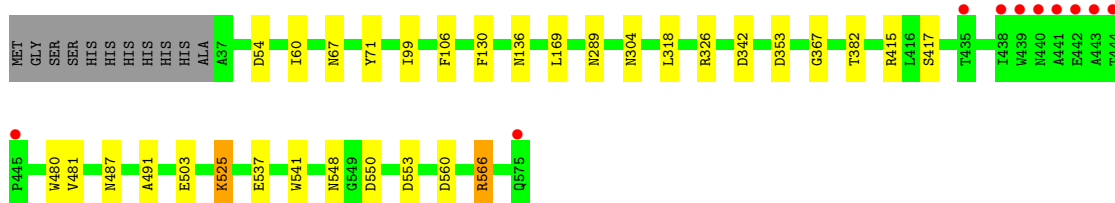
- Molecule 1: Beta-galactosidase, putative, bgl35A



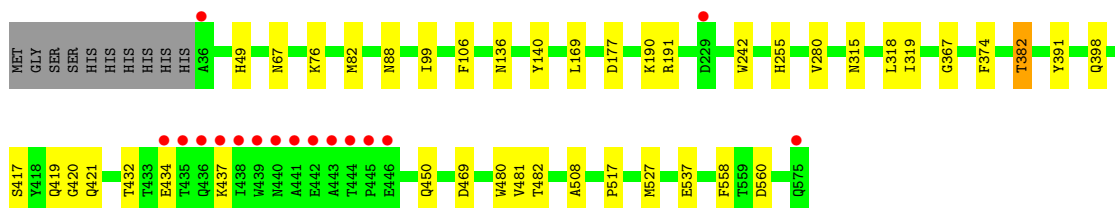
- Molecule 1: Beta-galactosidase, putative, bgl35A



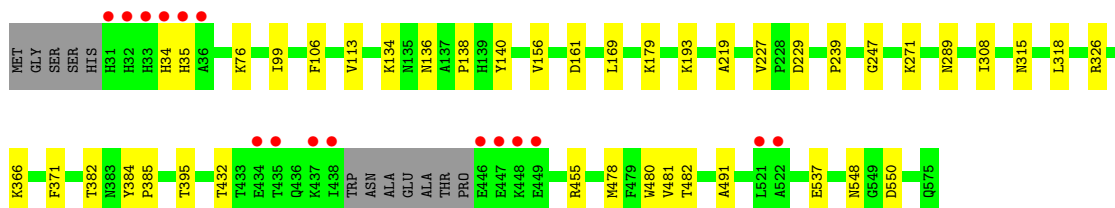
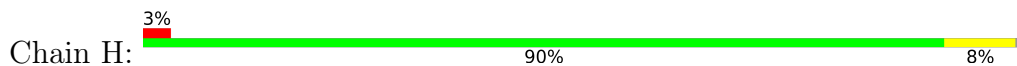
- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



4 Data and refinement statistics

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 – 1.46 116.10 – 1.46	Depositor EDS
% Data completeness (in resolution range)	96.3 (116.10-1.46) 96.4 (116.10-1.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.126 , 0.172 0.135 , 0.176	Depositor DCC
R_{free} test set	43376 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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
F_o, F_c correlation	0.98	EDS
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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, N8V, NA

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	1.21	8/4403 (0.2%)	1.29	6/6002 (0.1%)
1	B	1.19	9/4378 (0.2%)	1.30	13/5965 (0.2%)
1	C	1.17	8/4428 (0.2%)	1.28	7/6026 (0.1%)
1	D	1.22	7/4433 (0.2%)	1.31	10/6039 (0.2%)
1	E	1.24	11/4418 (0.2%)	1.34	19/6014 (0.3%)
1	F	1.21	4/4523 (0.1%)	1.31	12/6153 (0.2%)
1	G	1.22	8/4495 (0.2%)	1.31	14/6116 (0.2%)
1	H	1.21	8/4475 (0.2%)	1.27	10/6094 (0.2%)
All	All	1.21	63/35553 (0.2%)	1.30	91/48409 (0.2%)

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 (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	34	HIS	CE1-NE2	9.06	1.41	1.32
1	H	326	ARG	C-O	7.83	1.34	1.24
1	A	139	HIS	CE1-NE2	7.78	1.40	1.32
1	F	525	LYS	CG-CD	-7.57	1.29	1.52
1	G	255	HIS	CE1-NE2	7.46	1.40	1.32
1	A	326	ARG	C-O	6.96	1.33	1.24
1	C	560	ASP	CG-OD1	-6.66	1.12	1.25
1	C	523	GLY	C-O	6.63	1.33	1.23
1	E	478	MET	C-O	6.61	1.32	1.24
1	C	195	HIS	CE1-NE2	6.55	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	326	ARG	C-O	6.50	1.32	1.24
1	E	520	GLU	C-O	6.50	1.31	1.23
1	D	527	MET	C-O	6.36	1.31	1.23
1	F	326	ARG	C-O	6.35	1.32	1.24
1	H	161	ASP	C-O	6.29	1.31	1.23
1	G	398	GLN	C-O	-6.17	1.16	1.24
1	D	560	ASP	CG-OD2	-6.17	1.13	1.25
1	B	326	ARG	C-O	6.16	1.32	1.24
1	A	49	HIS	CE1-NE2	6.13	1.38	1.32
1	G	49	HIS	CE1-NE2	6.08	1.38	1.32
1	D	569	MET	C-O	5.93	1.31	1.23
1	E	513	VAL	C-O	-5.92	1.17	1.24
1	E	110	PHE	C-O	-5.92	1.17	1.24
1	F	60	ILE	C-O	5.90	1.29	1.23
1	B	560	ASP	CG-OD1	-5.89	1.14	1.25
1	G	450	GLN	C-O	5.85	1.31	1.24
1	C	307	HIS	CE1-NE2	5.84	1.38	1.32
1	H	478	MET	C-O	5.82	1.31	1.24
1	E	40	PRO	C-O	-5.80	1.16	1.23
1	G	242	TRP	C-O	5.78	1.30	1.24
1	E	195	HIS	CE1-NE2	5.78	1.38	1.32
1	F	560	ASP	CG-OD1	-5.75	1.14	1.25
1	A	212	VAL	C-O	5.62	1.30	1.24
1	E	514	GLU	C-O	-5.47	1.17	1.23
1	B	493	GLY	C-O	5.46	1.29	1.23
1	D	403	TYR	C-O	-5.44	1.17	1.24
1	B	520	GLU	C-O	5.43	1.30	1.23
1	B	303	ASP	C-O	-5.38	1.17	1.24
1	D	496	ILE	C-O	5.37	1.29	1.24
1	G	391	TYR	C-O	-5.33	1.18	1.24
1	A	372	SER	N-CA	5.33	1.52	1.46
1	B	255	HIS	CE1-NE2	5.31	1.37	1.32
1	H	308	ILE	C-O	5.29	1.30	1.24
1	E	500	ASP	C-O	-5.29	1.18	1.23
1	B	100	GLU	N-CA	5.28	1.52	1.46
1	H	156	VAL	C-O	5.26	1.30	1.24
1	C	390	VAL	C-O	-5.24	1.18	1.24
1	D	381	TYR	C-O	-5.23	1.17	1.23
1	E	363	THR	C-O	5.16	1.30	1.24
1	E	531	VAL	C-O	-5.15	1.18	1.24
1	B	561	ARG	CD-NE	-5.13	1.39	1.46
1	A	440	ASN	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	527	MET	C-N	-5.11	1.27	1.33
1	E	484	PRO	C-O	-5.11	1.17	1.23
1	A	573	SER	C-O	5.10	1.30	1.23
1	H	35	HIS	CE1-NE2	-5.10	1.27	1.32
1	C	93	PRO	C-O	-5.10	1.18	1.23
1	B	330	THR	N-CA	5.08	1.52	1.46
1	C	290	PRO	C-O	-5.07	1.18	1.24
1	H	239	PRO	C-O	-5.06	1.17	1.23
1	G	177	ASP	N-CA	5.03	1.52	1.46
1	C	224	ASN	C-O	5.02	1.30	1.24
1	A	61	LEU	C-O	5.01	1.30	1.23

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	525	LYS	CB-CG-CD	7.56	128.69	111.30
1	B	238	LYS	CB-CA-C	7.51	120.10	108.61
1	E	159	ASP	CA-CB-CG	7.42	120.02	112.60
1	G	537	GLU	CB-CG-CD	7.30	125.01	112.60
1	H	227	VAL	N-CA-C	-6.96	102.55	109.02
1	E	537	GLU	CB-CG-CD	6.86	124.26	112.60
1	D	67	ASN	CA-CB-CG	6.78	119.38	112.60
1	E	136	ASN	CA-CB-CG	6.75	119.36	112.60
1	E	483	PRO	N-CA-CB	6.59	106.88	103.19
1	F	304	ASN	OD1-CG-ND2	6.48	129.08	122.60
1	F	67	ASN	CA-CB-CG	6.47	119.07	112.60
1	A	308	ILE	N-CA-C	-6.44	104.47	110.53
1	G	67	ASN	CA-CB-CG	6.41	119.01	112.60
1	E	401	GLN	CA-C-O	-6.39	113.78	120.55
1	B	67	ASN	CA-CB-CG	6.29	118.89	112.60
1	G	437	LYS	N-CA-C	-6.21	105.19	112.89
1	F	289	ASN	CA-CB-CG	6.20	118.80	112.60
1	E	67	ASN	CA-CB-CG	6.08	118.68	112.60
1	D	64	GLN	OE1-CD-NE2	6.06	128.66	122.60
1	D	135	ASN	O-C-N	6.04	130.04	122.55
1	D	295	GLN	N-CA-C	-6.01	104.07	111.40
1	F	130	PHE	CA-CB-CG	5.99	119.79	113.80
1	G	280	VAL	O-C-N	5.95	129.27	123.03
1	E	343	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	G	88	ASN	CA-CB-CG	5.82	118.42	112.60
1	E	136	ASN	O-C-N	5.81	127.08	121.56
1	E	500	ASP	CA-CB-CG	5.80	118.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	GLN	CB-CG-CD	-5.79	102.76	112.60
1	E	371	PHE	CA-CB-CG	5.66	119.46	113.80
1	F	550	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	401	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	B	371	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	122	LYS	CB-CA-C	5.63	119.41	111.86
1	E	135	ASN	CA-CB-CG	5.63	118.23	112.60
1	E	281	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	G	469	ASP	CA-CB-CG	5.62	118.22	112.60
1	F	560	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	130	PHE	CA-CB-CG	5.59	119.39	113.80
1	E	384	TYR	CA-C-O	5.58	124.40	119.71
1	H	371	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	522	ALA	N-CA-C	-5.56	103.93	111.55
1	E	560	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	560	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	229	ASP	N-CA-C	-5.52	105.26	111.28
1	C	500	ASP	CA-CB-CG	5.52	118.12	112.60
1	G	434	GLU	CA-C-N	5.51	127.66	120.28
1	G	434	GLU	C-N-CA	5.51	127.66	120.28
1	F	553	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	549	GLY	CA-C-N	5.49	127.90	120.38
1	D	549	GLY	C-N-CA	5.49	127.90	120.38
1	F	487	ASN	OD1-CG-ND2	5.39	128.00	122.60
1	H	134	LYS	CB-CA-C	5.39	118.48	110.62
1	B	198	ILE	CA-C-O	-5.38	114.03	119.20
1	F	289	ASN	N-CA-CB	-5.38	103.80	110.79
1	C	67	ASN	CA-CB-CG	5.36	117.96	112.60
1	G	319	ILE	CA-C-O	-5.34	114.81	120.53
1	D	82	MET	CG-SD-CE	-5.34	89.16	100.90
1	E	130	PHE	CA-CB-CG	5.34	119.14	113.80
1	B	88	ASN	CA-CB-CG	5.32	117.92	112.60
1	A	482	THR	CA-CB-OG1	-5.31	101.63	109.60
1	B	220	GLN	N-CA-C	-5.30	105.50	111.28
1	B	317	ASP	CA-C-O	-5.29	114.81	120.42
1	G	560	ASP	CA-CB-CG	5.27	117.87	112.60
1	G	315	ASN	CA-CB-CG	-5.26	107.34	112.60
1	E	308	ILE	N-CA-C	-5.26	105.59	110.53
1	H	455	ARG	N-CA-C	-5.24	105.56	111.28
1	D	134	LYS	CB-CA-C	5.23	118.26	110.62
1	G	319	ILE	O-C-N	5.23	129.22	123.10
1	D	550	ASP	CA-C-O	-5.22	115.00	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	229	ASP	CA-CB-CG	5.18	117.78	112.60
1	E	553	ASP	CA-CB-CG	5.18	117.78	112.60
1	G	482	THR	CA-CB-OG1	-5.17	101.84	109.60
1	E	482	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	67	ASN	CA-CB-CG	5.17	117.77	112.60
1	B	281	ASN	CA-CB-CG	5.17	117.77	112.60
1	E	207	GLY	CA-C-O	-5.16	117.27	121.76
1	B	198	ILE	O-C-N	5.15	127.28	122.23
1	H	247	GLY	CA-C-O	-5.15	114.95	121.44
1	C	289	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	548	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	F	353	ASP	CA-C-N	5.10	127.32	120.58
1	F	353	ASP	C-N-CA	5.10	127.32	120.58
1	G	517	PRO	N-CA-CB	5.08	107.84	103.31
1	H	550	ASP	CA-CB-CG	5.08	117.68	112.60
1	H	432	THR	CA-CB-OG1	-5.07	102.00	109.60
1	C	377	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	177	ASP	N-CA-C	-5.04	105.67	111.07
1	D	455	ARG	NE-CZ-NH2	5.03	123.72	119.20
1	C	432	THR	CA-C-O	-5.02	115.20	120.92
1	H	395	THR	N-CA-C	-5.01	105.71	111.07
1	H	289	ASN	CA-CB-CG	5.00	117.60	112.60

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	10	0
1	B	4266	0	4088	13	0
1	C	4313	0	4151	15	0
1	D	4317	0	4139	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4305	0	4150	12	0
1	F	4406	0	4232	13	0
1	G	4382	0	4206	19	0
1	H	4356	0	4161	21	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	0	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	2	0
5	B	590	0	0	4	0
5	C	608	0	0	6	0
5	D	713	0	0	12	0
5	E	720	0	0	6	0
5	F	672	0	0	4	0
5	G	721	0	0	9	0
5	H	596	0	0	12	0
All	All	40015	0	33484	113	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 (113) 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:C:452:LYS:HE2	5:C:1086:HOH:O	1.56	1.06
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:D:76:LYS:HE2	5:D:936:HOH:O	1.80	0.80
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: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
4:D:609:N8V:H18	5:D:1017:HOH:O	1.92	0.70
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: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:HA	1:D:575:GLN:OE1	1.93	0.67
1:D:382[B]:THR:HG22	5:D:1067:HOH:O	1.94	0.67
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	0.63
1:C:34:HIS:HB3	5:D:869:HOH:O	1.99	0.62
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: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:E:419:GLN:C	5:E:706:HOH:O	2.49	0.54
1:B:480:TRP:CG	1:B:481:VAL:H	2.26	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: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:382[B]:THR:HG22	5:H:1057:HOH:O	2.09	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: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:E:480:TRP:CG	1:E:481:VAL:H	2.31	0.49
1:G:421:GLN:CA	5:G:703:HOH:O	2.28	0.48
1:A:480:TRP:CG	1:A:481:VAL:H	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415[A]:ARG:CZ	5:C:710:HOH:O	2.62	0.48
1:C:480:TRP:CG	1:C:481:VAL:H	2.31	0.48
1:D:45:ASN:ND2	5:D:711:HOH:O	2.47	0.47
1:H:480:TRP:CG	1:H:481:VAL:H	2.33	0.47
1:C:415[A]:ARG:NH2	5:C:710:HOH:O	2.48	0.47
1:E:420:GLY:N	5:E:706:HOH:O	2.48	0.47
1:G:480:TRP:CG	1:G:481:VAL:H	2.33	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:F:480:TRP:CG	1:F:481:VAL:H	2.33	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:384:TYR:CD1	1:B:385:PRO:HA	2.51	0.46
1:B:455:ARG:NH1	5:B:707:HOH:O	2.44	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:B:318:LEU:C	1:B:318:LEU:HD12	2.42	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: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: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:99:ILE:O	1:B:106:PHE:HA	2.18	0.43
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.53	0.43
1:F:415[A]:ARG:NH1	5:F:702[A]:HOH:O	2.03	0.43
1:C:367:GLY:HA2	1:C:417[A]:SER:OG	2.19	0.43
1:C:384:TYR:CG	1:C:385:PRO:HA	2.53	0.43
1:D:480:TRP:CG	1:D:481:VAL:H	2.36	0.43
1:A:63[A]:SER:HB3	1:A:85:MET:SD	2.58	0.42
1:F:318:LEU:C	1:F:318:LEU:HD12	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:318:LEU:C	1:E:318:LEU:HD12	2.44	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:113[B]:VAL:HG12	5:H:1111:HOH:O	2.19	0.41
1:H:481:VAL:O	1:H:482:THR:C	2.64	0.41
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:C:541:TRP:CG	1:C:566:ARG:HH11	2.39	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:G:318:LEU:C	1:G:318:LEU:HD12	2.46	0.41
1:G:419:GLN:C	5:G:709:HOH:O	2.64	0.41
1:D:367:GLY:HA2	1:D:417[A]:SER:OG	2.20	0.40
1:H:318:LEU:C	1:H:318:LEU:HD12	2.47	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:F:342:ASP:OD1	1:F:342:ASP:C	2.65	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 ⓘ

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	546/550 (99%)	530 (97%)	15 (3%)	1 (0%)	43	21
1	B	539/550 (98%)	519 (96%)	19 (4%)	1 (0%)	43	21
1	C	542/550 (98%)	520 (96%)	22 (4%)	0	100	100
1	D	546/550 (99%)	527 (96%)	19 (4%)	0	100	100
1	E	543/550 (99%)	527 (97%)	15 (3%)	1 (0%)	43	21
1	F	558/550 (102%)	537 (96%)	20 (4%)	1 (0%)	43	21
1	G	555/550 (101%)	533 (96%)	22 (4%)	0	100	100
1	H	550/550 (100%)	530 (96%)	18 (3%)	2 (0%)	30	11
All	All	4379/4400 (100%)	4223 (96%)	150 (3%)	6 (0%)	48	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	ALA
1	H	491	ALA
1	B	491	ALA
1	E	491	ALA
1	F	491	ALA
1	H	138	PRO

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	438/461 (95%)	436 (100%)	2 (0%)	81	64
1	B	439/461 (95%)	436 (99%)	3 (1%)	76	54
1	C	445/461 (96%)	442 (99%)	3 (1%)	76	54
1	D	445/461 (96%)	443 (100%)	2 (0%)	84	70
1	E	445/461 (96%)	442 (99%)	3 (1%)	76	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	453/461 (98%)	446 (98%)	7 (2%)	57 25
1	G	450/461 (98%)	446 (99%)	4 (1%)	70 46
1	H	448/461 (97%)	446 (100%)	2 (0%)	84 70
All	All	3563/3688 (97%)	3537 (99%)	26 (1%)	78 54

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	437	LYS
1	B	82[A]	MET
1	B	82[B]	MET
1	B	136	ASN
1	C	136	ASN
1	C	419	GLN
1	C	537	GLU
1	D	82	MET
1	D	136	ASN
1	E	136	ASN
1	E	173	THR
1	E	440	ASN
1	F	136	ASN
1	F	169[A]	LEU
1	F	169[B]	LEU
1	F	525	LYS
1	F	537	GLU
1	F	566[A]	ARG
1	F	566[B]	ARG
1	G	76	LYS
1	G	136	ASN
1	G	382[A]	THR
1	G	382[B]	THR
1	H	136	ASN
1	H	537	GLU

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

Mol	Chain	Res	Type
1	A	64	GLN
1	A	307	HIS

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Mol	Chain	Res	Type
1	A	440	ASN
1	A	487	ASN
1	B	498	GLN
1	C	64	GLN
1	C	233	GLN
1	C	354	GLN
1	C	487	ASN
1	D	105	GLN
1	D	354	GLN
1	D	451	HIS
1	E	105	GLN
1	E	275	ASN
1	E	451	HIS
1	F	275	ASN
1	F	498	GLN
1	G	64	GLN
1	G	275	ASN
1	G	354	GLN
1	G	419	GLN
1	H	31	HIS

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 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	E	605	-	3,3,3	1.07	0	3,3,3	0.74	0
4	N8V	A	606	-	20,20,20	1.35	3 (15%)	18,25,25	1.33	1 (5%)
3	ACT	F	604	-	3,3,3	1.24	0	3,3,3	0.95	0
3	ACT	A	602	-	3,3,3	1.37	0	3,3,3	0.58	0
3	ACT	H	602	-	3,3,3	1.46	1 (33%)	3,3,3	0.92	0
4	N8V	G	610	-	20,20,20	1.68	3 (15%)	18,25,25	1.74	3 (16%)
3	ACT	G	603	-	3,3,3	1.38	0	3,3,3	0.59	0
4	N8V	D	609	-	20,20,20	1.87	4 (20%)	18,25,25	1.54	3 (16%)
4	N8V	F	607	-	20,20,20	2.14	3 (15%)	18,25,25	1.58	3 (16%)
3	ACT	E	604	-	3,3,3	1.40	0	3,3,3	0.93	0
3	ACT	G	606	-	3,3,3	1.09	0	3,3,3	1.13	0
3	ACT	E	607	-	3,3,3	1.38	0	3,3,3	0.62	0
3	ACT	G	604	-	3,3,3	0.62	0	3,3,3	1.20	0
3	ACT	D	605	-	3,3,3	0.86	0	3,3,3	1.02	0
3	ACT	F	605	-	3,3,3	0.81	0	3,3,3	0.56	0
3	ACT	G	605	-	3,3,3	1.24	0	3,3,3	0.74	0
3	ACT	B	603	-	3,3,3	0.83	0	3,3,3	1.11	0
4	N8V	B	607	-	20,20,20	1.84	5 (25%)	18,25,25	1.37	2 (11%)
4	N8V	H	607	-	20,20,20	1.49	5 (25%)	18,25,25	1.31	3 (16%)
4	N8V	E	611	-	14,14,20	2.32	3 (21%)	12,19,25	1.42	2 (16%)
3	ACT	B	602	-	3,3,3	0.67	0	3,3,3	1.15	0
3	ACT	D	604	-	3,3,3	1.13	0	3,3,3	1.19	0
3	ACT	E	606	-	3,3,3	1.14	0	3,3,3	0.81	0
4	N8V	C	606	-	16,16,20	1.65	3 (18%)	14,21,25	1.92	2 (14%)
3	ACT	C	603	-	3,3,3	1.38	0	3,3,3	0.26	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	B	607	-	-	1/11/31/31	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	607	N8V	C4-C5	-7.86	1.45	1.51
4	E	611	N8V	C4-C5	-5.94	1.46	1.51
4	D	609	N8V	C4-C5	-5.88	1.46	1.51
4	B	607	N8V	C4-C5	-4.96	1.47	1.51
4	C	606	N8V	C2-C1	4.61	1.58	1.53
4	E	611	N8V	C2-C1	4.24	1.58	1.53
4	G	610	N8V	C1-N8	3.84	1.55	1.47
4	E	611	N8V	C1-N8	3.49	1.54	1.47
4	F	607	N8V	O4-C4	3.39	1.48	1.42
4	G	610	N8V	C10-C9	3.37	1.64	1.51
4	A	606	N8V	C1-C7	-3.28	1.45	1.50
4	D	609	N8V	C1-N8	3.28	1.54	1.47
4	H	607	N8V	C2-C1	3.08	1.56	1.53
4	B	607	N8V	O4-C4	2.94	1.47	1.42
4	D	609	N8V	C2-C1	2.81	1.56	1.53
4	H	607	N8V	O2-C2	2.71	1.49	1.43
4	B	607	N8V	C1-C7	2.68	1.54	1.50
4	H	607	N8V	C4-C5	-2.61	1.49	1.51
4	B	607	N8V	C2-C1	2.61	1.56	1.53
4	A	606	N8V	C4-C5	-2.58	1.49	1.51
4	A	606	N8V	C7-C5	2.58	1.36	1.32
4	B	607	N8V	C1-N8	2.53	1.52	1.47
4	F	607	N8V	O2-C2	2.52	1.49	1.43
4	D	609	N8V	C1-C7	-2.31	1.47	1.50
4	C	606	N8V	C7-C5	-2.28	1.29	1.32
4	H	607	N8V	O4-C4	2.22	1.46	1.42
3	H	602	ACT	CH3-C	2.14	1.57	1.49
4	C	606	N8V	C6-C5	2.11	1.56	1.50
4	H	607	N8V	C7-C5	2.08	1.35	1.32
4	G	610	N8V	C2-C1	2.08	1.55	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	606	N8V	C3-C4-C5	-5.96	102.30	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	609	N8V	C3-C4-C5	-4.97	103.86	111.67
4	G	610	N8V	C3-C4-C5	-4.95	103.89	111.67
4	F	607	N8V	C7-C1-N8	-4.27	104.63	110.71
4	E	611	N8V	C7-C1-N8	-3.69	105.46	110.71
4	G	610	N8V	C7-C1-N8	-3.23	106.11	110.71
4	A	606	N8V	C3-C4-C5	-3.19	106.65	111.67
4	H	607	N8V	C3-C4-C5	-3.17	106.68	111.67
4	B	607	N8V	C7-C1-N8	-2.91	106.57	110.71
4	C	606	N8V	C7-C1-N8	-2.80	106.72	110.71
4	B	607	N8V	C3-C4-C5	-2.69	107.44	111.67
4	F	607	N8V	C3-C4-C5	-2.60	107.58	111.67
4	H	607	N8V	O4-C4-C3	-2.43	105.49	110.53
4	D	609	N8V	O2-C2-C1	2.22	113.44	109.08
4	G	610	N8V	O3-C3-C4	-2.19	105.31	109.64
4	H	607	N8V	O4-C4-C5	2.15	114.85	110.75
4	E	611	N8V	O4-C4-C3	-2.07	106.22	110.53
4	D	609	N8V	O4-C4-C3	-2.06	106.25	110.53
4	F	607	N8V	C14-C13-C12	-2.01	104.23	114.37

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

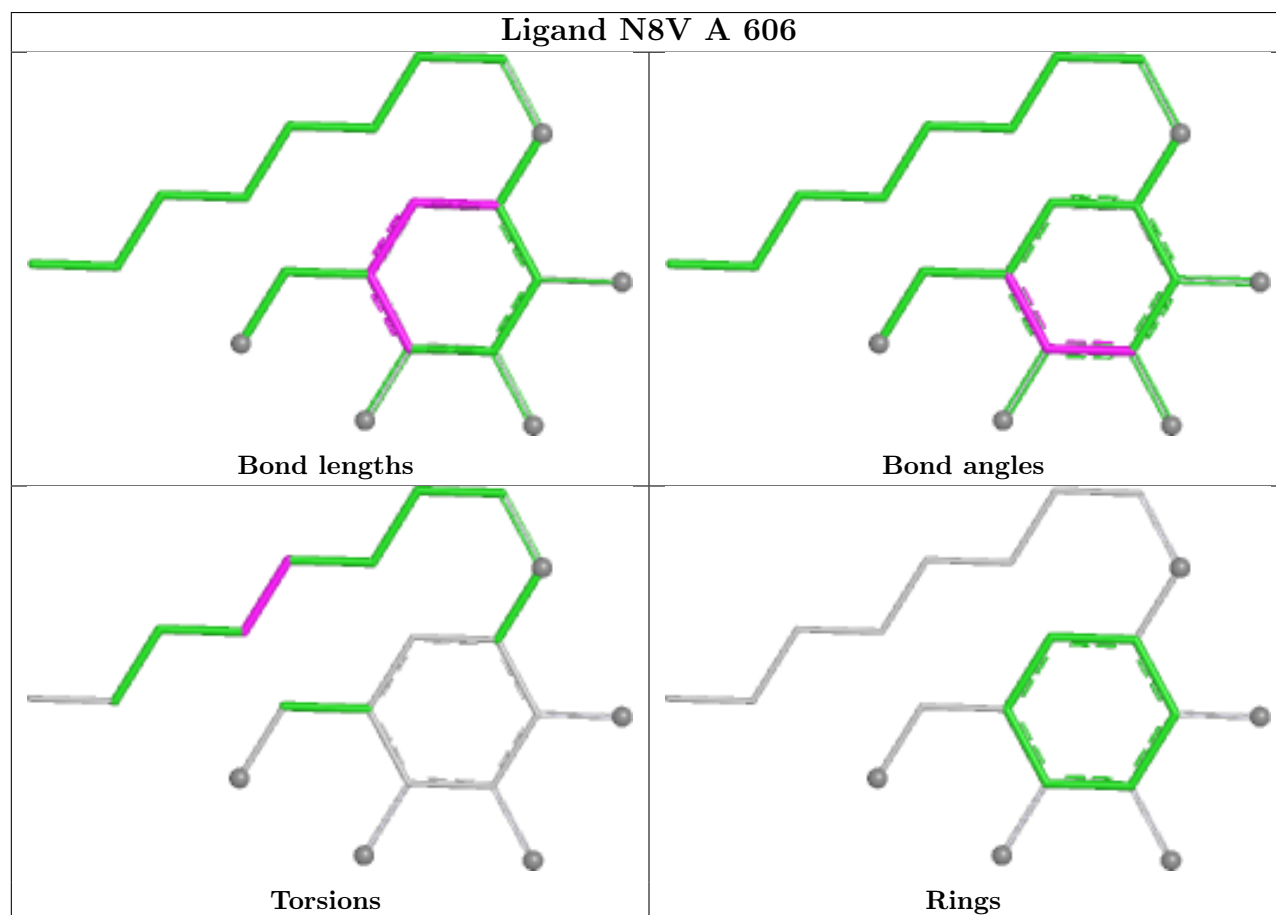
There are no ring outliers.

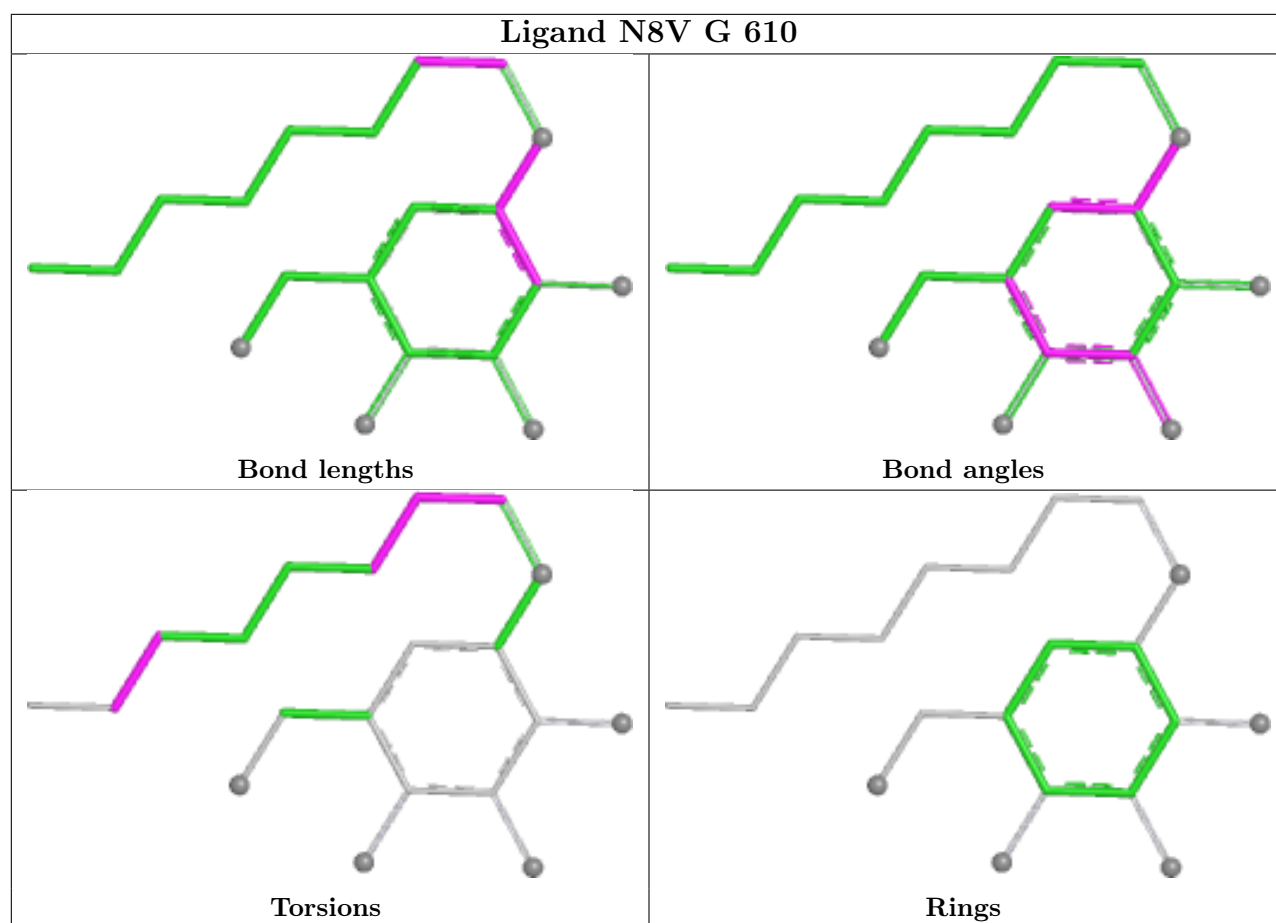
3 monomers are involved in 3 short contacts:

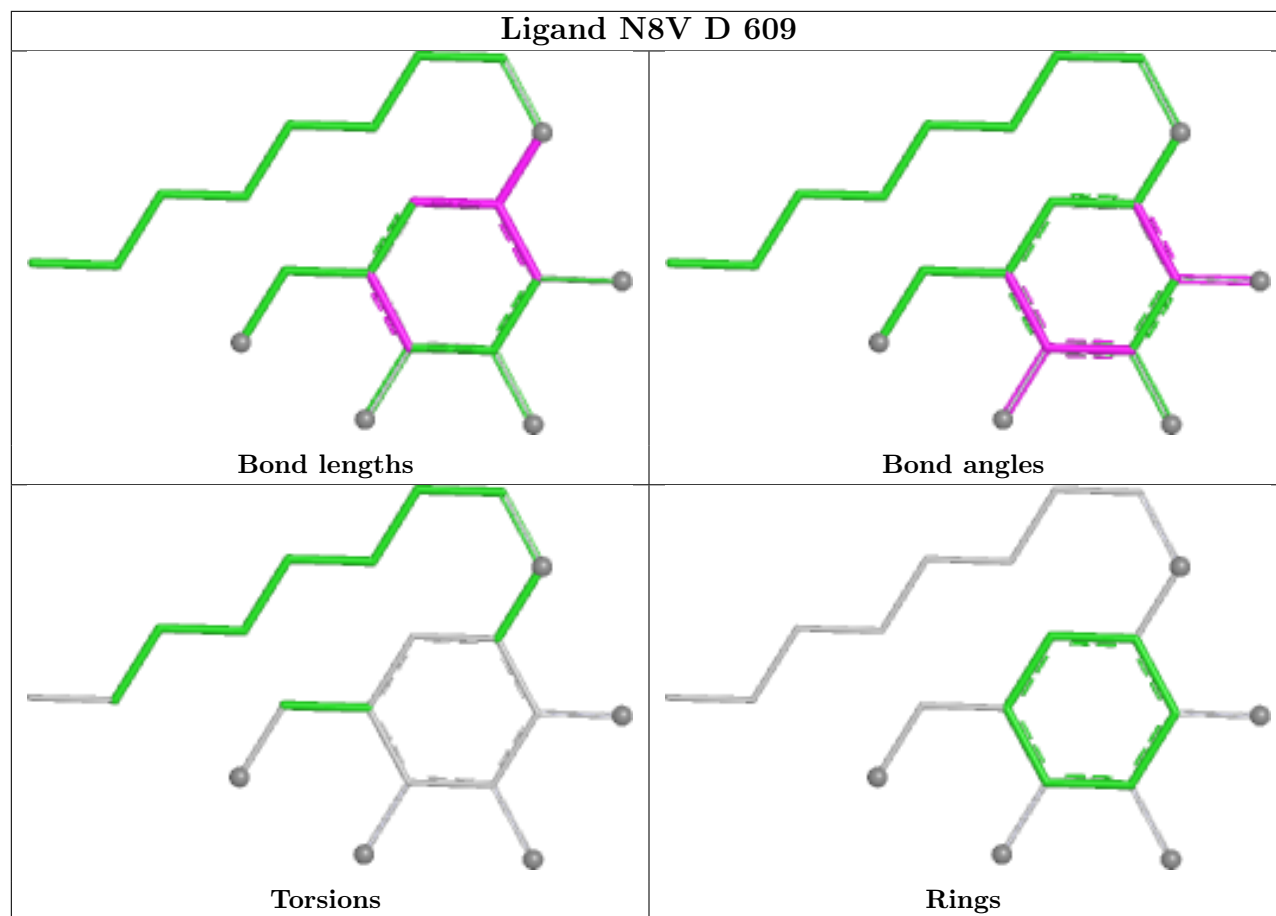
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	610	N8V	1	0
4	D	609	N8V	1	0
3	G	604	ACT	1	0

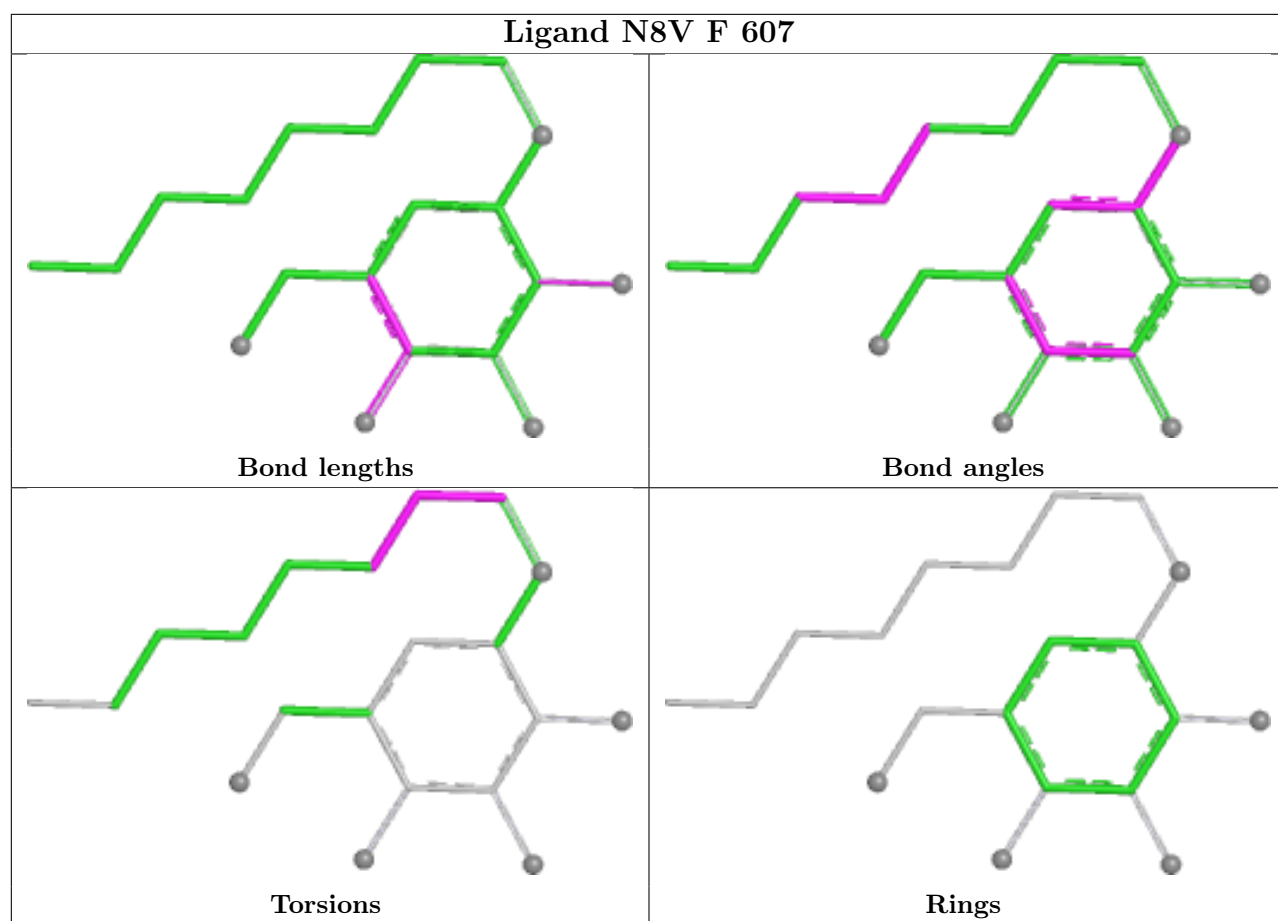
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

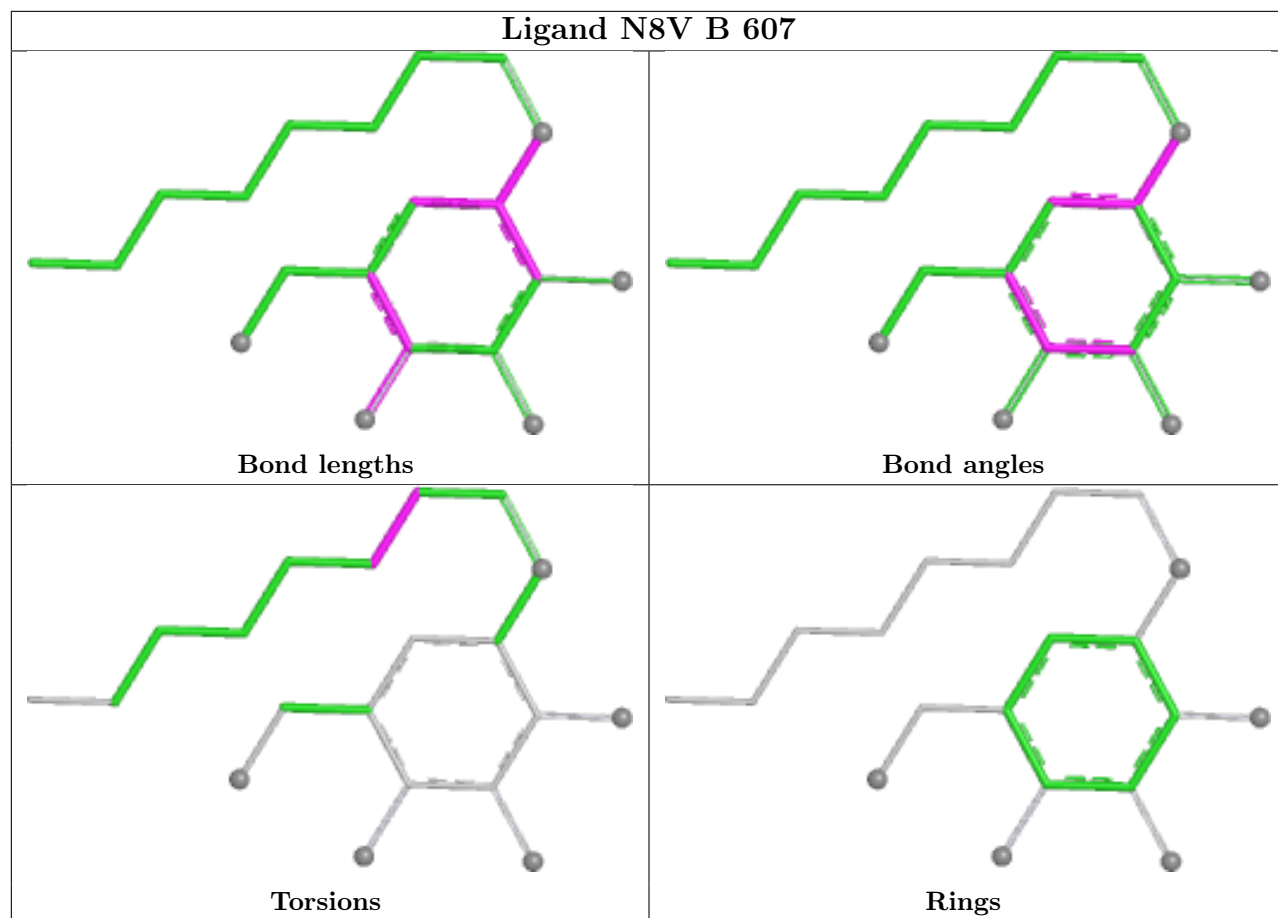
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

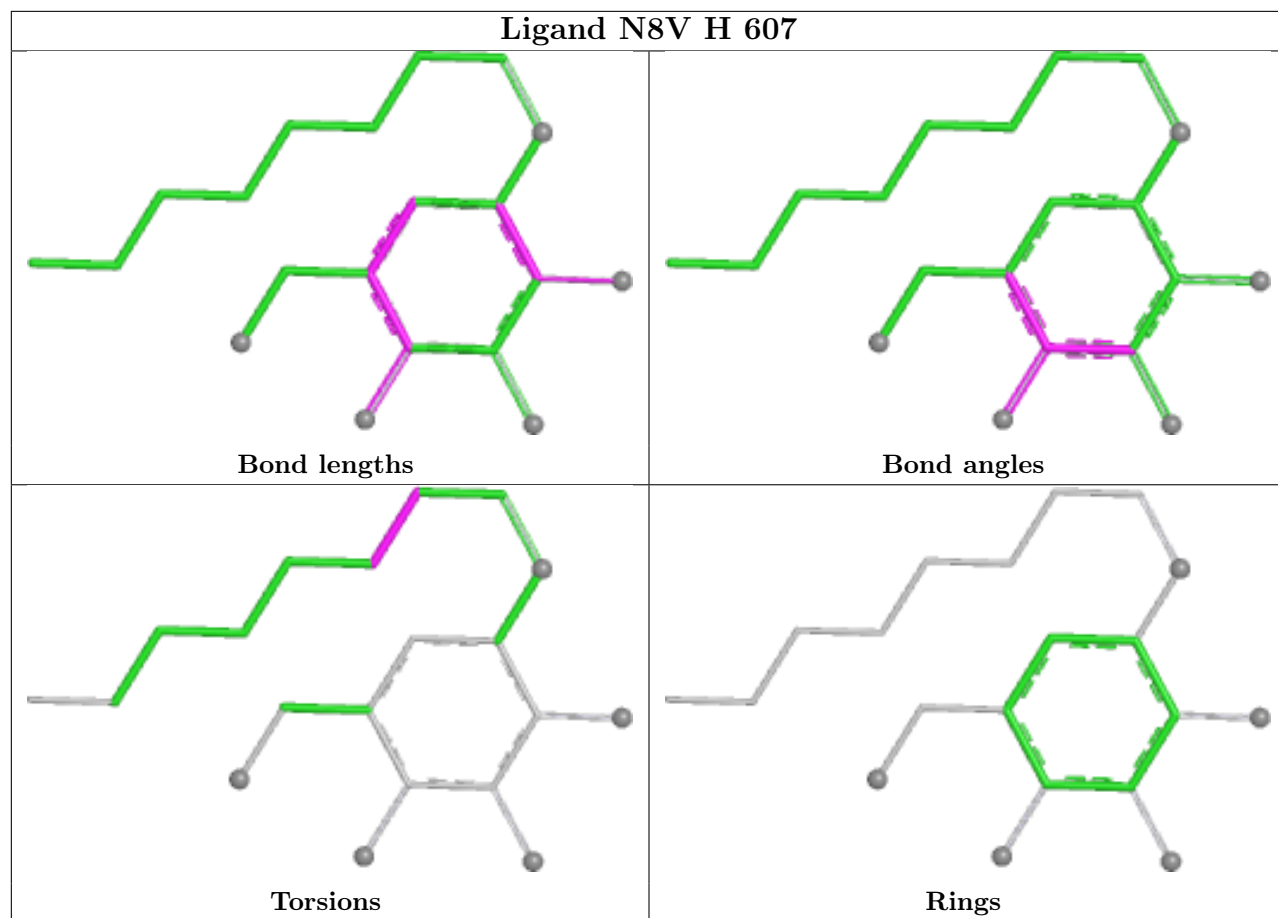


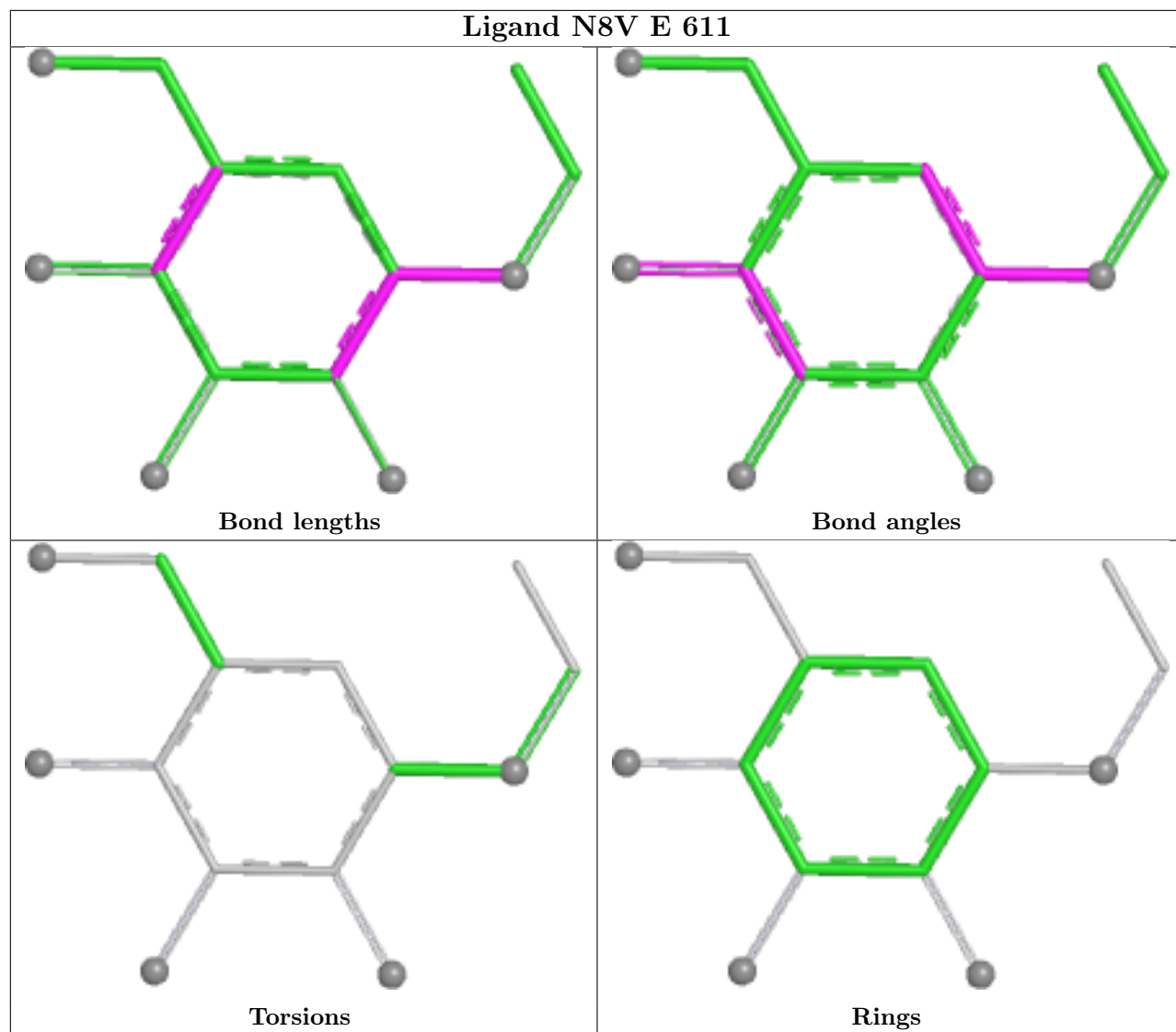


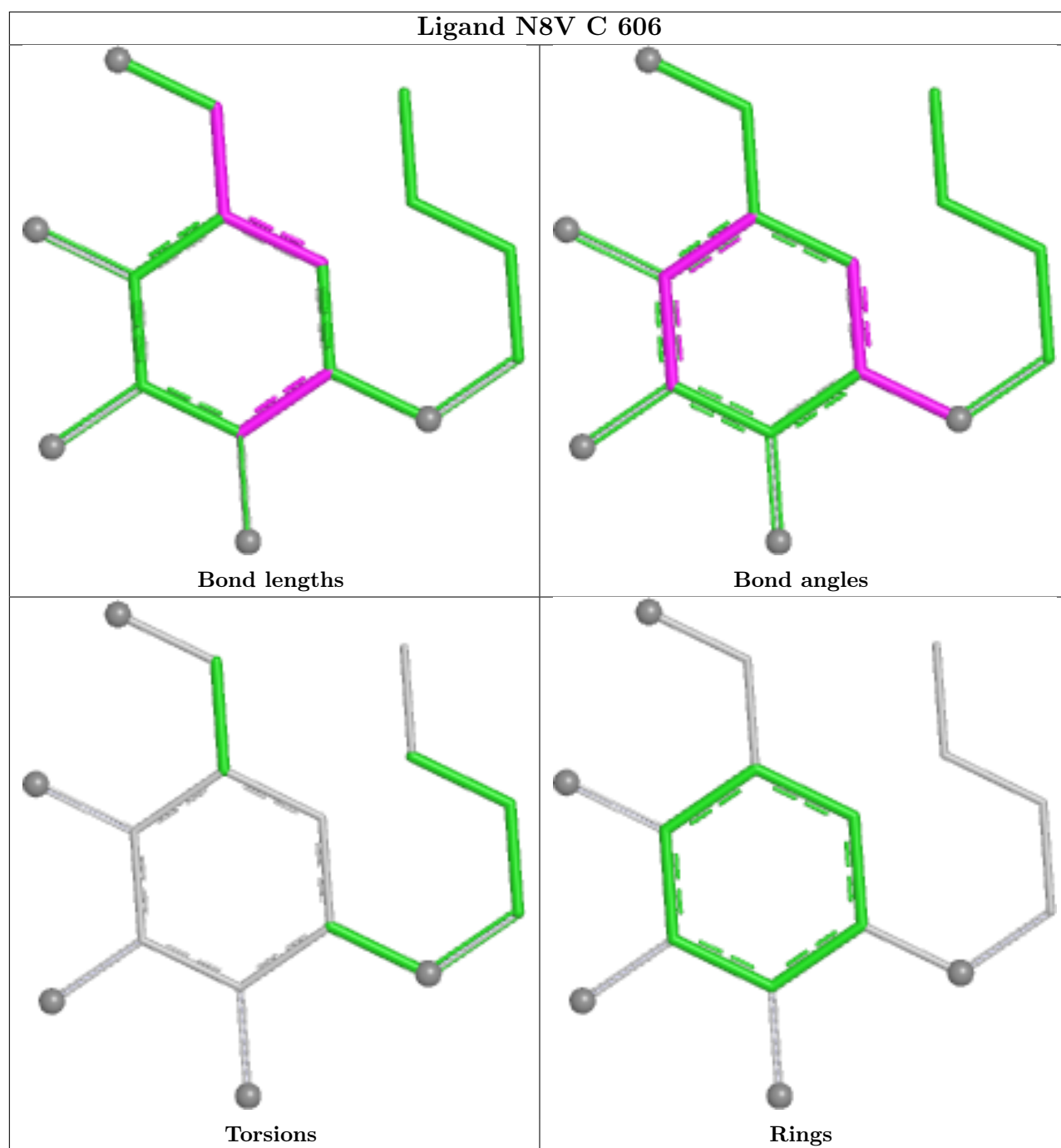












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	540/550 (98%)	0.01	23 (4%)	40	42	10, 24, 40, 60	50 (9%)
1	B	534/550 (97%)	-0.21	11 (2%)	63	66	10, 22, 36, 58	30 (5%)
1	C	536/550 (97%)	-0.19	13 (2%)	59	62	9, 22, 36, 65	35 (6%)
1	D	539/550 (98%)	-0.35	13 (2%)	59	62	9, 19, 33, 65	35 (6%)
1	E	538/550 (97%)	-0.41	7 (1%)	75	78	9, 19, 34, 49	33 (6%)
1	F	539/550 (98%)	-0.28	10 (1%)	66	68	7, 20, 39, 72	46 (8%)
1	G	540/550 (98%)	-0.32	16 (2%)	52	55	8, 19, 35, 63	43 (7%)
1	H	538/550 (97%)	-0.10	16 (2%)	52	55	10, 22, 35, 63	56 (10%)
All	All	4304/4400 (97%)	-0.23	109 (2%)	58	60	7, 21, 37, 72	328 (7%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	438	ILE	12.1
1	A	438	ILE	11.7
1	G	438	ILE	11.2
1	F	438	ILE	10.0
1	B	439	TRP	9.7
1	A	441	ALA	8.9
1	D	438	ILE	8.6
1	C	444	THR	8.6
1	G	36	ALA	8.3
1	E	439	TRP	8.3
1	D	435	THR	8.2
1	E	443	ALA	7.9
1	A	36	ALA	7.6
1	C	443	ALA	7.6
1	G	441	ALA	7.6
1	C	435	THR	7.6

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Mol	Chain	Res	Type	RSRZ
1	D	439	TRP	7.5
1	B	438	ILE	7.5
1	H	447	GLU	7.5
1	F	439	TRP	7.4
1	F	441	ALA	7.4
1	E	36	ALA	7.2
1	H	448	LYS	7.0
1	F	440	ASN	6.9
1	A	436	GLN	6.7
1	C	442	GLU	6.7
1	C	434	GLU	6.6
1	A	439	TRP	6.6
1	A	445	PRO	6.3
1	C	445	PRO	6.3
1	A	435	THR	6.3
1	G	443	ALA	6.1
1	H	435	THR	5.9
1	G	439	TRP	5.9
1	A	443	ALA	5.9
1	H	434	GLU	5.6
1	G	445	PRO	5.6
1	E	438	ILE	5.6
1	D	445	PRO	5.5
1	F	443	ALA	5.4
1	G	435	THR	5.3
1	H	31	HIS	5.3
1	H	446	GLU	5.2
1	G	437	LYS	5.2
1	A	437	LYS	5.1
1	G	434	GLU	5.1
1	B	440	ASN	5.0
1	E	440	ASN	5.0
1	D	441	ALA	4.9
1	G	444	THR	4.9
1	B	434	GLU	4.9
1	A	444	THR	4.9
1	B	446	GLU	4.8
1	B	575	GLN	4.8
1	F	442	GLU	4.8
1	C	433	THR	4.8
1	G	442	GLU	4.7
1	G	440	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	434	GLU	4.4
1	C	36	ALA	4.3
1	H	32	HIS	4.3
1	H	36	ALA	4.3
1	B	435	THR	4.3
1	D	442	GLU	4.2
1	B	436	GLN	4.1
1	D	444	THR	4.1
1	B	437	LYS	4.0
1	D	36	ALA	4.0
1	A	446	GLU	3.9
1	A	442	GLU	3.9
1	E	445	PRO	3.7
1	A	575	GLN	3.7
1	C	446	GLU	3.6
1	H	437	LYS	3.6
1	A	440	ASN	3.6
1	C	34	HIS	3.4
1	H	521	LEU	3.4
1	F	445	PRO	3.4
1	D	446	GLU	3.4
1	F	444	THR	3.3
1	A	237	LEU	3.3
1	D	443	ALA	3.3
1	A	523	GLY	3.3
1	F	435	THR	3.2
1	G	229[A]	ASP	3.2
1	A	521	LEU	3.0
1	C	521	LEU	2.9
1	B	447	GLU	2.8
1	A	236	GLN	2.8
1	A	448	LYS	2.8
1	A	433	THR	2.7
1	H	522	ALA	2.7
1	H	449	GLU	2.6
1	A	239	PRO	2.6
1	D	448	LYS	2.6
1	H	34	HIS	2.6
1	H	35	HIS	2.5
1	H	33	HIS	2.5
1	F	575	GLN	2.5
1	B	522	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	575	GLN	2.4
1	A	447	GLU	2.4
1	E	444	THR	2.3
1	C	35	HIS	2.3
1	G	575	GLN	2.2
1	D	440	ASN	2.2
1	C	575	GLN	2.2
1	G	446	GLU	2.1
1	G	436	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACT	E	607	4/4	0.86	0.19	20,24,25,26	4
3	ACT	F	604	4/4	0.86	0.16	30,32,32,33	4
3	ACT	F	605	4/4	0.88	0.15	22,27,27,28	4
3	ACT	G	604	4/4	0.88	0.21	43,47,48,53	4
3	ACT	D	604	4/4	0.90	0.13	31,32,38,40	0
3	ACT	H	602	4/4	0.90	0.12	26,27,29,31	4
3	ACT	G	606	4/4	0.91	0.10	31,31,31,34	4
3	ACT	E	604	4/4	0.92	0.14	20,21,22,24	4
3	ACT	G	605	4/4	0.92	0.12	30,34,35,36	4
3	ACT	E	605	4/4	0.93	0.12	31,32,34,37	4
3	ACT	C	603	4/4	0.93	0.19	18,20,21,22	4
3	ACT	D	605	4/4	0.94	0.10	25,25,40,46	4
3	ACT	E	606	4/4	0.94	0.10	29,43,45,47	0
3	ACT	A	602	4/4	0.94	0.09	27,29,29,34	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	G	603	4/4	0.95	0.17	21,22,26,27	4
3	ACT	B	602	4/4	0.96	0.07	32,32,33,34	4
3	ACT	B	603	4/4	0.96	0.10	29,31,33,36	4
2	NA	C	602	1/1	0.97	0.06	35,35,35,35	0
4	N8V	D	609	20/20	0.97	0.09	14,17,39,40	6
2	NA	B	605	1/1	0.98	0.07	42,42,42,42	0
2	NA	H	605	1/1	0.98	0.04	35,35,35,35	1
2	NA	B	606	1/1	0.98	0.08	35,35,35,35	0
4	N8V	B	607	20/20	0.98	0.08	16,19,35,36	6
4	N8V	C	606	16/20	0.98	0.08	16,18,35,40	3
2	NA	C	601	1/1	0.98	0.06	43,43,43,43	0
4	N8V	E	611	14/20	0.98	0.05	15,16,29,35	0
4	N8V	F	607	20/20	0.98	0.06	14,17,38,41	5
4	N8V	G	610	20/20	0.98	0.07	13,16,31,32	6
4	N8V	H	607	20/20	0.98	0.07	15,20,48,51	5
2	NA	H	606	1/1	0.99	0.04	39,39,39,39	0
2	NA	A	604	1/1	0.99	0.10	36,36,36,36	0
2	NA	A	605	1/1	0.99	0.06	31,31,31,31	0
2	NA	B	604	1/1	0.99	0.08	25,25,25,25	0
2	NA	C	604	1/1	0.99	0.10	25,25,25,25	0
2	NA	D	601	1/1	0.99	0.07	22,22,22,22	0
2	NA	D	606	1/1	0.99	0.12	23,23,23,23	0
2	NA	D	607	1/1	0.99	0.11	27,27,27,27	0
2	NA	D	608	1/1	0.99	0.05	24,24,24,24	0
2	NA	E	603	1/1	0.99	0.03	22,22,22,22	0
2	NA	E	608	1/1	0.99	0.09	28,28,28,28	0
2	NA	E	609	1/1	0.99	0.04	40,40,40,40	0
2	NA	E	610	1/1	0.99	0.04	22,22,22,22	0
2	NA	F	601	1/1	0.99	0.06	25,25,25,25	0
2	NA	F	602	1/1	0.99	0.04	25,25,25,25	0
2	NA	F	603	1/1	0.99	0.03	20,20,20,20	0
2	NA	G	601	1/1	0.99	0.07	25,25,25,25	0
2	NA	G	602	1/1	0.99	0.05	20,20,20,20	0
4	N8V	A	606	20/20	0.99	0.06	17,20,35,37	7
2	NA	G	607	1/1	0.99	0.04	27,27,27,27	0
2	NA	G	608	1/1	0.99	0.05	23,23,23,23	0
2	NA	G	609	1/1	0.99	0.03	25,25,25,25	0
2	NA	H	601	1/1	0.99	0.04	32,32,32,32	0
2	NA	H	603	1/1	0.99	0.09	24,24,24,24	0
2	NA	H	604	1/1	0.99	0.06	27,27,27,27	0
2	NA	A	601	1/1	0.99	0.06	32,32,32,32	0
2	NA	C	605	1/1	1.00	0.08	27,27,27,27	0

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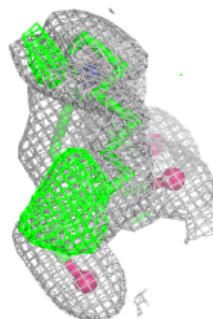
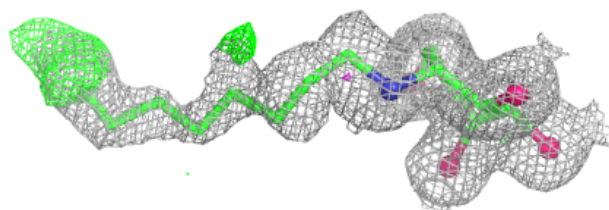
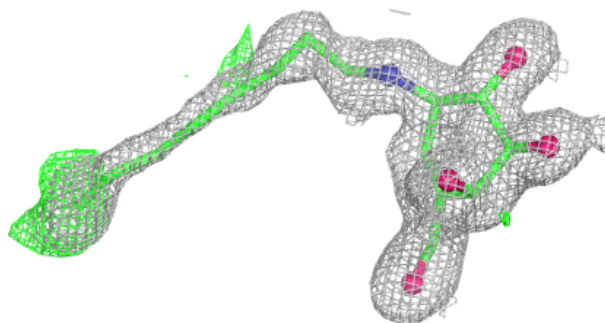
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	A	603	1/1	1.00	0.08	25,25,25,25	0
2	NA	E	601	1/1	1.00	0.03	21,21,21,21	0
2	NA	E	602	1/1	1.00	0.03	20,20,20,20	0
2	NA	F	606	1/1	1.00	0.05	26,26,26,26	0
2	NA	D	602	1/1	1.00	0.04	22,22,22,22	0
2	NA	D	603	1/1	1.00	0.04	20,20,20,20	0
2	NA	B	601	1/1	1.00	0.10	32,32,32,32	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.

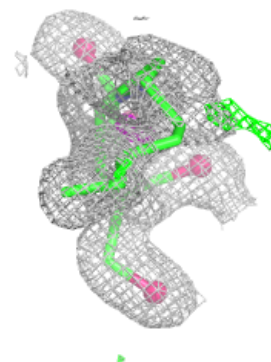
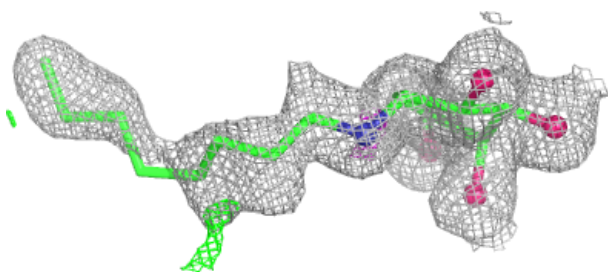
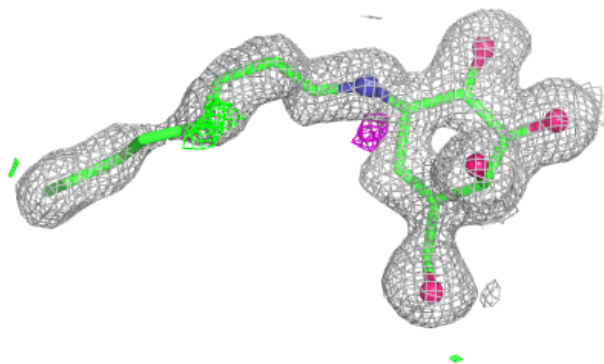
Electron density around N8V D 609:

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

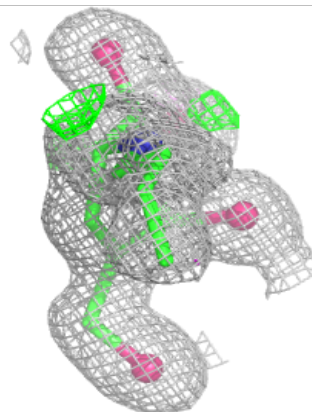
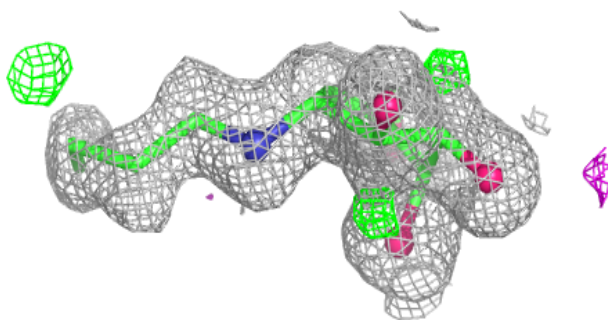
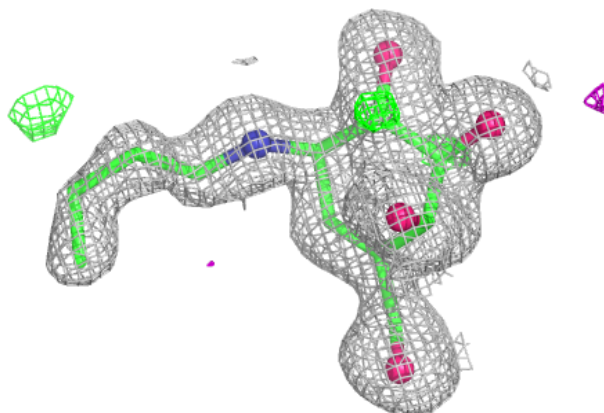


Electron density around N8V B 607:

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

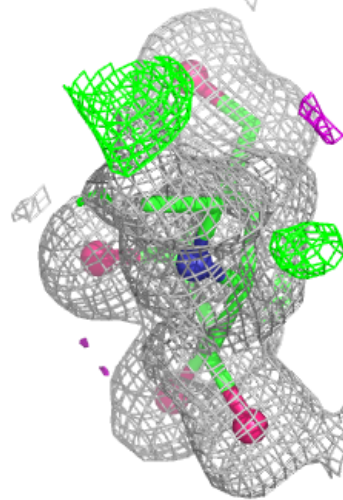
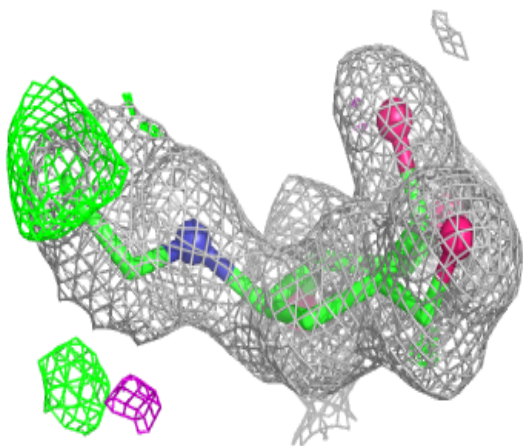
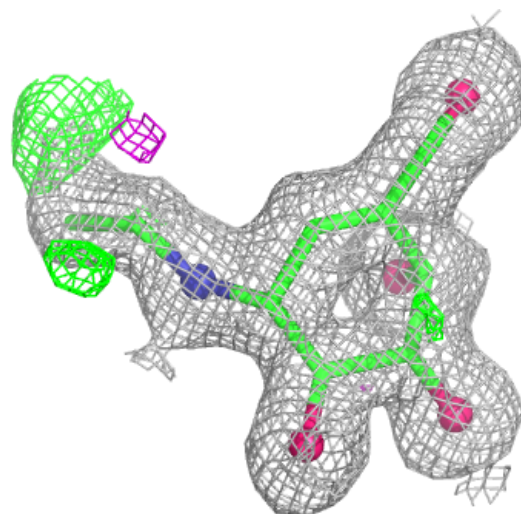
**Electron density around N8V C 606:**

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



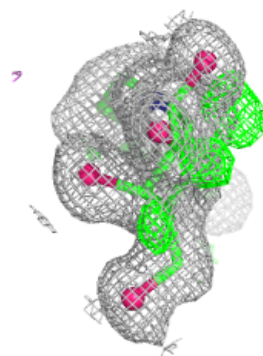
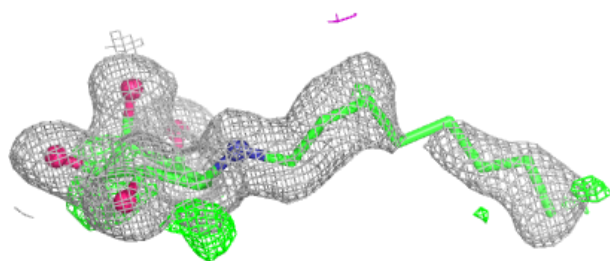
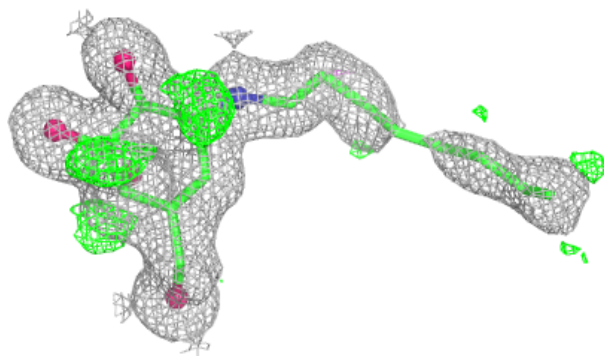
Electron density around N8V E 611:

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

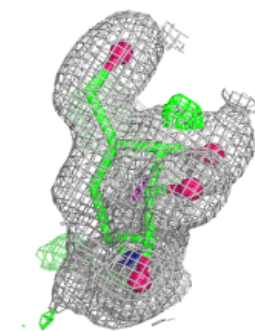
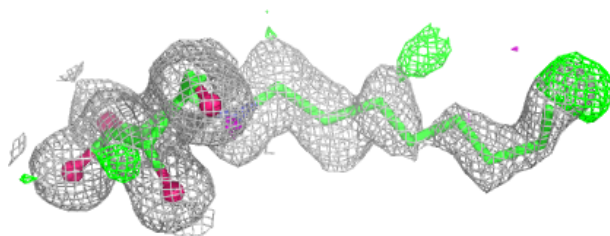
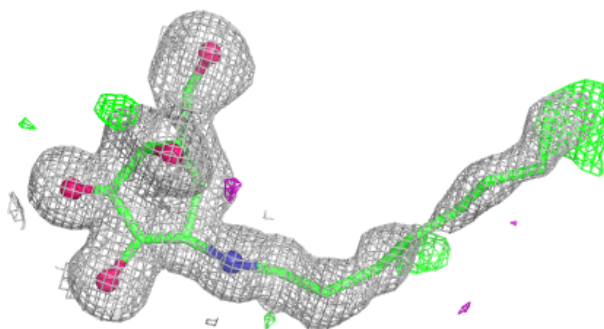


Electron density around N8V F 607:

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

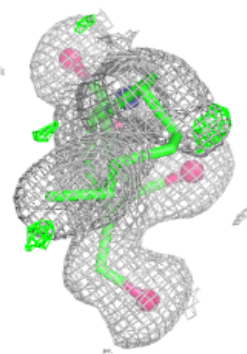
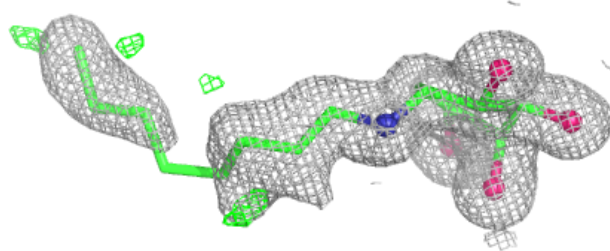
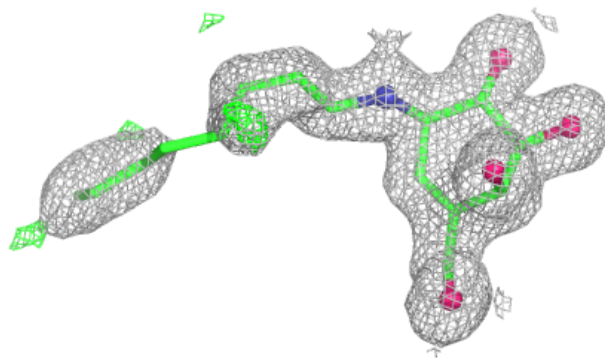
**Electron density around N8V G 610:**

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

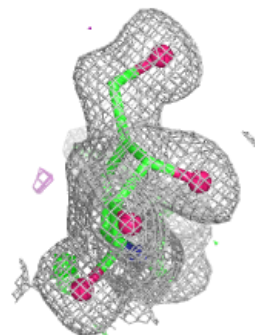
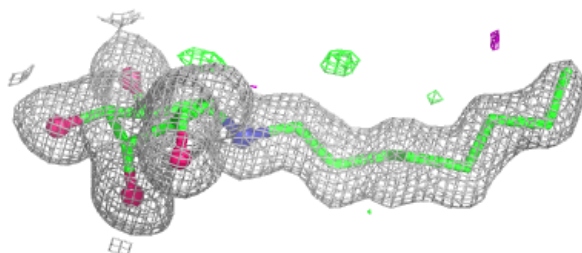
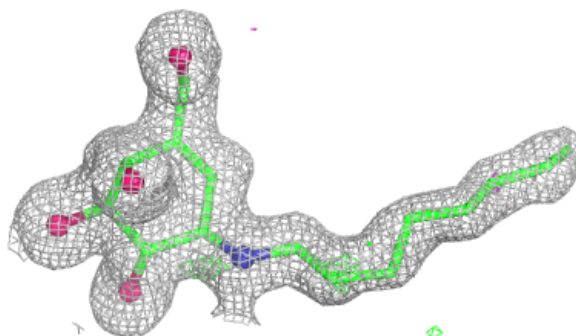


Electron density around N8V H 607:

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

**Electron density around N8V 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.