Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 02:21 PM JST

PDB ID	:	8WKL
Title	:	Rauvolfia serpentina strictosidine synthase (RsSTR) in complex with a non-reactive tryptamine substitute crystallized in P1211 space group
Authors	:	Nitin, K.; Rajakumara, E.
Deposited on	:	2023-09-28
Resolution	:	2.67 Å(reported)

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

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

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

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

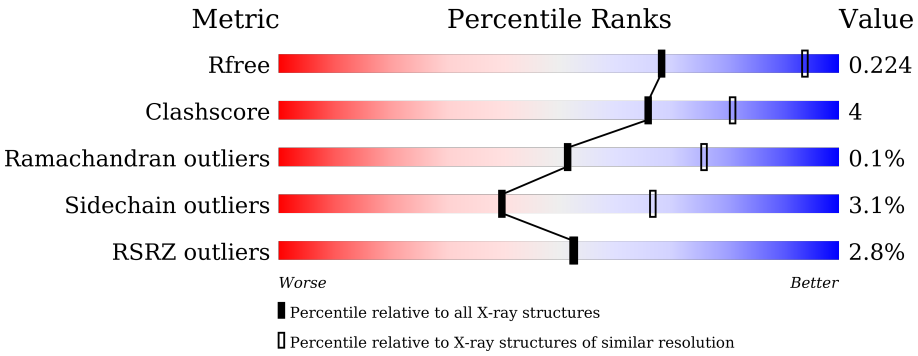
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	81% 12% • 5%
1	B	318	3% 81% 12% • 5%
1	C	318	84% 9% • 5%
1	D	318	83% 12% 5%
1	E	318	4% 85% 8% • 5%
1	F	318	4% 82% 12% • •

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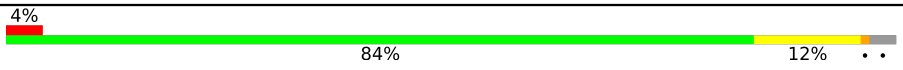
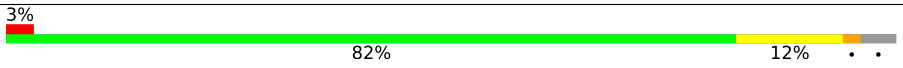
Mol	Chain	Length	Quality of chain
1	G	318	
1	H	318	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	F66	A	401	-	-	-	X
2	F66	B	401	-	-	-	X
2	F66	G	401	-	-	-	X
3	PEG	F	402	-	-	-	X
3	PEG	H	402	-	-	-	X

2 Entry composition (i)

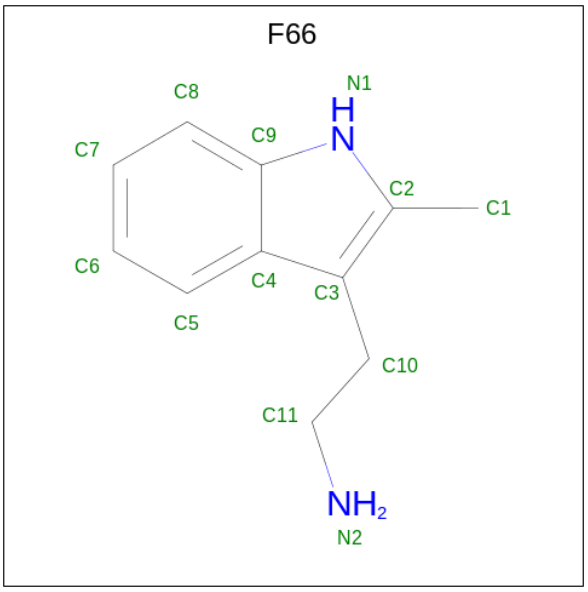
There are 4 unique types of molecules in this entry. The entry contains 19548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Strictosidine synthase.

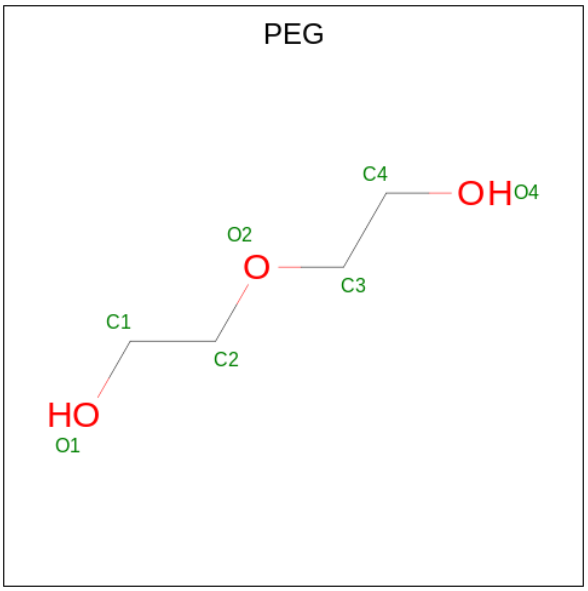
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	1	0
			2389	1535	387	462	5			
1	B	302	Total	C	N	O	S	0	2	0
			2386	1533	388	461	4			
1	C	302	Total	C	N	O	S	0	1	0
			2380	1529	386	460	5			
1	D	302	Total	C	N	O	S	0	2	0
			2395	1538	391	461	5			
1	E	302	Total	C	N	O	S	0	1	0
			2381	1529	387	460	5			
1	F	304	Total	C	N	O	S	0	1	0
			2391	1534	389	463	5			
1	G	307	Total	C	N	O	S	0	0	0
			2407	1546	391	465	5			
1	H	304	Total	C	N	O	S	0	0	0
			2383	1529	387	462	5			

- Molecule 2 is 2-(2-methyl-1H-indol-3-yl)ethanamine (three-letter code: F66) (formula: $C_{11}H_{14}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 13 11 2	0	0
2	B	1	Total C N 13 11 2	0	0
2	C	1	Total C N 13 11 2	0	0
2	D	1	Total C N 13 11 2	0	0
2	E	1	Total C N 13 11 2	0	0
2	F	1	Total C N 13 11 2	0	0
2	G	1	Total C N 13 11 2	0	0
2	H	1	Total C N 13 11 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	45	Total O 45 45	0	0
4	B	41	Total O 41 41	0	0
4	C	31	Total O 31 31	0	0
4	D	51	Total O 51 51	0	0
4	E	22	Total O 22 22	0	0
4	F	35	Total O 35 35	0	0

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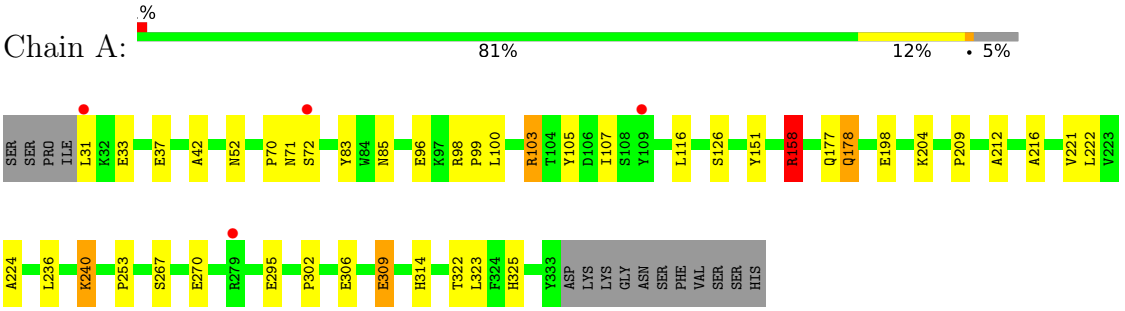
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	20	Total O 20 20	0	0
4	H	45	Total O 45 45	0	0

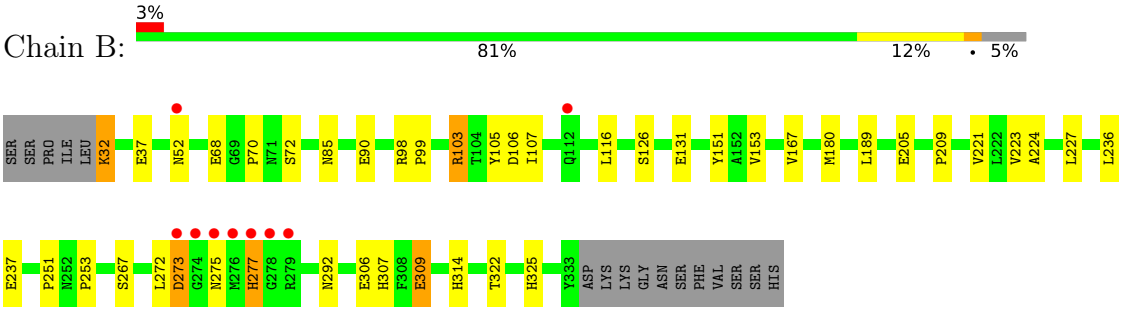
3 Residue-property plots

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.

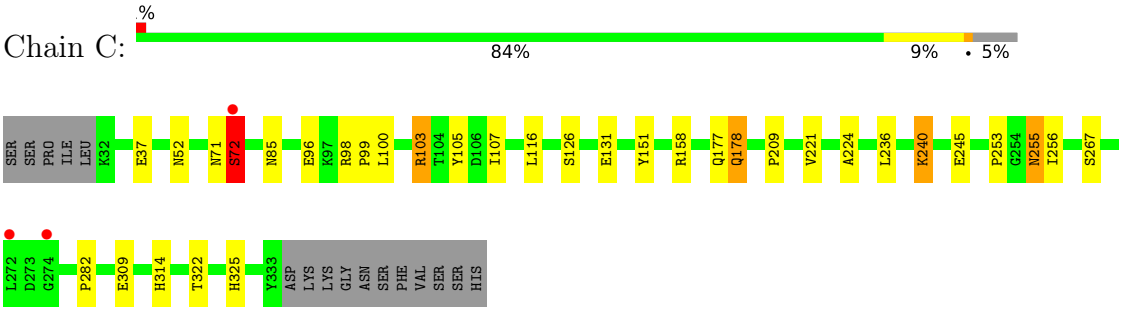
• Molecule 1: Strictosidine synthase



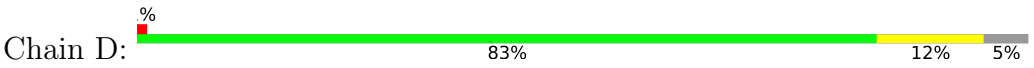
• Molecule 1: Strictosidine synthase

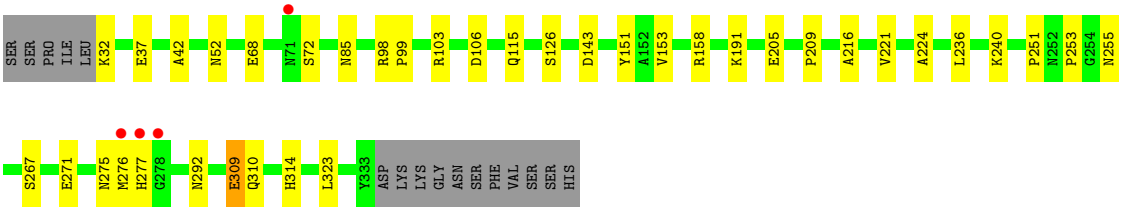


• Molecule 1: Strictosidine synthase

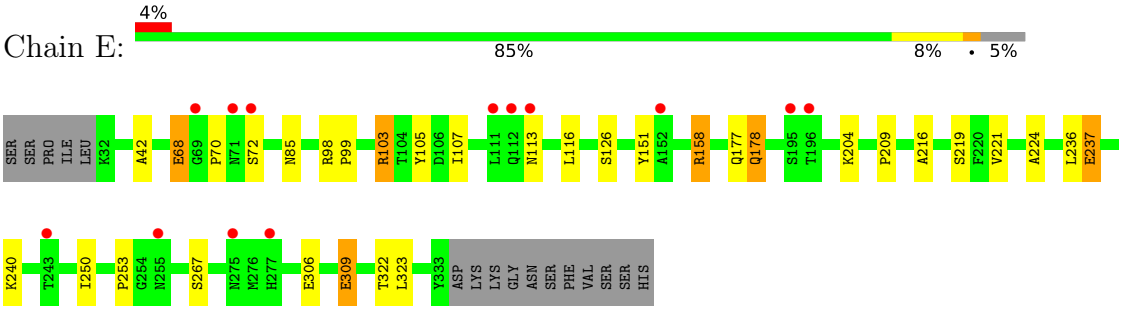


• Molecule 1: Strictosidine synthase

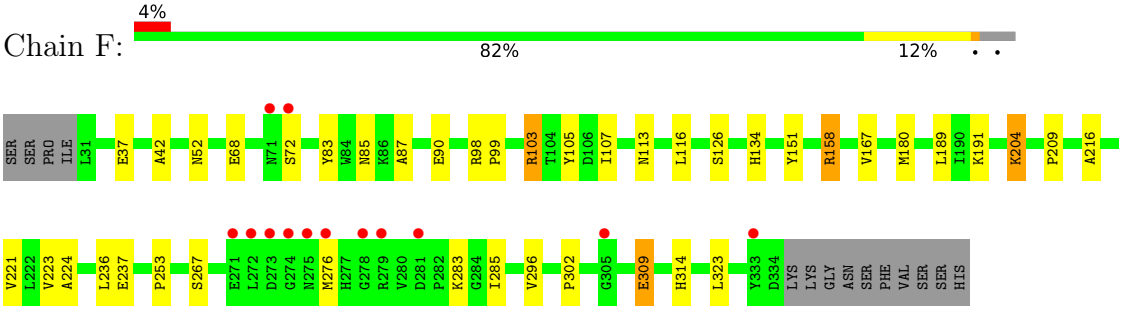




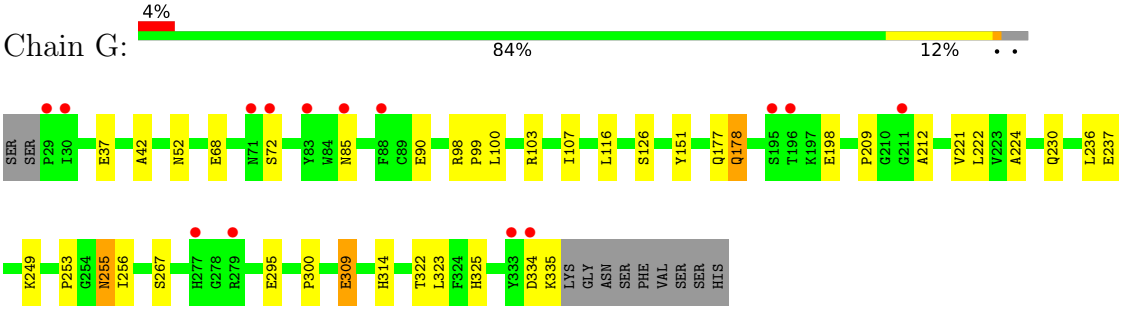
• Molecule 1: Strictosidine synthase



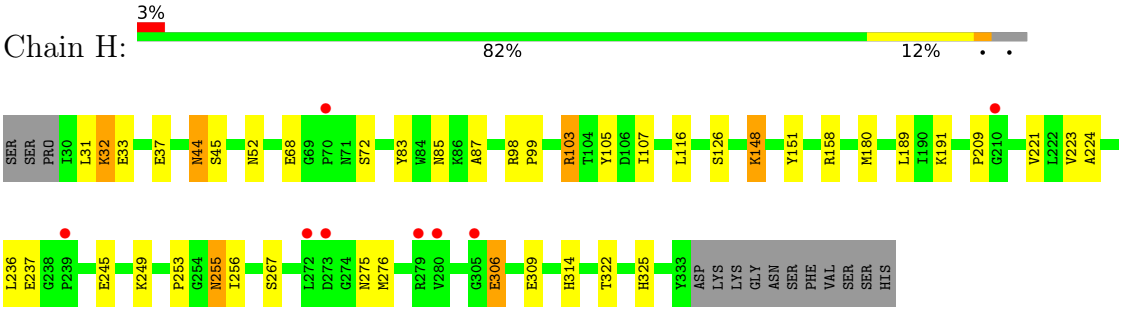
• Molecule 1: Strictosidine synthase



• Molecule 1: Strictosidine synthase



• Molecule 1: Strictosidine synthase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.49Å 82.64Å 171.84Å 90.00° 98.52° 90.00°	Depositor
Resolution (Å)	26.43 – 2.67 26.41 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.43-2.67) 100.0 (26.41-2.67)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.196 , 0.218 0.201 , 0.224	Depositor DCC
R_{free} test set	3459 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19548	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9080e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, F66

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	1.02	11/2457 (0.4%)	0.61	0/3344
1	B	0.96	8/2458 (0.3%)	0.60	1/3346 (0.0%)
1	C	0.94	7/2448 (0.3%)	0.61	0/3332
1	D	0.99	4/2467 (0.2%)	0.62	0/3356
1	E	0.89	2/2449 (0.1%)	0.59	0/3333
1	F	0.96	6/2459 (0.2%)	0.62	0/3347
1	G	0.91	5/2473 (0.2%)	0.59	0/3368
1	H	0.96	8/2448 (0.3%)	0.62	0/3334
All	All	0.95	51/19659 (0.3%)	0.61	1/26760 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	309	GLU	CD-OE2	11.96	1.38	1.25
1	D	271	GLU	CD-OE2	-10.03	1.14	1.25
1	B	131	GLU	CD-OE2	9.71	1.36	1.25
1	A	198	GLU	CG-CD	9.04	1.65	1.51
1	F	37	GLU	CD-OE1	8.86	1.35	1.25
1	A	306[A]	GLU	CD-OE1	-8.50	1.16	1.25
1	A	306[B]	GLU	CD-OE1	-8.50	1.16	1.25
1	E	306	GLU	CD-OE1	8.40	1.34	1.25
1	H	237	GLU	CD-OE1	-7.90	1.17	1.25
1	A	37	GLU	CD-OE1	7.89	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	90	GLU	CD-OE2	-7.82	1.17	1.25
1	H	306	GLU	CD-OE2	7.77	1.34	1.25
1	C	131	GLU	CD-OE2	7.64	1.34	1.25
1	B	309	GLU	CD-OE2	7.36	1.33	1.25
1	A	309	GLU	CD-OE2	7.33	1.33	1.25
1	F	309	GLU	CD-OE2	7.27	1.33	1.25
1	G	90	GLU	CD-OE2	-6.87	1.18	1.25
1	E	309	GLU	CD-OE2	6.81	1.33	1.25
1	D	205	GLU	CD-OE2	6.72	1.33	1.25
1	H	37	GLU	CD-OE1	6.63	1.32	1.25
1	B	32	LYS	CD-CE	6.61	1.67	1.51
1	A	240	LYS	CB-CG	6.48	1.70	1.52
1	B	306	GLU	CD-OE1	6.46	1.32	1.25
1	B	90	GLU	CD-OE2	-6.42	1.18	1.25
1	C	96	GLU	CD-OE1	6.32	1.32	1.25
1	G	198	GLU	CD-OE2	6.31	1.32	1.25
1	C	240	LYS	CB-CG	6.20	1.69	1.52
1	C	245	GLU	CD-OE1	6.07	1.32	1.25
1	B	205	GLU	CD-OE1	6.03	1.32	1.25
1	A	198	GLU	CD-OE2	6.03	1.32	1.25
1	H	45	SER	CA-CB	-6.01	1.44	1.52
1	B	237	GLU	CD-OE1	6.00	1.32	1.25
1	A	96	GLU	CD-OE1	5.99	1.32	1.25
1	F	204	LYS	CD-CE	5.97	1.66	1.51
1	G	237	GLU	CD-OE1	5.91	1.32	1.25
1	F	237	GLU	CD-OE1	5.85	1.32	1.25
1	A	295	GLU	CD-OE1	5.84	1.32	1.25
1	A	270	GLU	CD-OE1	5.79	1.32	1.25
1	H	33	GLU	CD-OE2	5.47	1.31	1.25
1	H	245	GLU	CD-OE1	5.43	1.31	1.25
1	B	37	GLU	CD-OE2	5.41	1.31	1.25
1	C	96	GLU	CD-OE2	5.38	1.31	1.25
1	C	72	SER	CA-CB	5.36	1.60	1.52
1	C	37	GLU	CG-CD	-5.32	1.44	1.51
1	H	306	GLU	CG-CD	5.23	1.59	1.51
1	F	283	LYS	CD-CE	5.20	1.64	1.51
1	D	37	GLU	CD-OE1	-5.19	1.20	1.25
1	G	37	GLU	CD-OE1	5.18	1.31	1.25
1	A	33	GLU	CD-OE1	-5.14	1.20	1.25
1	G	309	GLU	CD-OE2	5.08	1.31	1.25
1	H	32	LYS	C-O	-5.01	1.13	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	277	HIS	CB-CA-C	5.19	120.78	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	72	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2389	0	2289	18	0
1	B	2386	0	2284	22	0
1	C	2380	0	2275	17	0
1	D	2395	0	2302	16	0
1	E	2381	0	2280	16	0
1	F	2391	0	2285	25	0
1	G	2407	0	2299	17	0
1	H	2383	0	2264	26	0
2	A	13	0	0	0	0
2	B	13	0	0	0	0
2	C	13	0	0	1	0
2	D	13	0	0	0	0
2	E	13	0	0	0	0
2	F	13	0	0	0	0
2	G	13	0	0	0	0
2	H	13	0	0	0	0
3	B	7	0	10	0	0
3	D	14	0	20	2	0
3	E	7	0	10	0	0
3	F	7	0	10	1	0
3	H	7	0	10	0	0
4	A	45	0	0	1	0
4	B	41	0	0	0	0
4	C	31	0	0	1	0
4	D	51	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	22	0	0	2	0
4	F	35	0	0	1	0
4	G	20	0	0	0	0
4	H	45	0	0	0	0
All	All	19548	0	18338	151	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 4.

All (151) 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:D:277:HIS:HE1	4:D:528:HOH:O	1.55	0.87
1:A:151:TYR:OH	1:A:309:GLU:OE1	2.10	0.70
1:F:134:HIS:CD2	3:F:402:PEG:H32	2.26	0.69
1:F:151:TYR:OH	1:F:309:GLU:OE1	2.11	0.68
1:G:151:TYR:OH	1:G:309:GLU:OE1	2.12	0.68
1:D:151:TYR:OH	1:D:309:GLU:OE1	2.11	0.68
1:E:151:TYR:OH	1:E:309:GLU:OE1	2.12	0.67
1:C:151:TYR:OH	1:C:309:GLU:OE1	2.12	0.67
1:D:255:ASN:HD22	1:D:310:GLN:HB2	1.60	0.66
1:A:83:TYR:O	1:A:83:TYR:CD2	2.49	0.66
1:B:151:TYR:OH	1:B:309:GLU:OE1	2.12	0.66
1:H:151:TYR:OH	1:H:309:GLU:OE1	2.14	0.65
1:B:272:LEU:O	1:B:273:ASP:HB2	1.97	0.65
1:C:282:PRO:HD2	4:C:525:HOH:O	1.96	0.65
1:F:285:ILE:HD12	1:F:296:VAL:HG22	1.79	0.64
1:C:158:ARG:CB	1:C:158:ARG:HH11	2.10	0.64
1:F:285:ILE:CD1	1:F:296:VAL:HG22	2.28	0.63
1:B:277:HIS:ND1	1:B:307:HIS:CE1	2.66	0.63
1:H:158:ARG:HH11	1:H:158:ARG:CB	2.12	0.63
1:D:158:ARG:NE	1:D:216:ALA:O	2.31	0.62
1:G:68:GLU:HB2	1:G:72:SER:HB2	1.81	0.61
1:F:68:GLU:HB2	1:F:72:SER:HB2	1.82	0.61
1:D:68:GLU:HB2	1:D:72:SER:HB2	1.83	0.61
1:H:189:LEU:HD22	1:H:223:VAL:CG2	2.31	0.61
1:B:180:MET:HE3	1:B:227:LEU:HD21	1.84	0.59
1:B:277:HIS:HA	1:B:307:HIS:HE1	1.68	0.59
1:E:219:SER:HA	1:E:237:GLU:HG2	1.85	0.59
1:H:68:GLU:HB2	1:H:72:SER:HB2	1.86	0.58
1:H:148:LYS:HE3	1:H:148:LYS:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:GLU:HB2	1:E:72:SER:HB2	1.85	0.58
1:B:68:GLU:HB2	1:B:72:SER:HB2	1.87	0.57
1:D:251:PRO:HG3	1:F:83:TYR:CE2	2.40	0.57
1:C:255:ASN:HD22	1:C:256:ILE:H	1.53	0.56
1:H:322:THR:HG21	1:H:325:HIS:HB2	1.86	0.56
1:G:255:ASN:HD22	1:G:256:ILE:H	1.54	0.56
1:F:180:MET:HG3	1:F:276:MET:CE	2.36	0.55
1:E:103:ARG:HD2	1:E:105:TYR:CE1	2.42	0.55
1:H:255:ASN:HD22	1:H:256:ILE:H	1.54	0.54
1:A:209:PRO:HA	1:A:224:ALA:O	2.09	0.53
1:B:103:ARG:HD2	1:B:105:TYR:CE1	2.43	0.52
1:H:209:PRO:HA	1:H:224:ALA:O	2.10	0.52
1:B:209:PRO:HA	1:B:224:ALA:O	2.09	0.52
1:D:209:PRO:HA	1:D:224:ALA:O	2.09	0.52
1:H:189:LEU:HD22	1:H:223:VAL:HG21	1.90	0.52
1:C:209:PRO:HA	1:C:224:ALA:O	2.09	0.52
1:E:209:PRO:HA	1:E:224:ALA:O	2.09	0.52
1:F:209:PRO:HA	1:F:224:ALA:O	2.09	0.52
1:G:209:PRO:HA	1:G:224:ALA:O	2.09	0.52
1:D:255:ASN:HD22	1:D:310:GLN:HE21	1.57	0.52
1:F:103:ARG:HD2	1:F:105:TYR:CE1	2.44	0.51
1:H:180:MET:HG3	1:H:276:MET:CE	2.40	0.51
1:E:219:SER:HA	1:E:237:GLU:CG	2.42	0.50
1:D:292:ASN:HB3	1:F:87:ALA:CB	2.42	0.49
1:E:158:ARG:NH2	1:E:216:ALA:O	2.42	0.49
1:F:189:LEU:HD22	1:F:223:VAL:CG2	2.44	0.47
1:F:52:ASN:OD1	1:F:314:HIS:NE2	2.47	0.47
2:C:401:F66:N2	2:C:401:F66:C5	2.77	0.47
1:A:158:ARG:NH2	1:A:216:ALA:O	2.48	0.47
1:C:52:ASN:OD1	1:C:314:HIS:NE2	2.47	0.47
1:C:158:ARG:HH11	1:C:158:ARG:HB2	1.79	0.47
1:G:300:PRO:HB2	1:H:31:LEU:HD12	1.96	0.47
1:E:322:THR:HG22	4:E:502:HOH:O	2.15	0.47
1:G:334:ASP:O	1:G:335:LYS:C	2.52	0.46
1:B:189:LEU:HD22	1:B:223:VAL:CG2	2.46	0.46
1:A:177:GLN:HB3	1:A:178:GLN:HE21	1.79	0.46
1:B:322:THR:HG21	1:B:325[A]:HIS:HB2	1.98	0.46
1:C:177:GLN:HB3	1:C:178:GLN:HE21	1.80	0.46
1:A:70:PRO:O	1:A:71:ASN:CB	2.64	0.46
1:B:52:ASN:OD1	1:B:314:HIS:NE2	2.47	0.45
1:A:52:ASN:OD1	1:A:314:HIS:NE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:GLN:HB3	1:E:178:GLN:HE21	1.82	0.45
1:G:177:GLN:HB3	1:G:178:GLN:HE21	1.81	0.45
1:G:98:ARG:N	1:G:99:PRO:CD	2.80	0.45
1:F:221:VAL:CG2	1:F:236:LEU:HD11	2.47	0.45
1:E:221:VAL:CG2	1:E:236:LEU:HD11	2.47	0.45
1:F:158:ARG:HD3	1:F:216:ALA:O	2.17	0.45
1:G:52:ASN:OD1	1:G:314:HIS:NE2	2.48	0.45
1:A:322:THR:HG21	1:A:325:HIS:HB2	1.98	0.44
1:F:98:ARG:N	1:F:99:PRO:CD	2.81	0.44
1:C:322:THR:HG21	1:C:325:HIS:HB2	1.99	0.44
1:D:98:ARG:N	1:D:99:PRO:CD	2.80	0.44
1:H:255:ASN:HD22	1:H:256:ILE:N	2.16	0.44
1:A:98:ARG:N	1:A:99:PRO:CD	2.80	0.44
1:B:251:PRO:HG3	1:H:83:TYR:CE2	2.52	0.44
1:E:253:PRO:HA	1:E:267:SER:O	2.18	0.44
1:H:98:ARG:N	1:H:99:PRO:CD	2.81	0.44
1:B:221:VAL:CG2	1:B:236:LEU:HD11	2.48	0.44
1:B:253:PRO:HA	1:B:267:SER:O	2.18	0.44
1:G:253:PRO:HA	1:G:267:SER:O	2.18	0.44
1:H:253:PRO:HA	1:H:267:SER:O	2.18	0.44
1:B:98:ARG:N	1:B:99:PRO:CD	2.81	0.44
1:E:98:ARG:N	1:E:99:PRO:CD	2.81	0.44
1:H:44:ASN:HD22	1:H:44:ASN:H	1.66	0.44
1:A:253:PRO:HA	1:A:267:SER:O	2.18	0.43
1:C:255:ASN:HD22	1:C:256:ILE:N	2.16	0.43
1:D:42:ALA:HB1	1:D:323:LEU:HA	2.00	0.43
1:H:31:LEU:HD23	1:H:32:LYS:H	1.83	0.43
1:B:292:ASN:OD1	1:H:87:ALA:HB2	2.18	0.43
1:C:221:VAL:CG2	1:C:236:LEU:HD11	2.47	0.43
1:C:253:PRO:HA	1:C:267:SER:O	2.18	0.43
1:F:285:ILE:CD1	1:F:296:VAL:HG13	2.48	0.43
1:A:83:TYR:O	1:A:83:TYR:CG	2.71	0.43
1:C:71:ASN:O	1:C:72:SER:CB	2.66	0.43
1:D:253:PRO:HA	1:D:267:SER:O	2.19	0.43
1:G:255:ASN:HD22	1:G:256:ILE:N	2.17	0.43
1:C:98:ARG:N	1:C:99:PRO:CD	2.81	0.43
1:D:221:VAL:CG2	1:D:236:LEU:HD11	2.48	0.43
1:H:52:ASN:OD1	1:H:314:HIS:NE2	2.48	0.43
1:C:158:ARG:HH11	1:C:158:ARG:HB3	1.80	0.43
1:F:42:ALA:HB1	1:F:323:LEU:HA	2.01	0.43
1:G:221:VAL:CG2	1:G:236:LEU:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:VAL:CG2	1:H:236:LEU:HD11	2.48	0.43
1:F:189:LEU:HD22	1:F:223:VAL:HG21	2.00	0.43
1:G:322:THR:HG21	1:G:325:HIS:HB2	2.01	0.43
1:A:302:PRO:HB3	1:B:70:PRO:HG2	2.00	0.42
1:A:221:VAL:CG2	1:A:236:LEU:HD11	2.49	0.42
1:F:180:MET:HG3	1:F:276:MET:HE2	2.00	0.42
1:E:151:TYR:HE2	4:E:517:HOH:O	2.02	0.42
1:F:107:ILE:HB	1:F:116:LEU:HD11	2.02	0.42
1:D:52:ASN:OD1	1:D:314:HIS:NE2	2.48	0.42
1:F:253:PRO:HA	1:F:267:SER:O	2.18	0.42
1:H:158:ARG:HH11	1:H:158:ARG:HB2	1.80	0.42
1:E:42:ALA:HB1	1:E:323:LEU:HA	2.01	0.42
1:D:292:ASN:OD1	1:F:87:ALA:HB2	2.19	0.42
1:F:151:TYR:HB2	1:F:167:VAL:HG23	2.02	0.42
1:H:44:ASN:ND2	1:H:103:ARG:HH12	2.17	0.42
1:B:189:LEU:HD22	1:B:223:VAL:HG21	2.01	0.41
1:D:106:ASP:HB3	1:D:153:VAL:HG12	2.03	0.41
3:D:402:PEG:H12	1:F:87:ALA:HB1	2.01	0.41
1:B:277:HIS:CA	1:B:307:HIS:HE1	2.32	0.41
1:A:100:LEU:HB2	4:A:530:HOH:O	2.20	0.41
1:E:107:ILE:HB	1:E:116:LEU:HD11	2.03	0.41
1:A:107:ILE:HB	1:A:116:LEU:HD11	2.03	0.41
1:C:103:ARG:HD2	1:C:105:TYR:CE2	2.55	0.41
1:G:42:ALA:HB1	1:G:323:LEU:HA	2.02	0.41
1:B:107:ILE:HB	1:B:116:LEU:HD11	2.03	0.41
1:G:230:GLN:HB3	1:G:249:LYS:HD3	2.02	0.41
1:H:103:ARG:HD2	1:H:105:TYR:CE2	2.55	0.41
1:C:107:ILE:HB	1:C:116:LEU:HD11	2.03	0.41
1:H:31:LEU:HD23	1:H:32:LYS:N	2.36	0.41
1:H:158:ARG:HH11	1:H:158:ARG:HB3	1.83	0.41
3:D:402:PEG:H11	4:F:528:HOH:O	2.21	0.40
1:E:70:PRO:HG2	1:F:302:PRO:HB3	2.03	0.40
1:H:107:ILE:HB	1:H:116:LEU:HD11	2.03	0.40
1:A:42:ALA:HB1	1:A:323:LEU:HA	2.03	0.40
1:A:103:ARG:HD2	1:A:105:TYR:CE2	2.55	0.40
1:B:151:TYR:HB2	1:B:167:VAL:HG23	2.03	0.40
1:G:107:ILE:HB	1:G:116:LEU:HD11	2.03	0.40
1:A:212:ALA:HA	1:A:222:LEU:O	2.22	0.40
1:B:106:ASP:HB3	1:B:153:VAL:HG12	2.03	0.40
1:G:212:ALA:HA	1:G:222:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/318 (95%)	289 (96%)	13 (4%)	0	100	100
1	B	302/318 (95%)	287 (95%)	14 (5%)	1 (0%)	41	64
1	C	301/318 (95%)	289 (96%)	11 (4%)	1 (0%)	41	64
1	D	302/318 (95%)	290 (96%)	12 (4%)	0	100	100
1	E	301/318 (95%)	290 (96%)	11 (4%)	0	100	100
1	F	303/318 (95%)	291 (96%)	12 (4%)	0	100	100
1	G	305/318 (96%)	294 (96%)	11 (4%)	0	100	100
1	H	302/318 (95%)	291 (96%)	11 (4%)	0	100	100
All	All	2418/2544 (95%)	2321 (96%)	95 (4%)	2 (0%)	51	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	SER
1	B	273	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/275 (94%)	252 (97%)	8 (3%)	40	67
1	B	260/275 (94%)	255 (98%)	5 (2%)	57	80
1	C	258/275 (94%)	251 (97%)	7 (3%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	262/275 (95%)	252 (96%)	10 (4%)	33 59
1	E	259/275 (94%)	248 (96%)	11 (4%)	30 55
1	F	260/275 (94%)	253 (97%)	7 (3%)	44 71
1	G	261/275 (95%)	254 (97%)	7 (3%)	44 71
1	H	257/275 (94%)	247 (96%)	10 (4%)	32 58
All	All	2077/2200 (94%)	2012 (97%)	65 (3%)	40 67

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	85	ASN
1	A	103	ARG
1	A	126	SER
1	A	158	ARG
1	A	178	GLN
1	A	204	LYS
1	A	240	LYS
1	B	32	LYS
1	B	85	ASN
1	B	103	ARG
1	B	126	SER
1	B	275	ASN
1	C	85	ASN
1	C	100	LEU
1	C	103	ARG
1	C	126	SER
1	C	178	GLN
1	C	240	LYS
1	C	255	ASN
1	D	32	LYS
1	D	85	ASN
1	D	103	ARG
1	D	115	GLN
1	D	126	SER
1	D	143	ASP
1	D	191	LYS
1	D	240	LYS
1	D	275	ASN
1	D	276	MET

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Mol	Chain	Res	Type
1	E	68	GLU
1	E	85	ASN
1	E	103	ARG
1	E	113	ASN
1	E	126	SER
1	E	158	ARG
1	E	178	GLN
1	E	204	LYS
1	E	237	GLU
1	E	240	LYS
1	E	250	ILE
1	F	85	ASN
1	F	103	ARG
1	F	113	ASN
1	F	126	SER
1	F	158	ARG
1	F	191	LYS
1	F	204	LYS
1	G	85	ASN
1	G	100	LEU
1	G	103	ARG
1	G	126	SER
1	G	178	GLN
1	G	255	ASN
1	G	295	GLU
1	H	44	ASN
1	H	85	ASN
1	H	103	ARG
1	H	126	SER
1	H	148	LYS
1	H	191	LYS
1	H	249	LYS
1	H	255	ASN
1	H	275	ASN
1	H	306	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	178	GLN
1	A	307	HIS

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Mol	Chain	Res	Type
1	B	114	ASN
1	B	307	HIS
1	C	137	GLN
1	C	178	GLN
1	C	255	ASN
1	D	114	ASN
1	D	255	ASN
1	D	277	HIS
1	D	312	GLN
1	E	114	ASN
1	E	178	GLN
1	F	112	GLN
1	F	113	ASN
1	F	114	ASN
1	G	114	ASN
1	G	178	GLN
1	G	255	ASN
1	G	307	HIS
1	H	44	ASN
1	H	114	ASN
1	H	177	GLN
1	H	255	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	D	402	-	6,6,6	0.99	0	5,5,5	0.15	0
3	PEG	H	402	-	6,6,6	0.98	0	5,5,5	0.10	0
2	F66	D	401	-	11,14,14	1.17	1 (9%)	11,19,19	0.95	0
3	PEG	D	403	-	6,6,6	0.80	0	5,5,5	0.08	0
2	F66	B	401	-	11,14,14	1.18	0	11,19,19	0.94	0
3	PEG	E	402	-	6,6,6	0.81	0	5,5,5	0.08	0
2	F66	E	401	-	11,14,14	1.15	1 (9%)	11,19,19	0.93	0
3	PEG	F	402	-	6,6,6	1.33	0	5,5,5	0.16	0
2	F66	G	401	-	11,14,14	1.00	0	11,19,19	0.93	1 (9%)
2	F66	C	401	-	11,14,14	1.80	2 (18%)	11,19,19	0.91	1 (9%)
2	F66	F	401	-	11,14,14	0.78	0	11,19,19	0.84	0
3	PEG	B	402	-	6,6,6	0.92	0	5,5,5	0.09	0
2	F66	H	401	-	11,14,14	1.46	2 (18%)	11,19,19	0.93	0
2	F66	A	401	-	11,14,14	1.17	1 (9%)	11,19,19	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	402	-	-	2/4/4/4	-
3	PEG	H	402	-	-	2/4/4/4	-
2	F66	D	401	-	-	3/3/3/3	0/2/2/2
3	PEG	D	403	-	-	4/4/4/4	-
2	F66	B	401	-	-	1/3/3/3	0/2/2/2
3	PEG	E	402	-	-	2/4/4/4	-
2	F66	E	401	-	-	0/3/3/3	0/2/2/2
3	PEG	F	402	-	-	4/4/4/4	-
2	F66	G	401	-	-	1/3/3/3	0/2/2/2
2	F66	C	401	-	-	0/3/3/3	0/2/2/2
2	F66	F	401	-	-	1/3/3/3	0/2/2/2
3	PEG	B	402	-	-	1/4/4/4	-
2	F66	H	401	-	-	0/3/3/3	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	F66	A	401	-	-	3/3/3/3	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	F66	C10-C3	-4.68	1.44	1.52
2	H	401	F66	C10-C3	-2.97	1.47	1.52
2	E	401	F66	C10-C3	-2.41	1.48	1.52
2	H	401	F66	C3-C2	-2.29	1.35	1.39
2	C	401	F66	C3-C2	-2.26	1.35	1.39
2	A	401	F66	C10-C3	-2.19	1.48	1.52
2	D	401	F66	C7-C8	2.05	1.41	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	F66	C7-C8-C9	-2.01	117.19	120.08
2	G	401	F66	C7-C8-C9	-2.00	117.20	120.08

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	F66	C3-C10-C11-N2
2	A	401	F66	C11-C10-C3-C4
2	A	401	F66	C11-C10-C3-C2
2	F	401	F66	C3-C10-C11-N2
3	E	402	PEG	O2-C3-C4-O4
3	D	402	PEG	O2-C3-C4-O4
3	H	402	PEG	O1-C1-C2-O2
3	H	402	PEG	O2-C3-C4-O4
3	B	402	PEG	O1-C1-C2-O2
3	D	402	PEG	O1-C1-C2-O2
3	E	402	PEG	O1-C1-C2-O2
3	F	402	PEG	O1-C1-C2-O2
3	F	402	PEG	O2-C3-C4-O4
3	D	403	PEG	O1-C1-C2-O2
3	F	402	PEG	C1-C2-O2-C3
2	D	401	F66	C3-C10-C11-N2
2	G	401	F66	C3-C10-C11-N2
2	D	401	F66	C11-C10-C3-C4

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Mol	Chain	Res	Type	Atoms
2	D	401	F66	C11-C10-C3-C2
2	B	401	F66	C3-C10-C11-N2
3	D	403	PEG	C1-C2-O2-C3
3	F	402	PEG	C4-C3-O2-C2
3	D	403	PEG	O2-C3-C4-O4
3	D	403	PEG	C4-C3-O2-C2

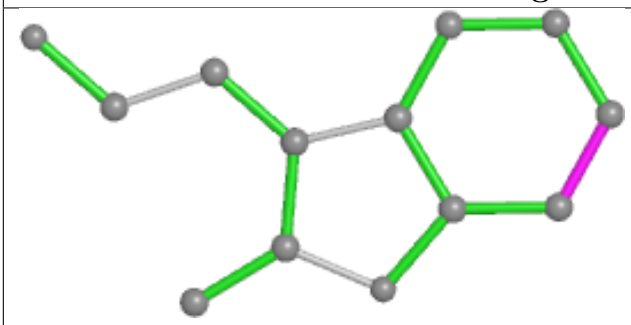
There are no ring outliers.

3 monomers are involved in 4 short contacts:

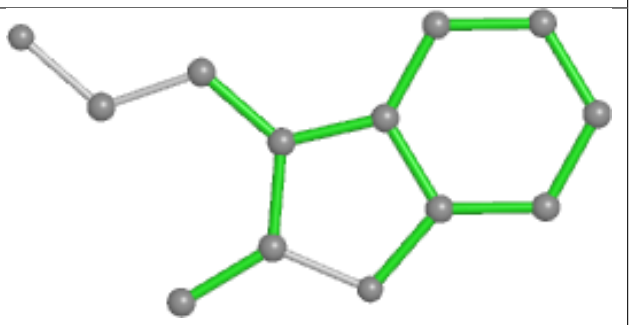
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	PEG	2	0
3	F	402	PEG	1	0
2	C	401	F66	1	0

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.

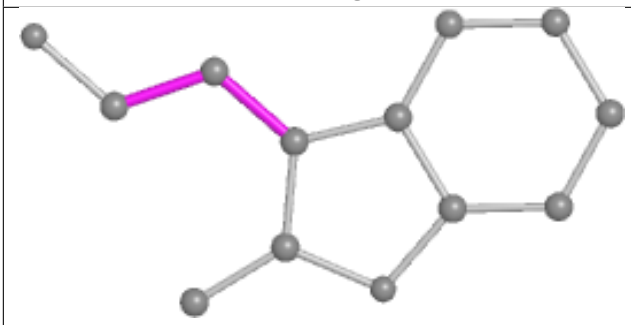
Ligand F66 D 401



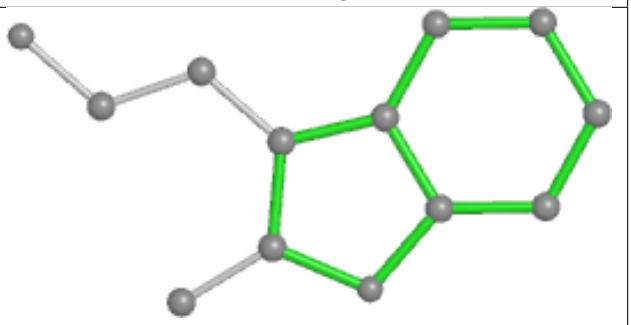
Bond lengths



Bond angles

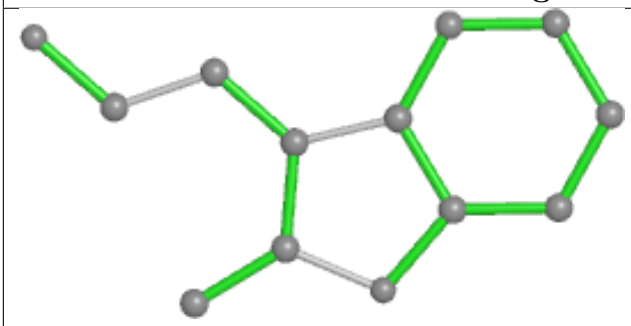


Torsions

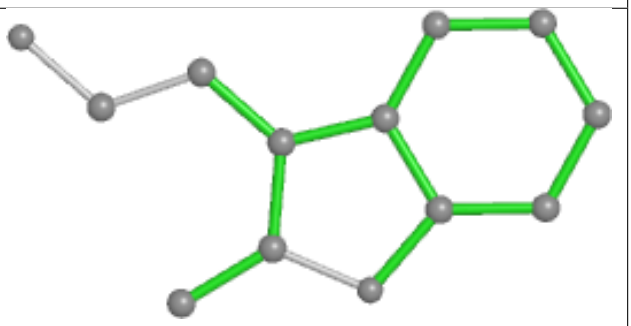


Rings

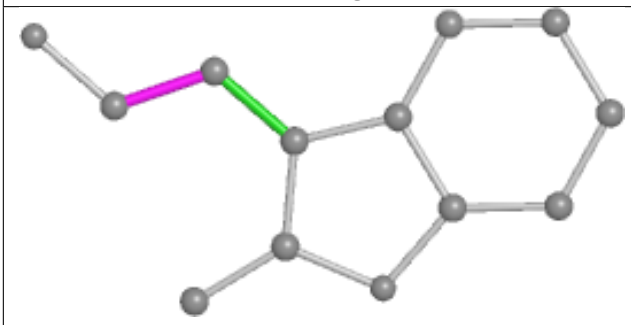
Ligand F66 B 401



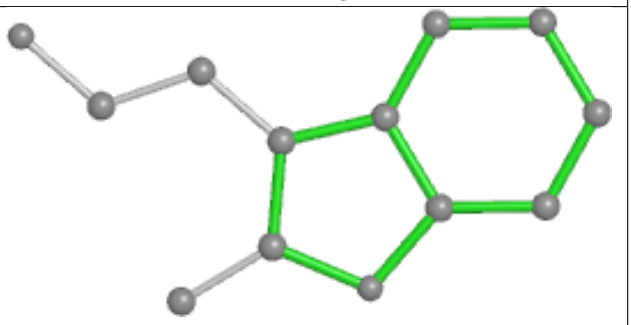
Bond lengths



Bond angles

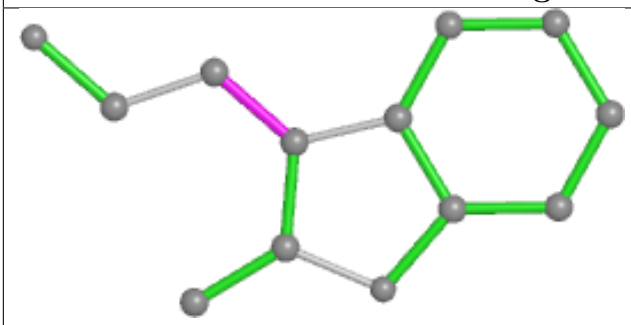


Torsions

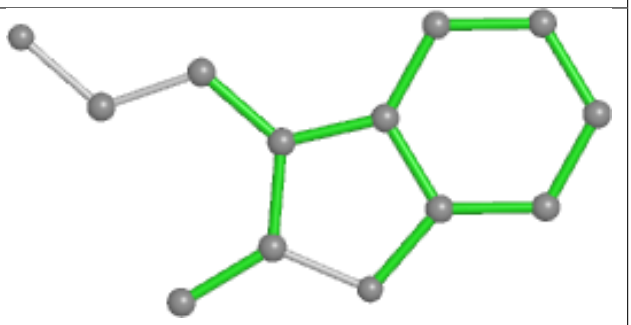


Rings

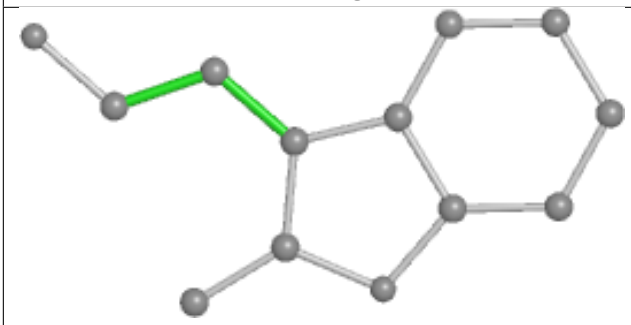
Ligand F66 E 401



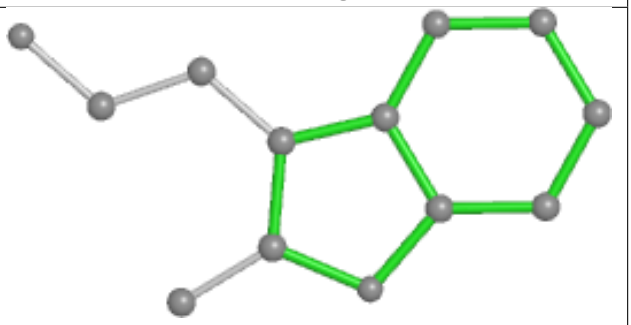
Bond lengths



Bond angles

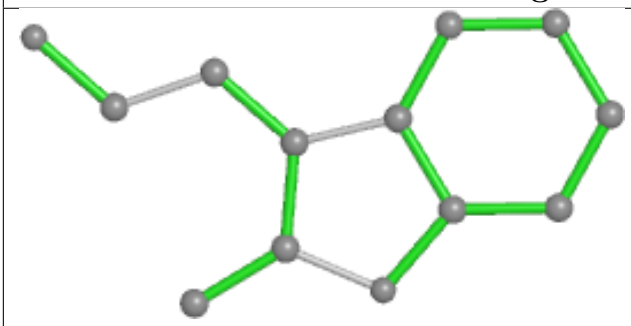


Torsions

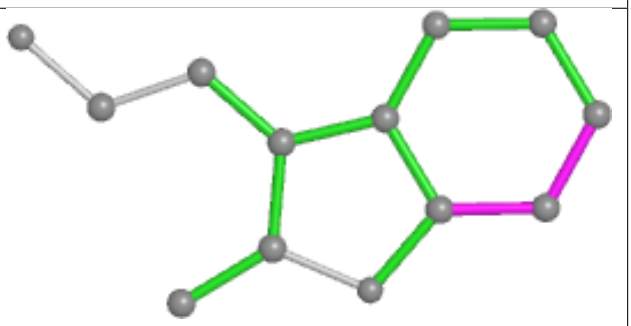


Rings

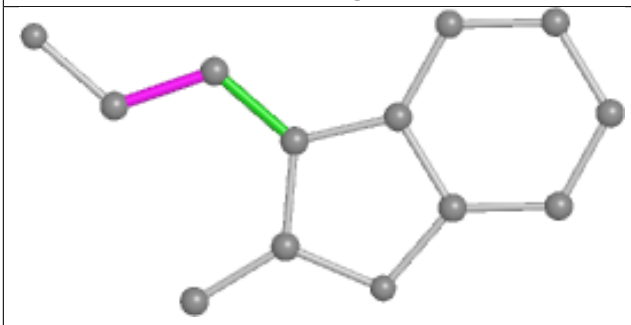
Ligand F66 G 401



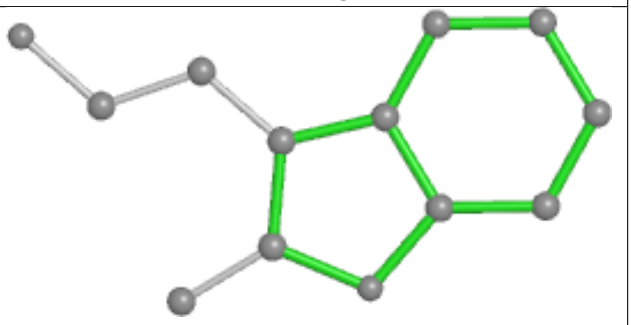
Bond lengths



Bond angles

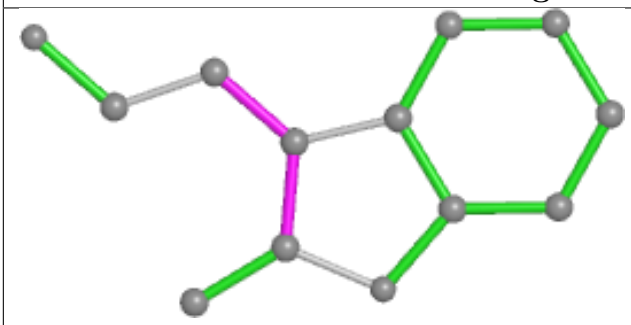


Torsions

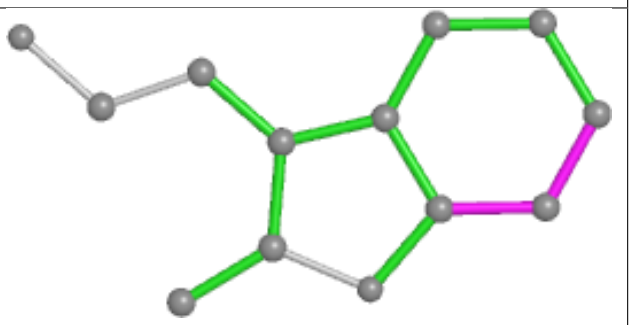


Rings

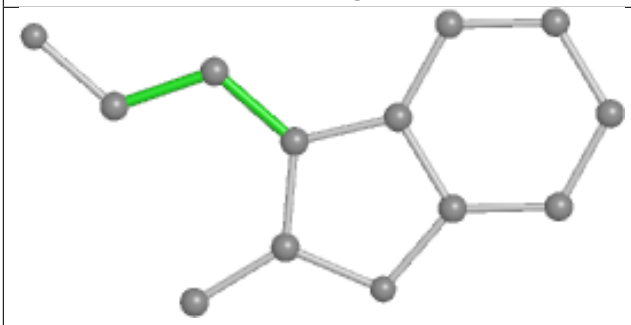
Ligand F66 C 401



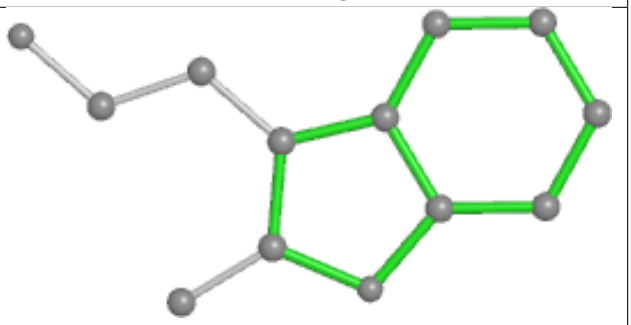
Bond lengths



Bond angles

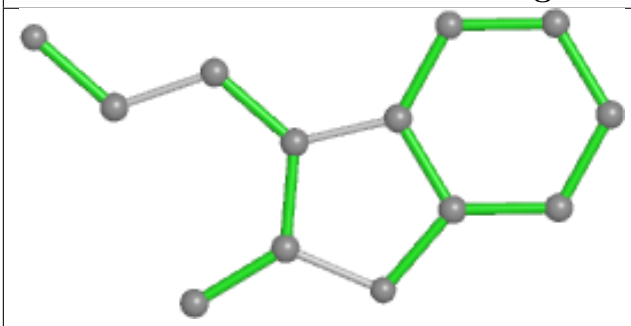


Torsions

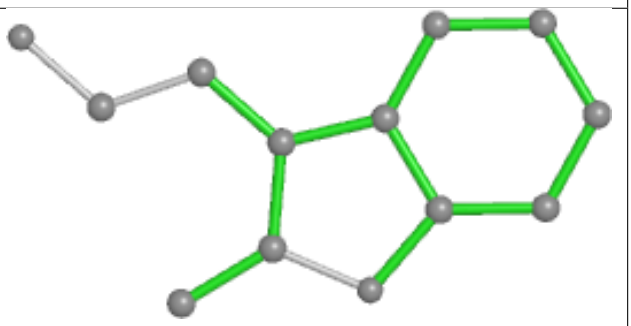


Rings

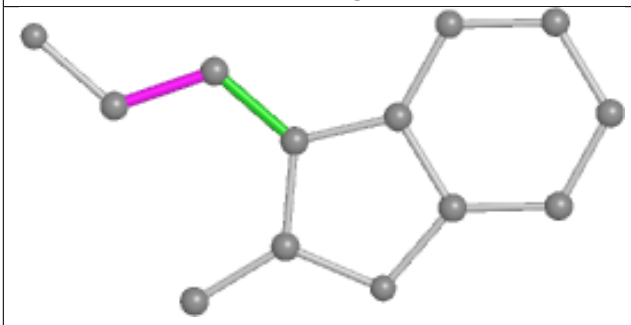
Ligand F66 F 401



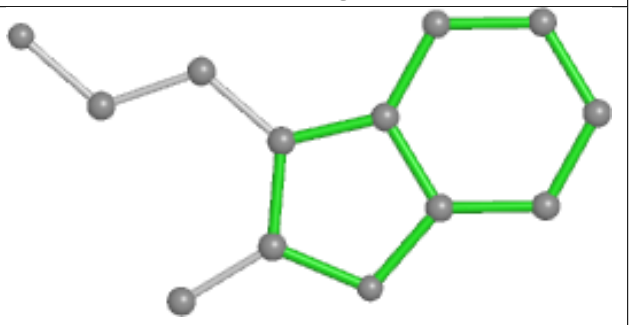
Bond lengths



Bond angles

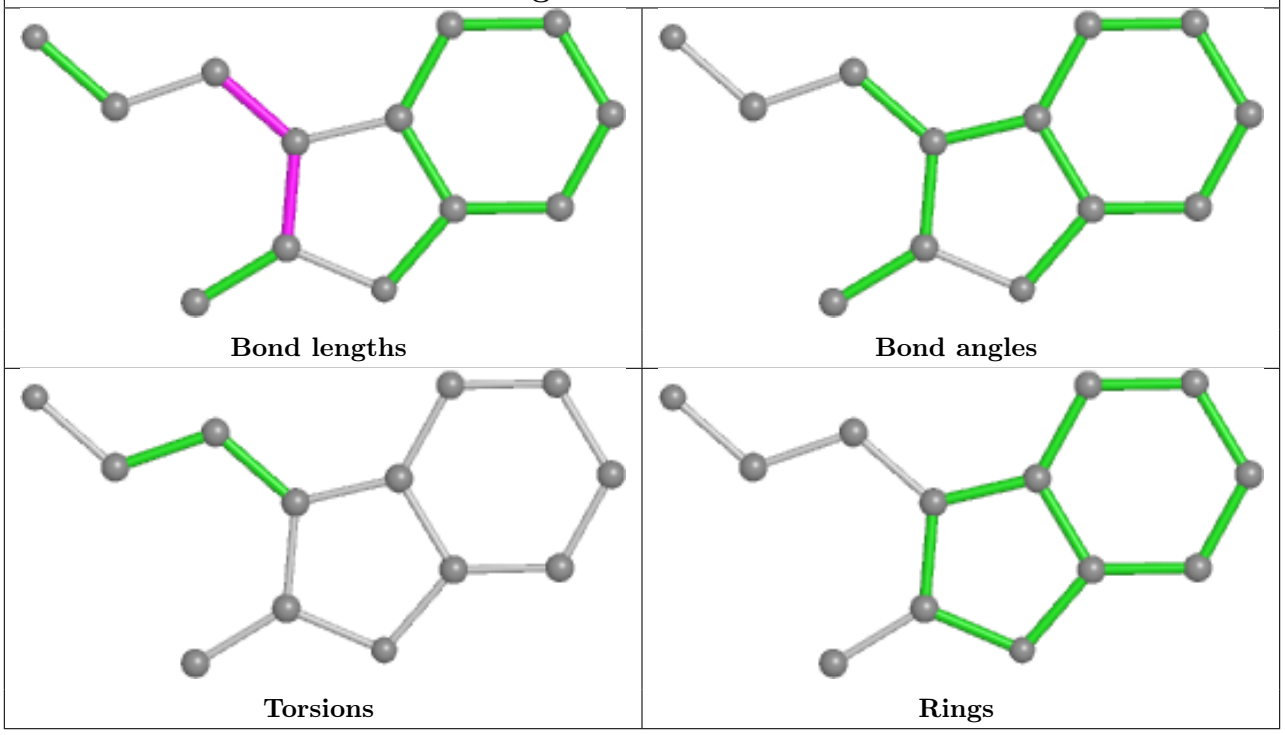


Torsions

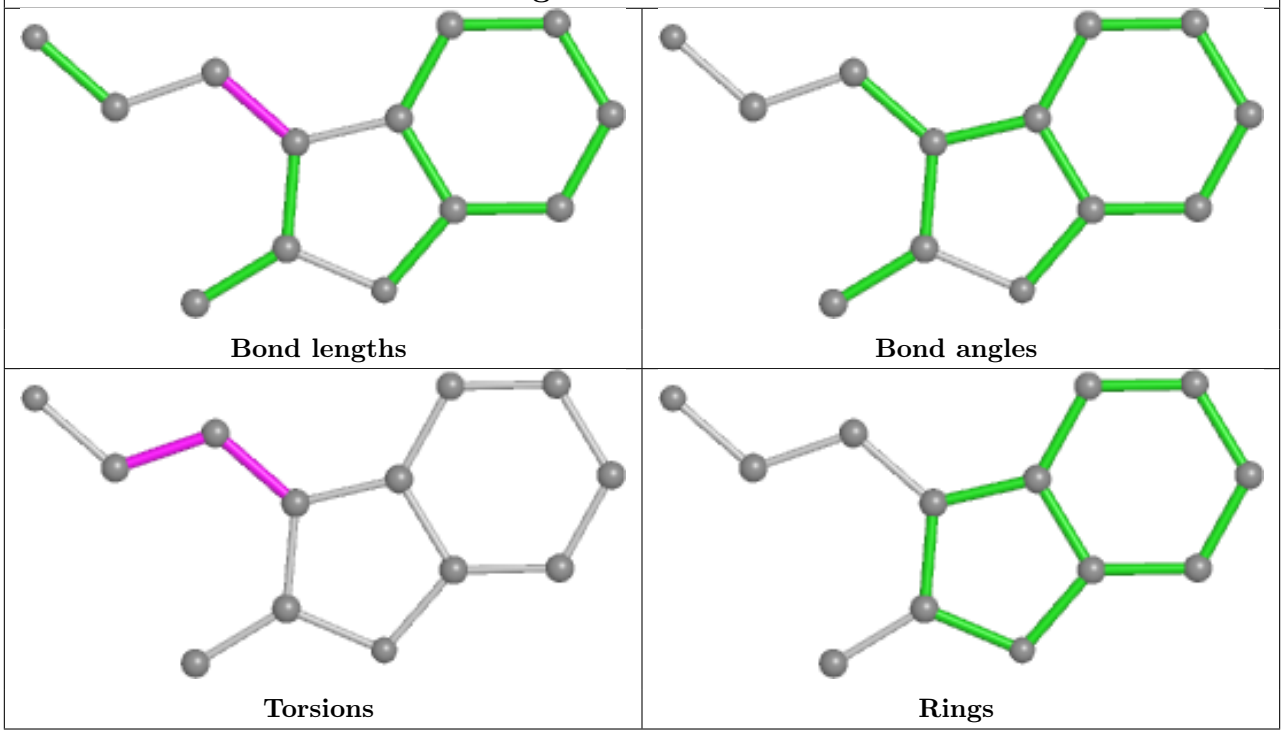


Rings

Ligand F66 H 401



Ligand F66 A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	303/318 (95%)	-0.23	4 (1%)	77 78	21, 38, 70, 89	0
1	B	302/318 (94%)	-0.17	9 (2%)	50 49	23, 39, 74, 132	0
1	C	302/318 (94%)	-0.21	3 (0%)	82 82	26, 42, 72, 91	0
1	D	302/318 (94%)	-0.25	4 (1%)	77 78	20, 38, 69, 121	0
1	E	302/318 (94%)	0.13	13 (4%)	35 33	30, 55, 88, 121	0
1	F	304/318 (95%)	0.05	13 (4%)	35 33	25, 54, 93, 117	0
1	G	307/318 (96%)	0.14	14 (4%)	32 30	32, 58, 88, 117	0
1	H	304/318 (95%)	-0.03	8 (2%)	56 55	26, 51, 82, 93	0
All	All	2426/2544 (95%)	-0.07	68 (2%)	53 52	20, 46, 84, 132	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	HIS	9.5
1	D	277	HIS	6.7
1	D	276	MET	6.2
1	B	276	MET	5.4
1	B	274	GLY	5.4
1	G	30	ILE	5.3
1	E	112	GLN	4.7
1	F	279	ARG	4.2
1	F	272	LEU	4.0
1	F	276	MET	3.9
1	G	333	TYR	3.8
1	E	72	SER	3.7
1	G	72	SER	3.5
1	F	72	SER	3.4
1	G	29	PRO	3.3
1	H	279	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	85	ASN	3.2
1	C	72	SER	3.2
1	H	280	VAL	3.1
1	G	71	ASN	3.1
1	A	72	SER	3.1
1	E	111	LEU	3.0
1	B	273	ASP	2.9
1	F	274	GLY	2.9
1	B	52	ASN	2.8
1	G	334	ASP	2.8
1	E	71	ASN	2.8
1	F	275	ASN	2.7
1	H	272	LEU	2.7
1	G	83	TYR	2.7
1	F	271	GLU	2.7
1	B	275	ASN	2.7
1	F	333	TYR	2.6
1	G	277	HIS	2.5
1	H	273	ASP	2.5
1	C	274	GLY	2.5
1	E	195	SER	2.5
1	B	278	GLY	2.5
1	F	71	ASN	2.4
1	F	273	ASP	2.4
1	G	88	PHE	2.4
1	B	279	ARG	2.4
1	C	272	LEU	2.4
1	G	279	ARG	2.4
1	H	239	PRO	2.3
1	A	31	LEU	2.3
1	A	279	ARG	2.3
1	F	278	GLY	2.3
1	H	305	GLY	2.3
1	F	281	ASP	2.3
1	F	305	GLY	2.2
1	G	211	GLY	2.2
1	D	278	GLY	2.2
1	H	70	PRO	2.2
1	E	113	ASN	2.2
1	A	109	TYR	2.2
1	E	277	HIS	2.2
1	D	71	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	195	SER	2.1
1	E	152	ALA	2.1
1	E	243	THR	2.1
1	E	255	ASN	2.1
1	E	196	THR	2.1
1	G	196	THR	2.1
1	E	69	GLY	2.1
1	B	112	GLN	2.1
1	E	275	ASN	2.0
1	H	210	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F66	A	401	13/13	0.64	0.43	78,83,92,92	0
2	F66	G	401	13/13	0.67	0.44	84,87,93,94	0
2	F66	B	401	13/13	0.68	0.41	74,81,85,86	0
3	PEG	B	402	7/7	0.73	0.28	64,67,70,73	0
3	PEG	H	402	7/7	0.73	0.50	70,85,96,96	0
2	F66	C	401	13/13	0.74	0.38	69,79,80,81	0
3	PEG	D	403	7/7	0.75	0.26	63,71,77,79	0
3	PEG	F	402	7/7	0.76	0.43	58,67,71,76	0
2	F66	E	401	13/13	0.78	0.38	76,83,93,94	0
2	F66	D	401	13/13	0.79	0.35	72,80,90,92	0
3	PEG	D	402	7/7	0.84	0.47	48,57,65,66	0
2	F66	F	401	13/13	0.84	0.41	109,115,122,125	0
3	PEG	E	402	7/7	0.86	0.20	58,63,65,69	0

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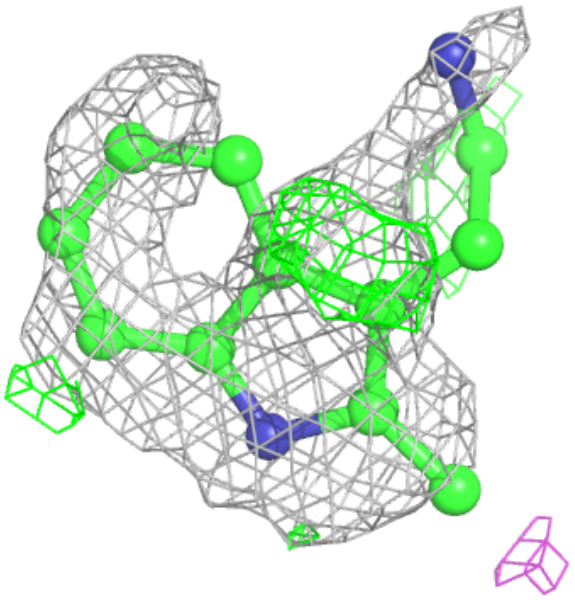
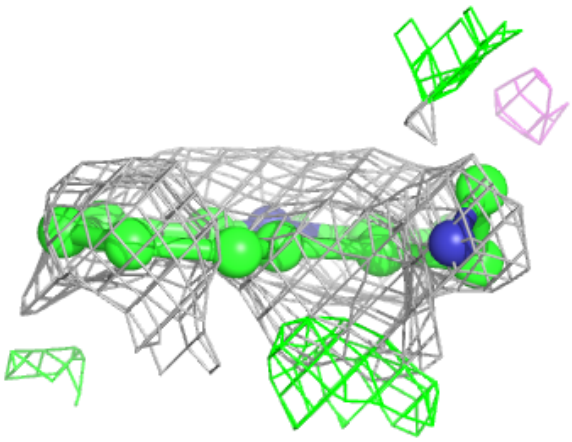
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	F66	H	401	13/13	0.87	0.30	70,75,79,79	0

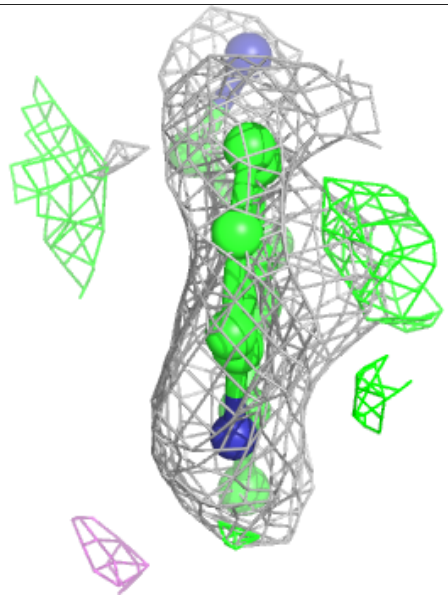
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around F66 A 401:

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

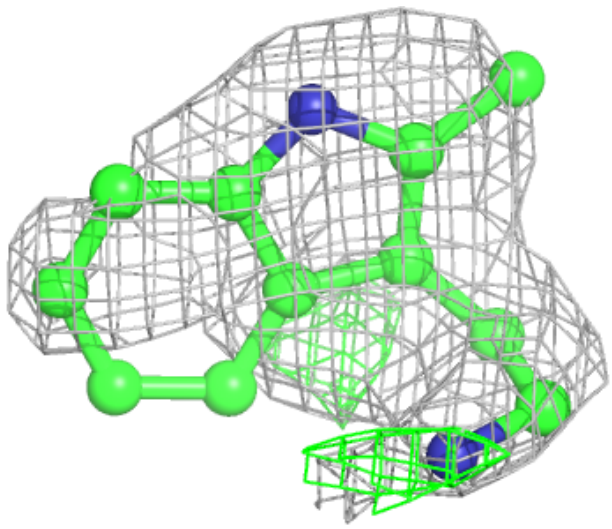


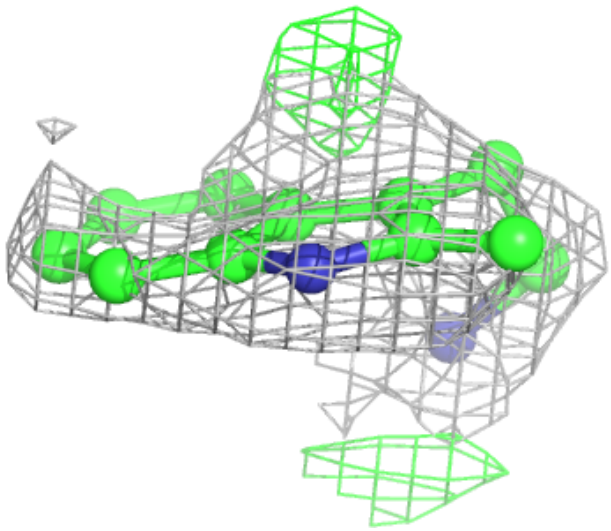


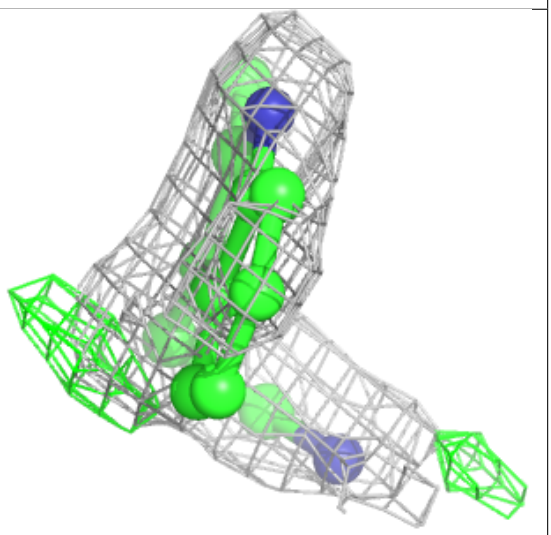


Electron density around F66 G 401:

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

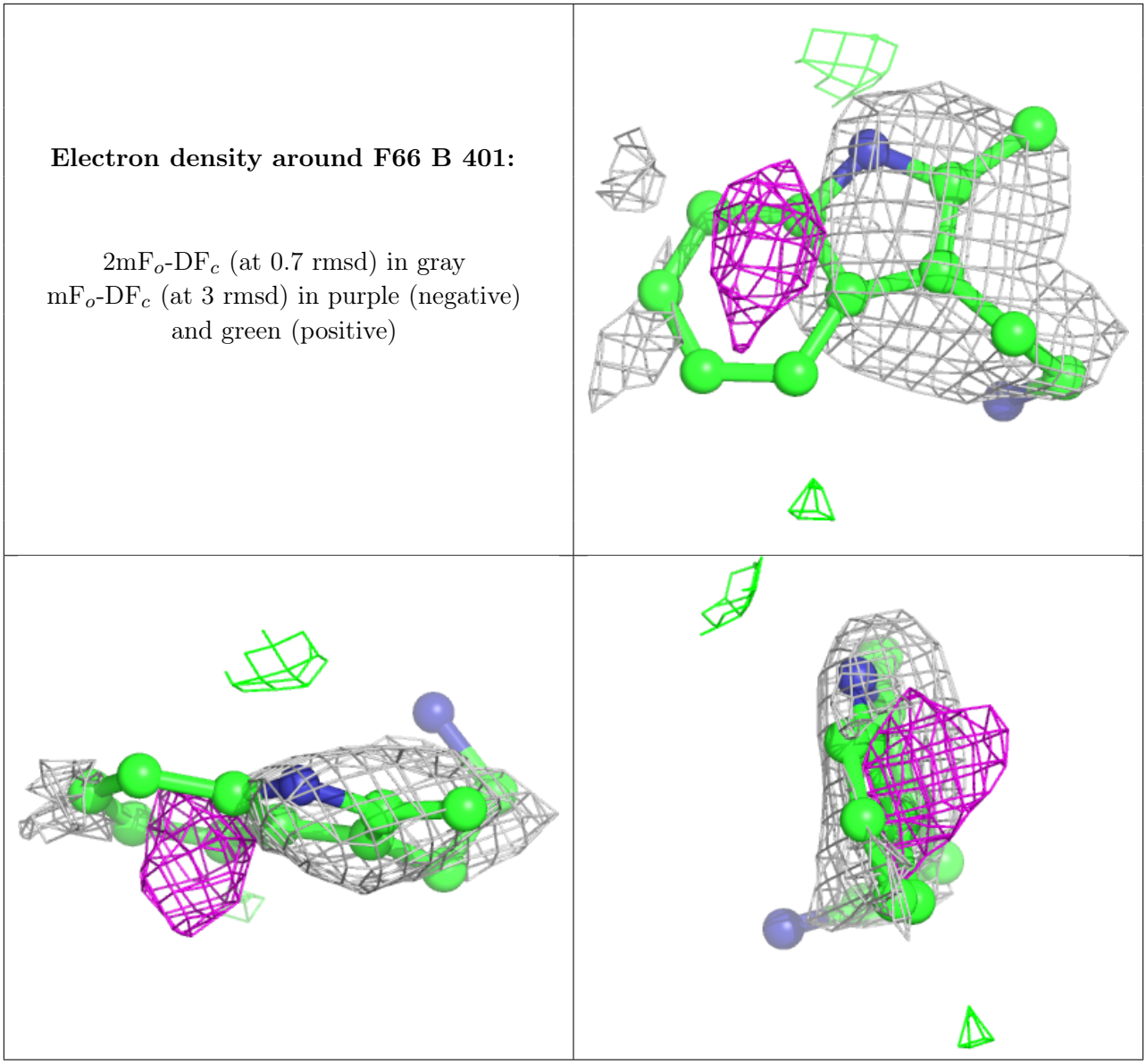






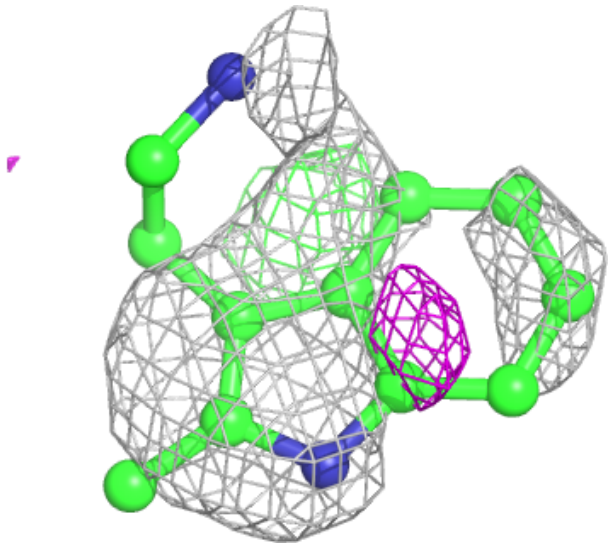
Electron density around F66 B 401:

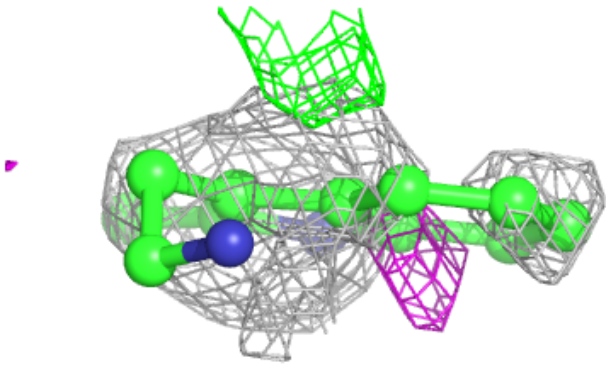
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

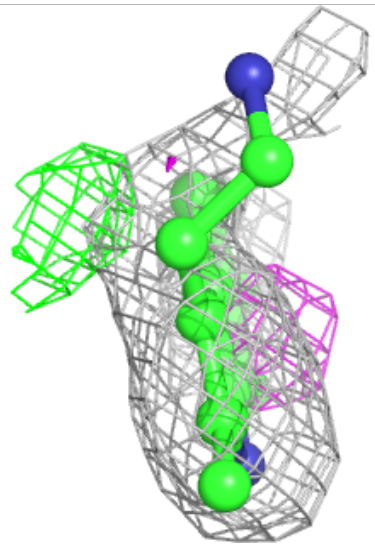


Electron density around F66 C 401:

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

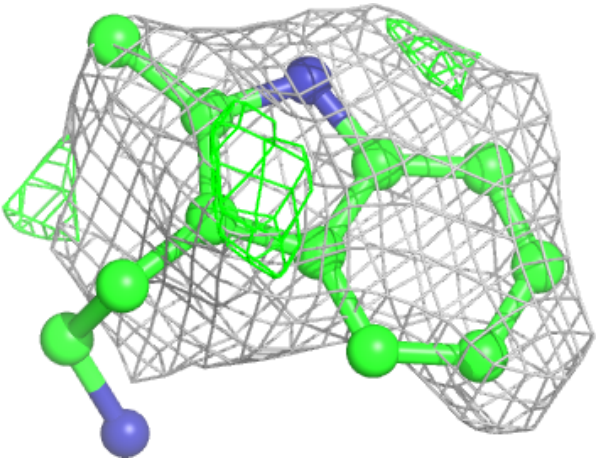


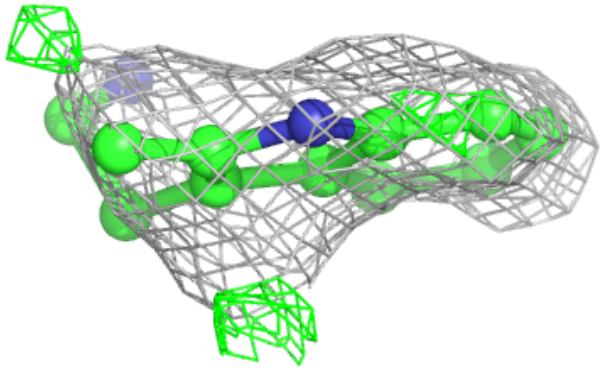


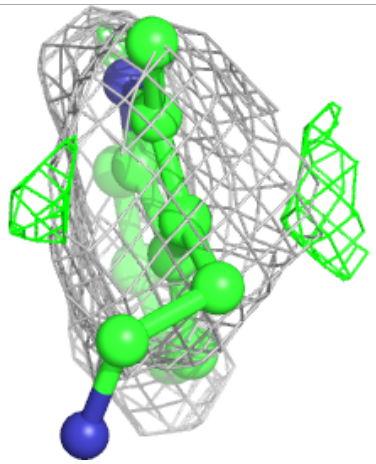


Electron density around F66 E 401:

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

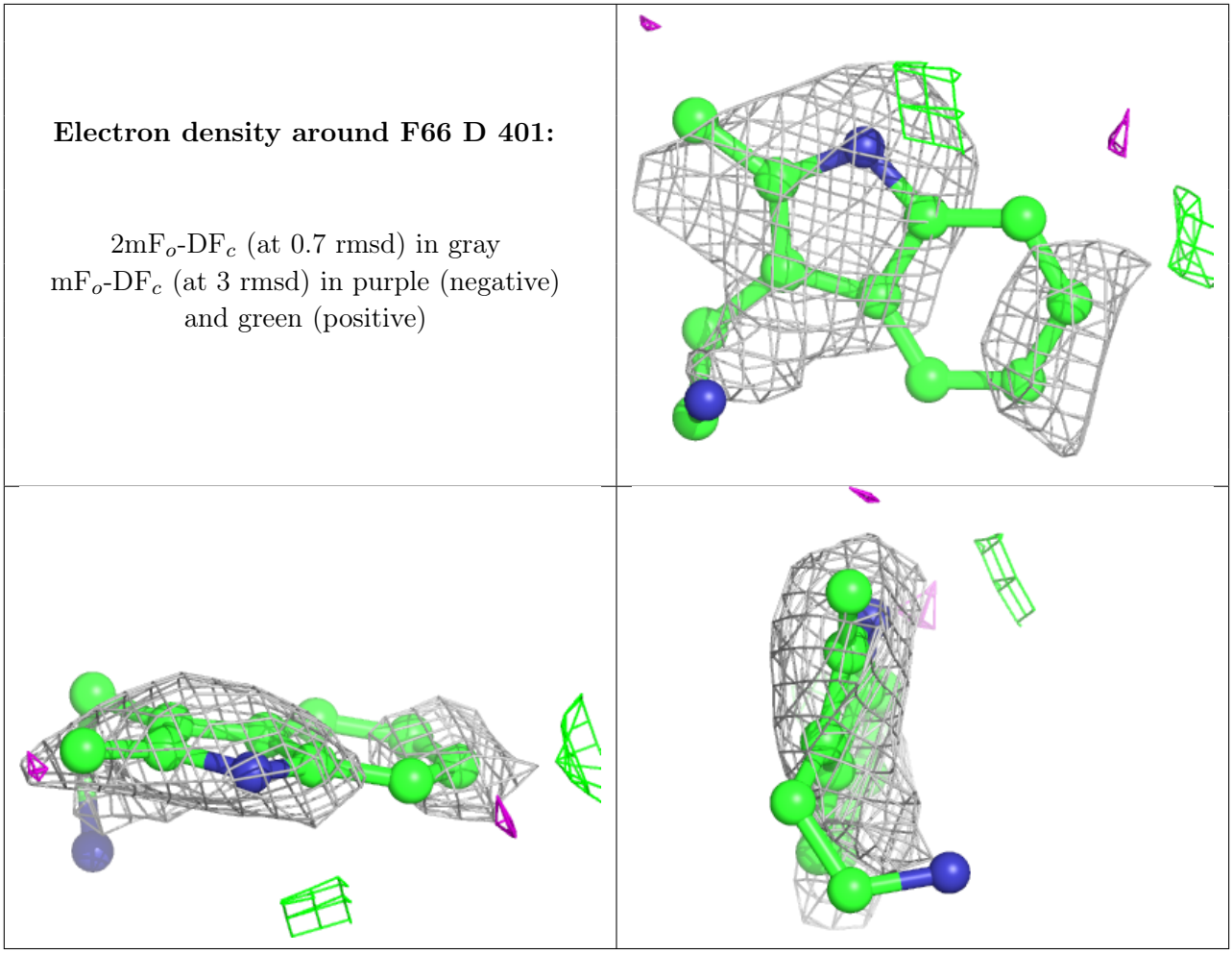






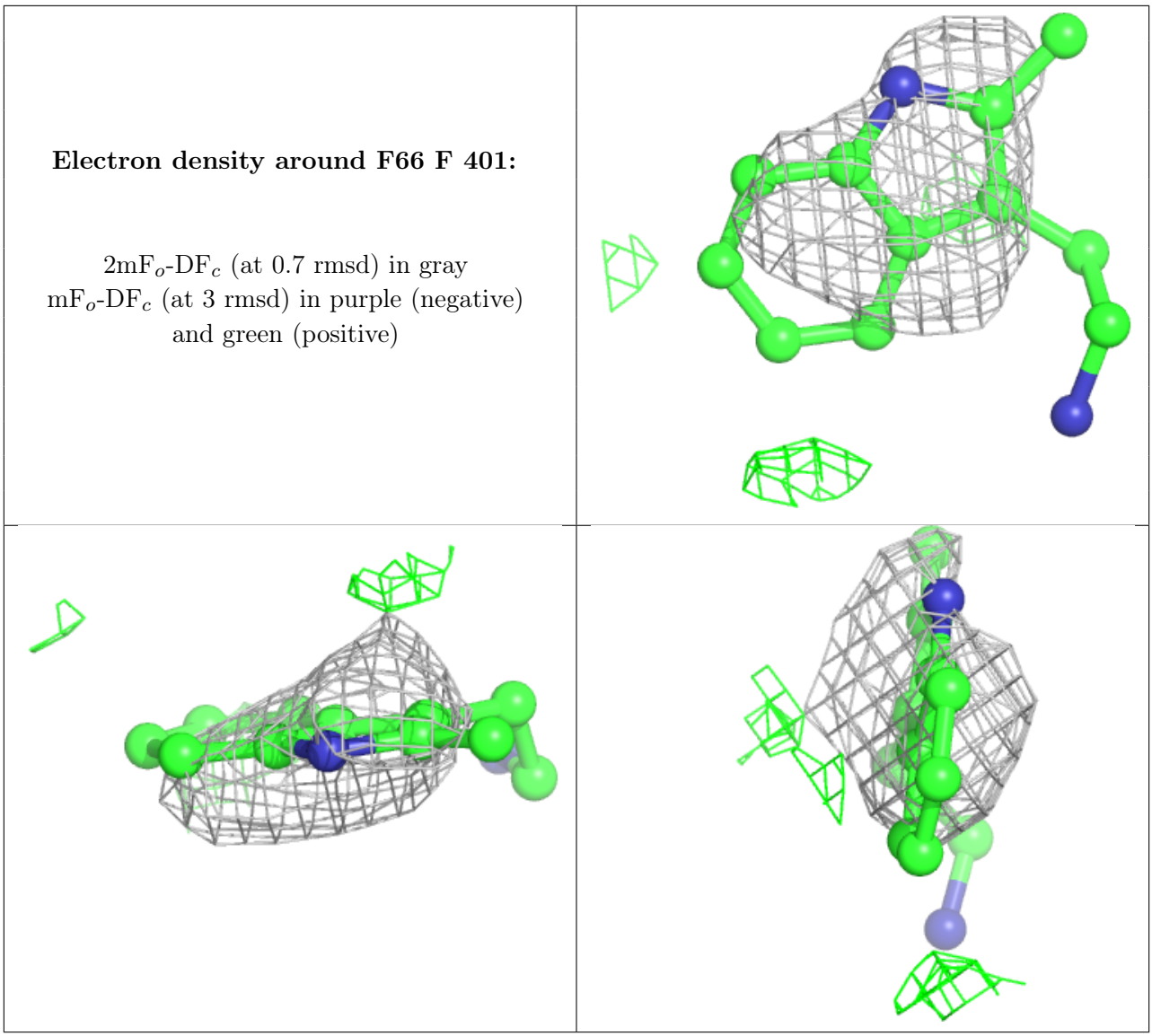
Electron density around F66 D 401:

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



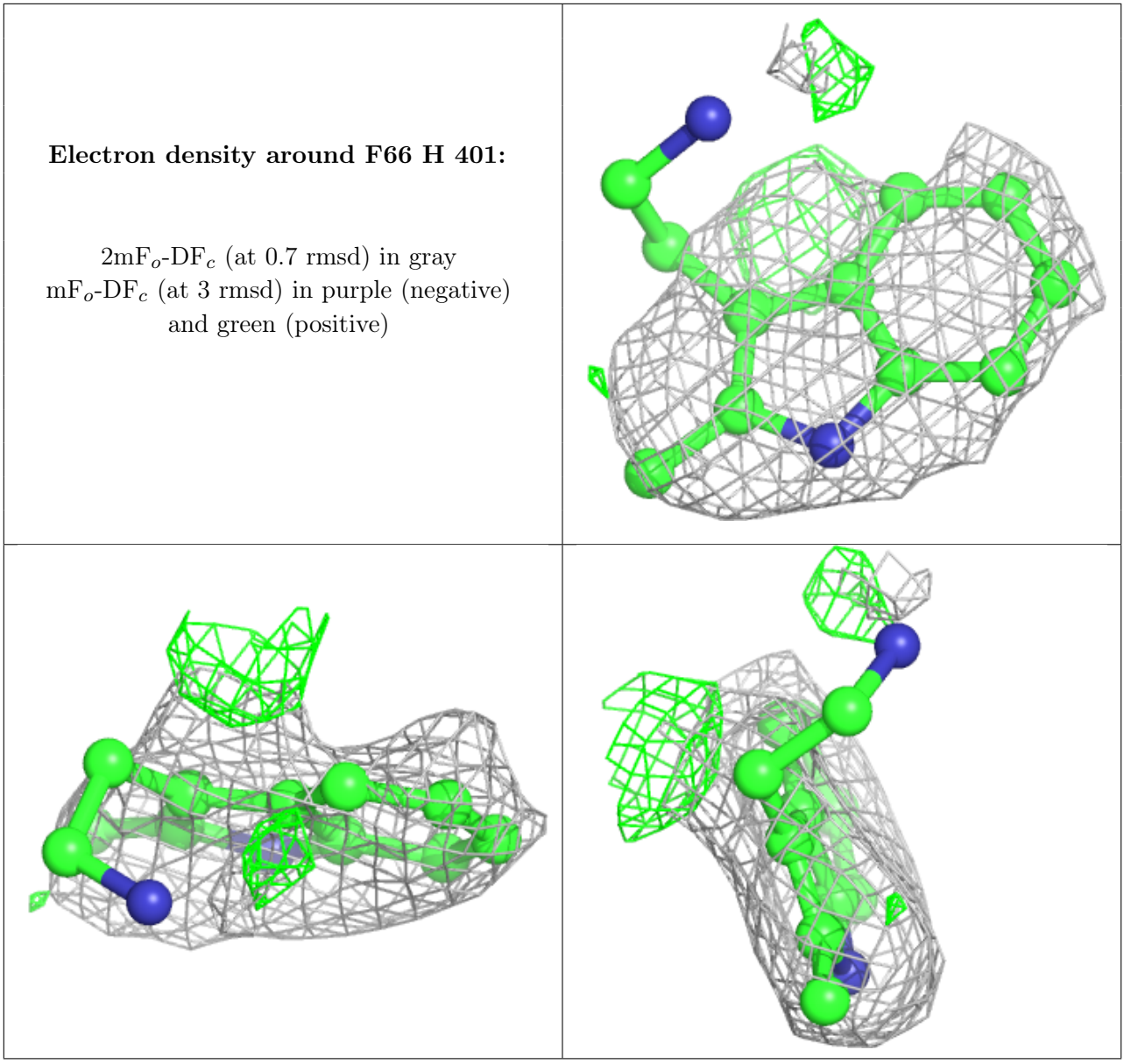
Electron density around F66 F 401:

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



Electron density around F66 H 401:

$2mF_o$-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

There are no such residues in this entry.