Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:34 PM UTC

PDB ID	:	6RT8 / pdb_00006rt8
Title	:	Structure of catharanthine synthase - an alpha-beta hydrolase from Catharanthus roseus with a cleaviminium intermediate bound
Authors	:	Caputi, L.; Franke, J.; Bussey, K.; Farrow, S.C.; Curcino Vieira, I.J.; Stevenson, C.E.M.; Lawson, D.M.; O'Connor, S.E.
Deposited on	:	2019-05-22
Resolution	:	2.19 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:

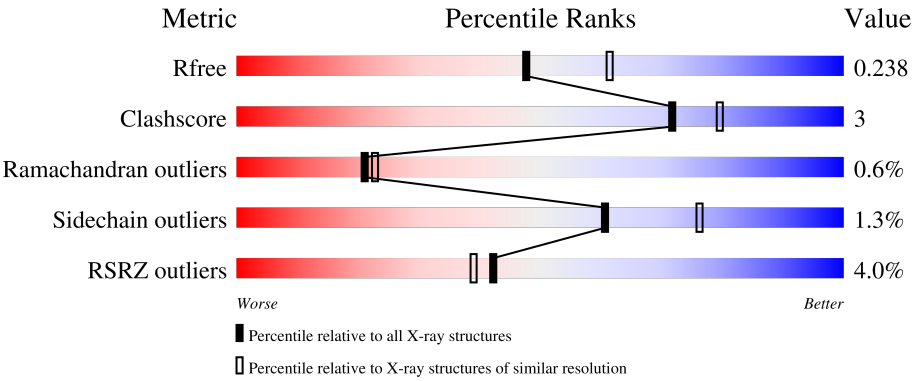
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	330	88% 7% • 5%
1	B	330	88% 6% • 5%
1	C	330	88% 6% • 5%
1	D	330	3% 88% 6% • 5%

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Mol	Chain	Length	Quality of chain
1	E	330	11% 85% 6% • 8%
1	F	330	3% 86% 8% • 5%
1	G	330	% 87% 7% • 5%
1	H	330	7% 88% 7% • 5%

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	KJE	A	401	X	-	-	-
2	KJE	B	401	X	-	-	-
2	KJE	C	401	X	-	-	-
2	KJE	D	401	X	-	-	-
2	KJE	E	401	X	-	-	-
2	KJE	F	401	X	-	-	-
2	KJE	G	401	X	-	-	-
2	KJE	H	401	X	-	-	-
3	P6G	E	402	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20132 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 Catharanthine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2461	1605	391	456	9			
1	B	314	Total	C	N	O	S	0	0	0
			2457	1602	393	453	9			
1	C	314	Total	C	N	O	S	0	0	0
			2464	1609	391	455	9			
1	D	314	Total	C	N	O	S	0	0	0
			2461	1605	392	455	9			
1	E	305	Total	C	N	O	S	0	0	0
			2313	1506	369	429	9			
1	F	313	Total	C	N	O	S	0	0	0
			2438	1588	385	456	9			
1	G	313	Total	C	N	O	S	0	0	0
			2455	1603	389	454	9			
1	H	314	Total	C	N	O	S	0	0	0
			2419	1580	385	445	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A2P1GIW2
A	1	PRO	-	expression tag	UNP A0A2P1GIW2
A	2	ALA	-	expression tag	UNP A0A2P1GIW2
A	3	SER	-	expression tag	UNP A0A2P1GIW2
A	4	GLN	-	expression tag	UNP A0A2P1GIW2
A	5	THR	-	expression tag	UNP A0A2P1GIW2
B	0	GLY	-	expression tag	UNP A0A2P1GIW2
B	1	PRO	-	expression tag	UNP A0A2P1GIW2
B	2	ALA	-	expression tag	UNP A0A2P1GIW2
B	3	SER	-	expression tag	UNP A0A2P1GIW2
B	4	GLN	-	expression tag	UNP A0A2P1GIW2
B	5	THR	-	expression tag	UNP A0A2P1GIW2
C	0	GLY	-	expression tag	UNP A0A2P1GIW2

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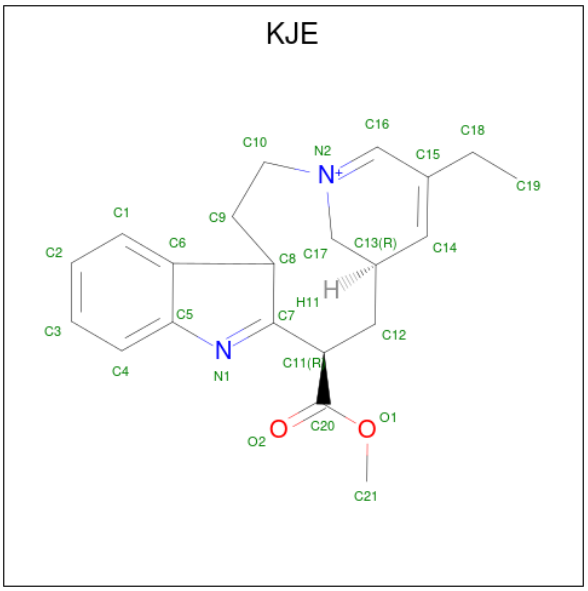
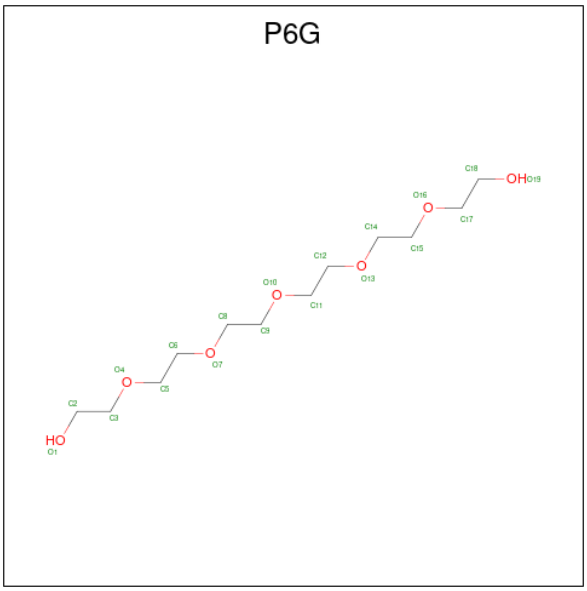
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	PRO	-	expression tag	UNP A0A2P1GIW2
C	2	ALA	-	expression tag	UNP A0A2P1GIW2
C	3	SER	-	expression tag	UNP A0A2P1GIW2
C	4	GLN	-	expression tag	UNP A0A2P1GIW2
C	5	THR	-	expression tag	UNP A0A2P1GIW2
D	0	GLY	-	expression tag	UNP A0A2P1GIW2
D	1	PRO	-	expression tag	UNP A0A2P1GIW2
D	2	ALA	-	expression tag	UNP A0A2P1GIW2
D	3	SER	-	expression tag	UNP A0A2P1GIW2
D	4	GLN	-	expression tag	UNP A0A2P1GIW2
D	5	THR	-	expression tag	UNP A0A2P1GIW2
E	0	GLY	-	expression tag	UNP A0A2P1GIW2
E	1	PRO	-	expression tag	UNP A0A2P1GIW2
E	2	ALA	-	expression tag	UNP A0A2P1GIW2
E	3	SER	-	expression tag	UNP A0A2P1GIW2
E	4	GLN	-	expression tag	UNP A0A2P1GIW2
E	5	THR	-	expression tag	UNP A0A2P1GIW2
F	0	GLY	-	expression tag	UNP A0A2P1GIW2
F	1	PRO	-	expression tag	UNP A0A2P1GIW2
F	2	ALA	-	expression tag	UNP A0A2P1GIW2
F	3	SER	-	expression tag	UNP A0A2P1GIW2
F	4	GLN	-	expression tag	UNP A0A2P1GIW2
F	5	THR	-	expression tag	UNP A0A2P1GIW2
G	0	GLY	-	expression tag	UNP A0A2P1GIW2
G	1	PRO	-	expression tag	UNP A0A2P1GIW2
G	2	ALA	-	expression tag	UNP A0A2P1GIW2
G	3	SER	-	expression tag	UNP A0A2P1GIW2
G	4	GLN	-	expression tag	UNP A0A2P1GIW2
G	5	THR	-	expression tag	UNP A0A2P1GIW2
H	0	GLY	-	expression tag	UNP A0A2P1GIW2
H	1	PRO	-	expression tag	UNP A0A2P1GIW2
H	2	ALA	-	expression tag	UNP A0A2P1GIW2
H	3	SER	-	expression tag	UNP A0A2P1GIW2
H	4	GLN	-	expression tag	UNP A0A2P1GIW2
H	5	THR	-	expression tag	UNP A0A2P1GIW2

- Molecule 2 is 18-carboxymethoxy-cleaviminium (CCD ID: KJE) (formula: $C_{21}H_{25}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	21	2	2		
2	B	1	Total	C	N	O	0	0
			25	21	2	2		
2	C	1	Total	C	N	O	0	0
			25	21	2	2		
2	D	1	Total	C	N	O	0	0
			25	21	2	2		
2	E	1	Total	C	N	O	0	0
			25	21	2	2		
2	F	1	Total	C	N	O	0	0
			25	21	2	2		
2	G	1	Total	C	N	O	0	0
			25	21	2	2		
2	H	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 3 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 19 12 7	0	0
3	C	1	Total C O 19 12 7	0	0
3	E	1	Total C O 19 12 7	0	0
3	H	1	Total C O 19 12 7	0	0

- Molecule 4 is water.

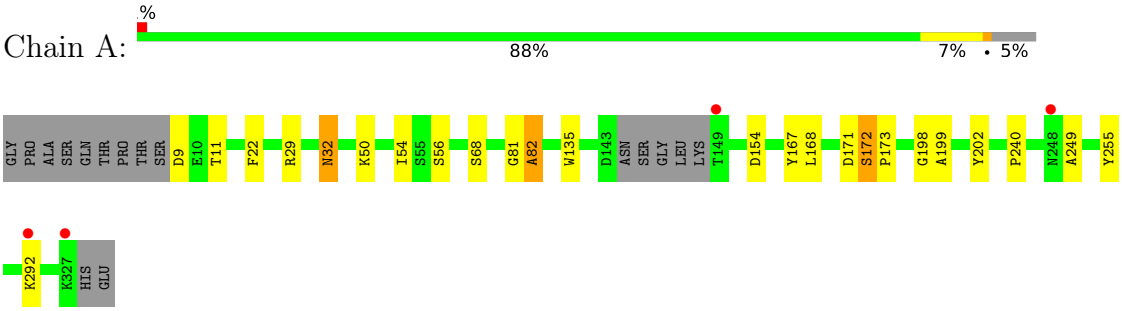
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	40	Total O 40 40	0	0
4	C	44	Total O 44 44	0	0
4	D	70	Total O 70 70	0	0
4	E	33	Total O 33 33	0	0
4	F	64	Total O 64 64	0	0
4	G	38	Total O 38 38	0	0
4	H	34	Total O 34 34	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

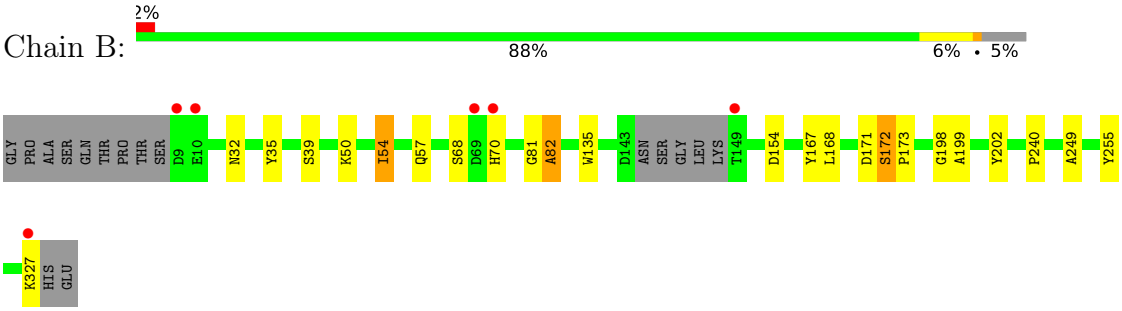
• Molecule 1: Catharanthine synthase

Chain A:



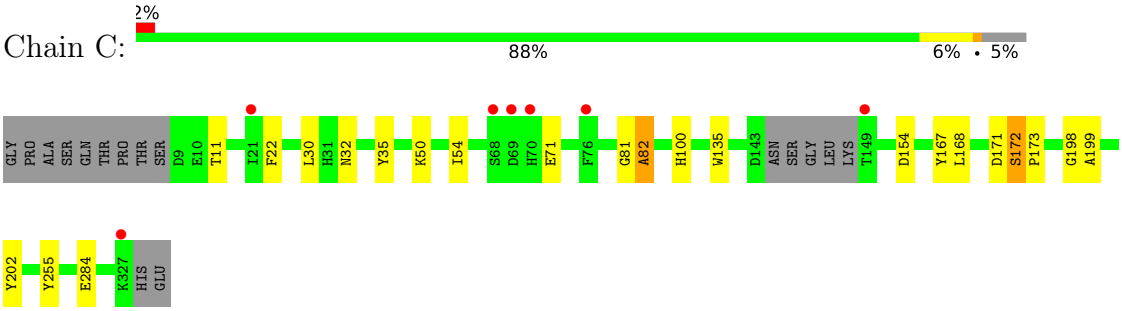
• Molecule 1: Catharanthine synthase

Chain B:



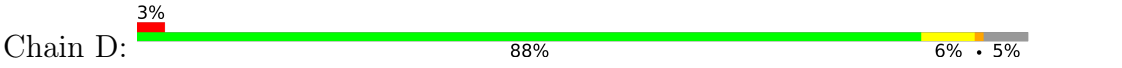
• Molecule 1: Catharanthine synthase

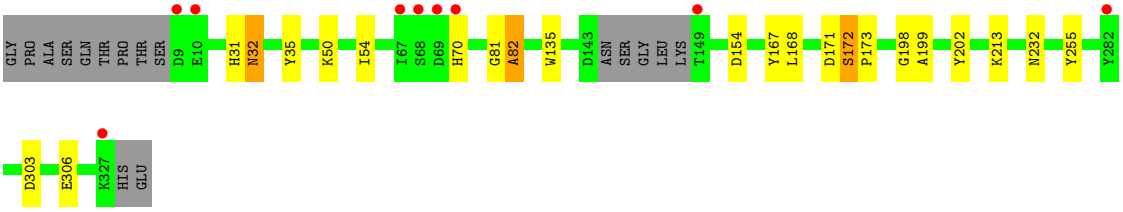
Chain C:



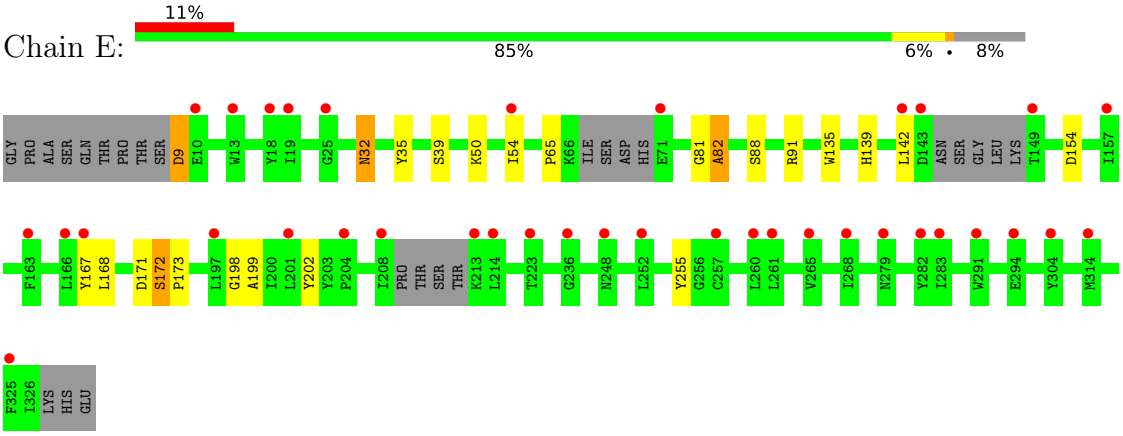
• Molecule 1: Catharanthine synthase

Chain D:

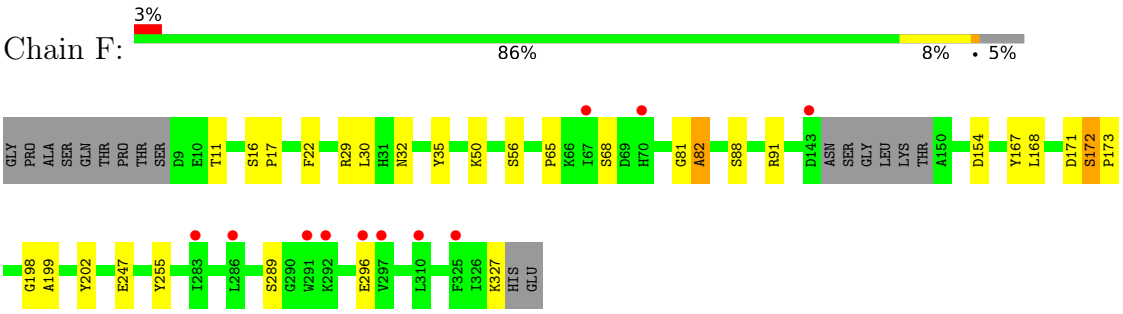




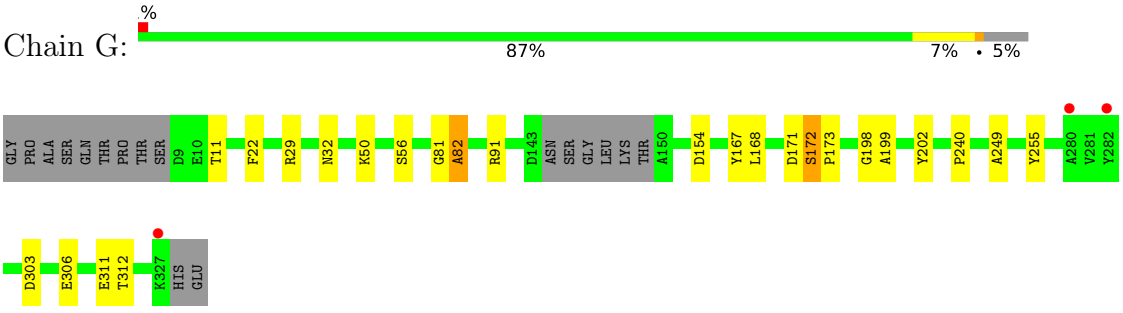
• Molecule 1: Catharanthine synthase



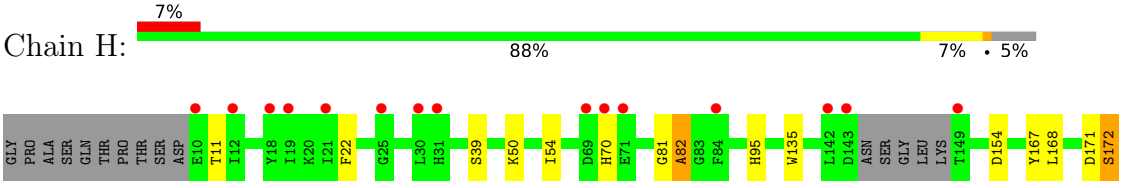
• Molecule 1: Catharanthine synthase

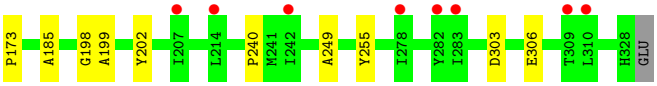


• Molecule 1: Catharanthine synthase



• Molecule 1: Catharanthine synthase




P173
A185
G198
A199
Y202
I207
L214
P240
M241
I242
A249
Y255
I278
Y282
I283
D303
E306
T309
L310
H328
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.54Å 121.03Å 157.98Å 90.00° 99.02° 90.00°	Depositor
Resolution (Å)	52.01 – 2.19 52.01 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.1 (52.01-2.19) 98.1 (52.01-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.194 , 0.234 0.202 , 0.238	Depositor DCC
R_{free} test set	7594 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å^2)	43.0	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20132	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, KJE

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	1.01	0/2534	1.31	2/3460 (0.1%)
1	B	1.03	0/2530	1.31	4/3455 (0.1%)
1	C	1.02	0/2537	1.30	1/3463 (0.0%)
1	D	1.01	1/2534 (0.0%)	1.31	3/3459 (0.1%)
1	E	1.04	0/2380	1.32	2/3256 (0.1%)
1	F	1.01	0/2511	1.30	4/3434 (0.1%)
1	G	1.02	0/2528	1.30	2/3452 (0.1%)
1	H	1.03	1/2491 (0.0%)	1.32	4/3406 (0.1%)
All	All	1.02	2/20045 (0.0%)	1.31	22/27385 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	95	HIS	CE1-NE2	5.29	1.37	1.32
1	D	31	HIS	C-O	5.03	1.30	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	296	GLU	CB-CG-CD	8.20	126.54	112.60
1	D	232	ASN	CA-CB-CG	-7.33	105.28	112.60
1	E	32	ASN	N-CA-CB	-5.91	100.79	109.95
1	D	70	HIS	CA-C-N	5.64	128.72	120.71
1	D	70	HIS	C-N-CA	5.64	128.72	120.71
1	E	65	PRO	CA-C-O	-5.43	115.28	121.96
1	H	70	HIS	CA-C-N	5.26	128.18	120.71
1	H	70	HIS	C-N-CA	5.26	128.18	120.71
1	B	54	ILE	N-CA-C	-5.24	107.65	111.90
1	F	65	PRO	CA-C-O	-5.17	115.60	121.96
1	C	71	GLU	CB-CG-CD	5.09	121.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	29	ARG	CA-C-N	5.07	127.34	120.44
1	F	29	ARG	C-N-CA	5.07	127.34	120.44
1	A	29	ARG	CA-C-N	5.04	127.29	120.44
1	A	29	ARG	C-N-CA	5.04	127.29	120.44
1	H	185	ALA	CA-C-N	5.04	125.53	119.94
1	H	185	ALA	C-N-CA	5.04	125.53	119.94
1	B	70	HIS	CA-C-N	5.04	127.86	120.71
1	B	70	HIS	C-N-CA	5.04	127.86	120.71
1	G	29	ARG	CA-C-N	5.03	127.27	120.44
1	G	29	ARG	C-N-CA	5.03	127.27	120.44
1	B	32	ASN	N-CA-CB	-5.01	102.19	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2461	0	2351	13	0
1	B	2457	0	2352	12	0
1	C	2464	0	2350	17	0
1	D	2461	0	2350	14	0
1	E	2313	0	2132	16	0
1	F	2438	0	2300	21	0
1	G	2455	0	2343	14	0
1	H	2419	0	2283	14	0
2	A	25	0	0	1	0
2	B	25	0	0	1	0
2	C	25	0	0	1	0
2	D	25	0	0	0	0
2	E	25	0	0	1	0
2	F	25	0	0	4	0
2	G	25	0	0	1	0
2	H	25	0	0	1	0
3	A	19	0	26	2	0
3	C	19	0	26	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	19	0	26	11	0
3	H	19	0	26	1	0
4	A	65	0	0	0	0
4	B	40	0	0	0	0
4	C	44	0	0	2	0
4	D	70	0	0	0	0
4	E	33	0	0	0	0
4	F	64	0	0	0	0
4	G	38	0	0	0	0
4	H	34	0	0	0	0
All	All	20132	0	18565	126	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 3.

All (126) 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)
3:C:402:P6G:H22	1:D:32:ASN:HD21	1.46	0.79
1:D:172:SER:HB2	1:D:173:PRO:HD3	1.68	0.76
1:H:172:SER:HB2	1:H:173:PRO:HD3	1.68	0.76
1:G:172:SER:HB2	1:G:173:PRO:HD3	1.69	0.73
1:A:172:SER:HB2	1:A:173:PRO:HD3	1.71	0.72
1:C:172:SER:HB2	1:C:173:PRO:HD3	1.72	0.72
1:A:172:SER:HB2	1:A:173:PRO:CD	2.20	0.71
1:D:172:SER:HB2	1:D:173:PRO:CD	2.21	0.71
1:B:172:SER:HB2	1:B:173:PRO:HD3	1.73	0.71
1:H:172:SER:HB2	1:H:173:PRO:CD	2.21	0.71
1:E:172:SER:HB2	1:E:173:PRO:HD3	1.73	0.71
3:C:402:P6G:H111	1:D:35:TYR:CB	2.20	0.71
1:C:172:SER:HB2	1:C:173:PRO:CD	2.21	0.70
1:F:172:SER:HB2	1:F:173:PRO:CD	2.20	0.70
1:E:172:SER:HB2	1:E:173:PRO:CD	2.21	0.70
1:F:172:SER:HB2	1:F:173:PRO:HD3	1.72	0.70
1:G:172:SER:HB2	1:G:173:PRO:CD	2.21	0.70
1:B:172:SER:HB2	1:B:173:PRO:CD	2.23	0.69
3:C:402:P6G:H111	1:D:35:TYR:HB3	1.82	0.62
3:E:402:P6G:H81	1:F:91:ARG:NH2	2.20	0.57
1:C:35:TYR:HB2	3:C:402:P6G:H91	1.87	0.57
2:F:401:KJE:O1	2:F:401:KJE:C14	2.53	0.56
2:G:401:KJE:O1	2:G:401:KJE:C14	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:SER:CB	1:A:173:PRO:CD	2.85	0.54
1:G:172:SER:CB	1:G:173:PRO:CD	2.86	0.54
1:D:172:SER:CB	1:D:173:PRO:CD	2.86	0.54
1:H:172:SER:CB	1:H:173:PRO:CD	2.86	0.54
1:C:35:TYR:HB2	3:C:402:P6G:C9	2.37	0.54
1:F:172:SER:CB	1:F:173:PRO:CD	2.86	0.53
1:C:172:SER:CB	1:C:173:PRO:CD	2.86	0.53
1:E:172:SER:CB	1:E:173:PRO:CD	2.87	0.53
3:E:402:P6G:H111	1:F:35:TYR:CB	2.39	0.53
1:B:172:SER:CB	1:B:173:PRO:CD	2.87	0.52
1:A:32:ASN:HD21	3:A:402:P6G:H171	1.74	0.52
2:A:401:KJE:C8	2:A:401:KJE:C17	2.87	0.52
2:F:401:KJE:C17	2:F:401:KJE:C8	2.88	0.51
1:E:139:HIS:O	1:E:142:LEU:HD13	2.12	0.50
1:F:168:LEU:O	1:F:199:ALA:HA	2.12	0.50
1:G:168:LEU:O	1:G:199:ALA:HA	2.12	0.50
1:A:168:LEU:O	1:A:199:ALA:HA	2.12	0.50
1:C:168:LEU:O	1:C:199:ALA:HA	2.12	0.49
1:B:168:LEU:O	1:B:199:ALA:HA	2.11	0.49
1:E:168:LEU:O	1:E:199:ALA:HA	2.13	0.49
3:E:402:P6G:H52	1:F:88:SER:HB2	1.95	0.48
1:F:30:LEU:HD12	1:F:30:LEU:N	2.28	0.48
1:D:168:LEU:O	1:D:199:ALA:HA	2.14	0.48
1:H:168:LEU:O	1:H:199:ALA:HA	2.13	0.48
1:D:81:GLY:O	1:D:82:ALA:HB3	2.14	0.48
1:B:81:GLY:O	1:B:82:ALA:HB3	2.13	0.48
1:G:81:GLY:O	1:G:82:ALA:HB3	2.14	0.48
1:C:30:LEU:HD12	1:C:30:LEU:N	2.28	0.47
1:D:167:TYR:HA	1:D:198:GLY:O	2.15	0.47
1:C:35:TYR:CB	3:C:402:P6G:H91	2.45	0.47
1:H:167:TYR:HA	1:H:198:GLY:O	2.15	0.47
1:E:35:TYR:CG	3:E:402:P6G:H91	2.49	0.47
1:E:167:TYR:HA	1:E:198:GLY:O	2.15	0.47
1:H:81:GLY:O	1:H:82:ALA:HB3	2.15	0.47
1:E:81:GLY:O	1:E:82:ALA:HB3	2.15	0.47
1:A:167:TYR:HA	1:A:198:GLY:O	2.15	0.47
1:E:32:ASN:HD21	3:E:402:P6G:H181	1.80	0.47
1:E:50:LYS:HE3	1:E:154:ASP:OD1	2.15	0.46
2:F:401:KJE:C17	2:F:401:KJE:C7	2.93	0.46
1:B:167:TYR:HA	1:B:198:GLY:O	2.15	0.46
1:C:30:LEU:HD12	1:C:30:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:TYR:HA	1:G:198:GLY:O	2.15	0.46
1:F:167:TYR:HA	1:F:198:GLY:O	2.16	0.46
1:C:167:TYR:HA	1:C:198:GLY:O	2.15	0.46
3:C:402:P6G:H111	1:D:35:TYR:HB2	1.96	0.46
3:E:402:P6G:H92	1:F:35:TYR:HB2	1.97	0.46
1:F:30:LEU:HD12	1:F:30:LEU:H	1.80	0.46
3:E:402:P6G:C8	1:F:91:ARG:NH2	2.79	0.46
1:F:81:GLY:O	1:F:82:ALA:HB3	2.15	0.46
1:B:50:LYS:HE3	1:B:154:ASP:OD1	2.17	0.45
3:E:402:P6G:H81	1:F:91:ARG:CZ	2.47	0.45
1:C:81:GLY:O	1:C:82:ALA:HB3	2.16	0.45
1:A:81:GLY:O	1:A:82:ALA:HB3	2.16	0.45
1:D:50:LYS:HE3	1:D:154:ASP:OD1	2.17	0.45
1:B:171:ASP:HA	1:B:202:TYR:O	2.17	0.45
1:F:50:LYS:HE3	1:F:154:ASP:OD1	2.17	0.45
1:A:50:LYS:HE3	1:A:154:ASP:OD1	2.17	0.44
1:C:50:LYS:HE3	1:C:154:ASP:OD1	2.16	0.44
1:E:171:ASP:HA	1:E:202:TYR:O	2.17	0.44
1:A:171:ASP:HA	1:A:202:TYR:O	2.18	0.44
1:C:100:HIS:CE1	4:C:506:HOH:O	2.71	0.44
1:C:171:ASP:HA	1:C:202:TYR:O	2.17	0.44
1:D:171:ASP:HA	1:D:202:TYR:O	2.18	0.44
1:G:11:THR:HA	1:G:22:PHE:HA	2.00	0.44
1:G:50:LYS:HE3	1:G:154:ASP:OD1	2.17	0.44
1:C:100:HIS:HE1	4:C:506:HOH:O	1.99	0.44
2:E:401:KJE:C17	2:E:401:KJE:C8	2.96	0.44
3:A:402:P6G:H112	1:B:35:TYR:CB	2.48	0.43
1:G:171:ASP:HA	1:G:202:TYR:O	2.18	0.43
1:A:240:PRO:HB3	1:A:249:ALA:HA	1.99	0.43
1:H:171:ASP:HA	1:H:202:TYR:O	2.18	0.43
1:E:9:ASP:N	1:E:9:ASP:OD1	2.51	0.43
1:F:171:ASP:HA	1:F:202:TYR:O	2.18	0.43
1:H:82:ALA:HA	2:H:401:KJE:C7	2.48	0.43
1:H:240:PRO:HB3	1:H:249:ALA:HA	2.00	0.43
1:E:91:ARG:NH2	3:E:402:P6G:H112	2.33	0.42
1:H:50:LYS:HE3	1:H:154:ASP:OD1	2.19	0.42
1:D:303:ASP:HB3	1:D:306:GLU:HG3	2.00	0.42
1:E:54:ILE:HG12	1:E:135:TRP:CD2	2.54	0.42
3:E:402:P6G:H111	1:F:35:TYR:HB2	2.01	0.42
1:G:311:GLU:HG3	1:G:312:THR:HG23	2.02	0.42
1:C:11:THR:HA	1:C:22:PHE:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:THR:HA	1:F:22:PHE:HA	2.02	0.42
1:G:303:ASP:HB3	1:G:306:GLU:HG3	2.02	0.41
1:G:56:SER:HA	1:H:39:SER:OG	2.20	0.41
1:C:54:ILE:HG12	1:C:135:TRP:CD2	2.56	0.41
1:G:240:PRO:HB3	1:G:249:ALA:HA	2.01	0.41
1:A:11:THR:HA	1:A:22:PHE:HA	2.03	0.41
2:B:401:KJE:C17	2:B:401:KJE:C8	2.97	0.41
1:H:303:ASP:HB3	1:H:306:GLU:HG3	2.02	0.41
1:D:54:ILE:HG12	1:D:135:TRP:CD2	2.55	0.41
1:E:88:SER:HB2	3:E:402:P6G:H151	2.03	0.41
1:B:240:PRO:HB3	1:B:249:ALA:HA	2.03	0.41
1:B:54:ILE:HG12	1:B:135:TRP:CD2	2.56	0.41
1:A:56:SER:HA	1:B:39:SER:OG	2.20	0.41
1:H:54:ILE:HG12	1:H:135:TRP:CD2	2.55	0.41
1:A:54:ILE:HG12	1:A:135:TRP:CD2	2.56	0.40
1:H:11:THR:HA	1:H:22:PHE:HA	2.02	0.40
1:F:82:ALA:HB2	2:F:401:KJE:C4	2.52	0.40
2:C:401:KJE:C17	2:C:401:KJE:C8	2.99	0.40
1:E:39:SER:OG	1:F:56:SER:HA	2.21	0.40
1:F:16:SER:HA	1:F:17:PRO:HA	1.92	0.40
1:G:91:ARG:HE	3:H:402:P6G:H62	1.87	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	310/330 (94%)	295 (95%)	13 (4%)	2 (1%)	21	23
1	B	310/330 (94%)	291 (94%)	17 (6%)	2 (1%)	21	23
1	C	310/330 (94%)	296 (96%)	12 (4%)	2 (1%)	21	23
1	D	310/330 (94%)	296 (96%)	12 (4%)	2 (1%)	21	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	297/330 (90%)	282 (95%)	13 (4%)	2 (1%)	18	19
1	F	309/330 (94%)	295 (96%)	12 (4%)	2 (1%)	21	23
1	G	309/330 (94%)	296 (96%)	11 (4%)	2 (1%)	21	23
1	H	310/330 (94%)	296 (96%)	12 (4%)	2 (1%)	21	23
All	All	2465/2640 (93%)	2347 (95%)	102 (4%)	16 (1%)	21	23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	B	172	SER
1	C	172	SER
1	D	172	SER
1	E	172	SER
1	F	172	SER
1	G	172	SER
1	H	172	SER
1	A	82	ALA
1	B	82	ALA
1	C	82	ALA
1	D	82	ALA
1	E	82	ALA
1	F	82	ALA
1	G	82	ALA
1	H	82	ALA

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	256/283 (90%)	251 (98%)	5 (2%)	48	64
1	B	256/283 (90%)	252 (98%)	4 (2%)	55	71
1	C	254/283 (90%)	251 (99%)	3 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	255/283 (90%)	252 (99%)	3 (1%)	63 78
1	E	228/283 (81%)	226 (99%)	2 (1%)	70 84
1	F	252/283 (89%)	246 (98%)	6 (2%)	43 58
1	G	254/283 (90%)	252 (99%)	2 (1%)	73 85
1	H	245/283 (87%)	244 (100%)	1 (0%)	84 92
All	All	2000/2264 (88%)	1974 (99%)	26 (1%)	61 76

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

Mol	Chain	Res	Type
1	A	9	ASP
1	A	32	ASN
1	A	68	SER
1	A	255	TYR
1	A	292	LYS
1	B	57	GLN
1	B	68	SER
1	B	255	TYR
1	B	327	LYS
1	C	32	ASN
1	C	255	TYR
1	C	284	GLU
1	D	32	ASN
1	D	213	LYS
1	D	255	TYR
1	E	9	ASP
1	E	255	TYR
1	F	32	ASN
1	F	68	SER
1	F	247	GLU
1	F	255	TYR
1	F	289	SER
1	F	327	LYS
1	G	32	ASN
1	G	255	TYR
1	H	255	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	D	32	ASN
1	E	57	GLN

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)

12 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	$\#\|Z\| > 2$
2	KJE	F	401	-	23,28,28	3.77	5 (21%)	22,40,40	2.01	6 (27%)
3	P6G	E	402	-	18,18,18	0.58	0	17,17,17	0.79	1 (5%)
2	KJE	G	401	-	23,28,28	4.00	4 (17%)	22,40,40	2.21	5 (22%)
2	KJE	A	401	-	23,28,28	3.34	4 (17%)	22,40,40	2.21	6 (27%)
2	KJE	E	401	-	23,28,28	4.18	4 (17%)	22,40,40	2.25	4 (18%)
2	KJE	C	401	-	23,28,28	3.52	4 (17%)	22,40,40	2.30	5 (22%)
2	KJE	H	401	-	23,28,28	4.24	4 (17%)	22,40,40	2.29	6 (27%)
2	KJE	B	401	-	23,28,28	3.72	4 (17%)	22,40,40	2.26	5 (22%)
2	KJE	D	401	-	23,28,28	3.79	4 (17%)	22,40,40	2.21	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	P6G	C	402	-	18,18,18	0.82	0	17,17,17	1.21	3 (17%)
3	P6G	A	402	-	18,18,18	0.85	0	17,17,17	0.93	0
3	P6G	H	402	-	18,18,18	0.66	0	17,17,17	0.92	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
2	KJE	F	401	-	2/2/7/9	3/11/45/45	0/2/4/4
3	P6G	E	402	-	-	8/16/16/16	-
2	KJE	G	401	-	2/2/7/9	4/11/45/45	0/2/4/4
2	KJE	A	401	-	2/2/7/9	2/11/45/45	0/2/4/4
2	KJE	E	401	-	2/2/7/9	4/11/45/45	0/2/4/4
2	KJE	C	401	-	2/2/7/9	1/11/45/45	0/2/4/4
2	KJE	H	401	-	2/2/7/9	2/11/45/45	0/2/4/4
2	KJE	B	401	-	2/2/7/9	4/11/45/45	0/2/4/4
2	KJE	D	401	-	2/2/7/9	4/11/45/45	0/2/4/4
3	P6G	C	402	-	-	9/16/16/16	-
3	P6G	A	402	-	-	4/16/16/16	-
3	P6G	H	402	-	-	9/16/16/16	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	KJE	C7-N1	14.01	1.38	1.29
2	D	401	KJE	C7-N1	13.91	1.38	1.29
2	H	401	KJE	C14-C15	13.72	1.44	1.33
2	G	401	KJE	C7-N1	13.63	1.38	1.29
2	E	401	KJE	C7-N1	13.56	1.38	1.29
2	E	401	KJE	C14-C15	13.55	1.44	1.33
2	C	401	KJE	C7-N1	12.53	1.37	1.29
2	G	401	KJE	C14-C15	12.34	1.43	1.33
2	F	401	KJE	C7-N1	12.31	1.37	1.29
2	B	401	KJE	C7-N1	12.21	1.37	1.29
2	F	401	KJE	C14-C15	11.67	1.43	1.33
2	B	401	KJE	C14-C15	11.48	1.42	1.33
2	A	401	KJE	C7-N1	11.30	1.36	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	KJE	C14-C15	10.13	1.41	1.33
2	A	401	KJE	C14-C15	9.71	1.41	1.33
2	C	401	KJE	C14-C15	9.60	1.41	1.33
2	F	401	KJE	C6-C8	-4.76	1.43	1.51
2	D	401	KJE	C6-C8	-4.59	1.43	1.51
2	B	401	KJE	C6-C8	-4.59	1.43	1.51
2	A	401	KJE	C6-C8	-4.53	1.44	1.51
2	C	401	KJE	C6-C8	-4.42	1.44	1.51
2	G	401	KJE	C6-C8	-4.39	1.44	1.51
2	E	401	KJE	C6-C8	-4.33	1.44	1.51
2	H	401	KJE	C6-C8	-4.06	1.44	1.51
2	E	401	KJE	C9-C8	-3.12	1.49	1.54
2	C	401	KJE	C9-C8	-2.95	1.49	1.54
2	B	401	KJE	C9-C8	-2.88	1.50	1.54
2	D	401	KJE	C9-C8	-2.68	1.50	1.54
2	A	401	KJE	C9-C8	-2.56	1.50	1.54
2	F	401	KJE	C9-C8	-2.50	1.50	1.54
2	G	401	KJE	C9-C8	-2.47	1.50	1.54
2	H	401	KJE	C9-C8	-2.42	1.50	1.54
2	F	401	KJE	C16-C15	-2.31	1.37	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	KJE	C6-C5-N1	-5.79	106.97	111.93
2	E	401	KJE	C6-C5-N1	-5.39	107.32	111.93
2	B	401	KJE	C6-C5-N1	-5.34	107.36	111.93
2	A	401	KJE	C6-C5-N1	-5.28	107.41	111.93
2	D	401	KJE	C6-C5-N1	-5.22	107.46	111.93
2	H	401	KJE	C5-N1-C7	5.19	110.06	106.19
2	E	401	KJE	C5-N1-C7	5.17	110.05	106.19
2	G	401	KJE	C6-C5-N1	-5.14	107.53	111.93
2	H	401	KJE	C9-C8-C6	5.08	124.70	114.53
2	H	401	KJE	C6-C5-N1	-4.99	107.66	111.93
2	G	401	KJE	C9-C8-C6	4.96	124.47	114.53
2	B	401	KJE	C9-C8-C6	4.79	124.11	114.53
2	C	401	KJE	C9-C8-C6	4.72	123.97	114.53
2	C	401	KJE	C5-N1-C7	4.71	109.70	106.19
2	F	401	KJE	C6-C5-N1	-4.69	107.92	111.93
2	B	401	KJE	C5-N1-C7	4.67	109.67	106.19
2	A	401	KJE	C9-C8-C6	4.64	123.81	114.53
2	G	401	KJE	C5-N1-C7	4.61	109.63	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	KJE	C9-C8-C6	4.42	123.38	114.53
2	A	401	KJE	C5-N1-C7	4.41	109.48	106.19
2	D	401	KJE	C9-C8-C6	4.36	123.26	114.53
2	F	401	KJE	C5-N1-C7	4.36	109.44	106.19
2	D	401	KJE	C5-N1-C7	4.33	109.42	106.19
2	H	401	KJE	C6-C8-C7	4.13	107.35	100.86
2	E	401	KJE	C6-C8-C7	4.03	107.20	100.86
2	G	401	KJE	C6-C8-C7	3.92	107.02	100.86
2	D	401	KJE	C6-C8-C7	3.61	106.53	100.86
2	B	401	KJE	C6-C8-C7	3.54	106.42	100.86
2	C	401	KJE	C6-C8-C7	3.54	106.42	100.86
2	F	401	KJE	C6-C8-C7	3.52	106.39	100.86
2	D	401	KJE	C17-C13-C14	3.48	113.22	108.52
2	F	401	KJE	C9-C8-C6	3.37	121.28	114.53
2	C	401	KJE	C17-C13-C14	3.29	112.96	108.52
2	A	401	KJE	C6-C8-C7	3.26	105.99	100.86
2	B	401	KJE	C17-C13-C14	2.86	112.38	108.52
3	C	402	P6G	O10-C11-C12	2.75	122.91	110.35
2	F	401	KJE	C17-C13-C14	2.58	112.00	108.52
2	A	401	KJE	C17-C13-C14	2.45	111.83	108.52
3	C	402	P6G	O10-C9-C8	2.42	121.40	110.35
2	G	401	KJE	C17-C13-C14	2.42	111.78	108.52
3	E	402	P6G	O13-C14-C15	-2.40	99.41	110.35
2	F	401	KJE	C2-C1-C6	-2.26	118.28	120.99
3	C	402	P6G	O16-C17-C18	2.25	120.04	110.11
2	D	401	KJE	C18-C15-C14	-2.20	117.52	122.75
2	H	401	KJE	C17-C13-C14	2.16	111.44	108.52
2	H	401	KJE	C16-C15-C14	-2.11	115.33	119.22
2	A	401	KJE	C18-C15-C14	-2.11	117.73	122.75

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	KJE	C8
2	A	401	KJE	N2
2	B	401	KJE	C8
2	B	401	KJE	N2
2	C	401	KJE	C8
2	C	401	KJE	N2
2	D	401	KJE	C8
2	D	401	KJE	N2
2	E	401	KJE	C8

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Mol	Chain	Res	Type	Atom
2	E	401	KJE	N2
2	F	401	KJE	C8
2	F	401	KJE	N2
2	G	401	KJE	C8
2	G	401	KJE	N2
2	H	401	KJE	C8
2	H	401	KJE	N2

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	KJE	C7-C11-C20-O2
2	B	401	KJE	C7-C11-C20-O2
2	B	401	KJE	C14-C15-C18-C19
2	C	401	KJE	C7-C11-C20-O2
2	D	401	KJE	C7-C11-C20-O2
2	E	401	KJE	C7-C11-C20-O2
2	E	401	KJE	C14-C15-C18-C19
2	F	401	KJE	C7-C11-C20-O2
2	G	401	KJE	C7-C11-C20-O2
2	H	401	KJE	C7-C11-C20-O2
2	H	401	KJE	C14-C15-C18-C19
2	G	401	KJE	C11-C20-O1-C21
2	F	401	KJE	C11-C20-O1-C21
3	A	402	P6G	C8-C9-O10-C11
2	G	401	KJE	O2-C20-O1-C21
3	C	402	P6G	O10-C11-C12-O13
3	C	402	P6G	O7-C8-C9-O10
3	E	402	P6G	O10-C11-C12-O13
3	H	402	P6G	O4-C5-C6-O7
2	E	401	KJE	C11-C20-O1-C21
3	H	402	P6G	O7-C8-C9-O10
2	D	401	KJE	C11-C20-O1-C21
3	H	402	P6G	O10-C11-C12-O13
3	A	402	P6G	O7-C8-C9-O10
2	F	401	KJE	O2-C20-O1-C21
2	D	401	KJE	O2-C20-O1-C21
3	E	402	P6G	O7-C8-C9-O10
3	C	402	P6G	C12-C11-O10-C9
3	A	402	P6G	O10-C11-C12-O13
3	C	402	P6G	O1-C2-C3-O4
3	H	402	P6G	C12-C11-O10-C9

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Mol	Chain	Res	Type	Atoms
2	E	401	KJE	O2-C20-O1-C21
3	C	402	P6G	O13-C14-C15-O16
2	A	401	KJE	C14-C15-C18-C19
2	D	401	KJE	C14-C15-C18-C19
3	A	402	P6G	O1-C2-C3-O4
3	C	402	P6G	C11-C12-O13-C14
3	E	402	P6G	C5-C6-O7-C8
3	H	402	P6G	C2-C3-O4-C5
3	E	402	P6G	C12-C11-O10-C9
3	E	402	P6G	O16-C17-C18-O19
3	H	402	P6G	O13-C14-C15-O16
3	C	402	P6G	O16-C17-C18-O19
3	H	402	P6G	O1-C2-C3-O4
2	B	401	KJE	C7-C8-C9-C10
2	G	401	KJE	C7-C8-C9-C10
2	B	401	KJE	O2-C20-O1-C21
3	E	402	P6G	O13-C14-C15-O16
3	C	402	P6G	C18-C17-O16-C15
3	E	402	P6G	C9-C8-O7-C6
3	E	402	P6G	C11-C12-O13-C14
3	H	402	P6G	C18-C17-O16-C15
3	C	402	P6G	C8-C9-O10-C11
3	H	402	P6G	C5-C6-O7-C8

There are no ring outliers.

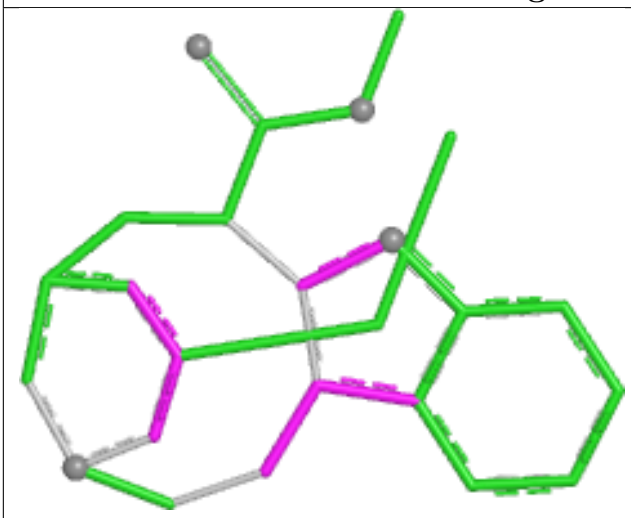
11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	KJE	4	0
3	E	402	P6G	11	0
2	G	401	KJE	1	0
2	A	401	KJE	1	0
2	E	401	KJE	1	0
2	C	401	KJE	1	0
2	H	401	KJE	1	0
2	B	401	KJE	1	0
3	C	402	P6G	7	0
3	A	402	P6G	2	0
3	H	402	P6G	1	0

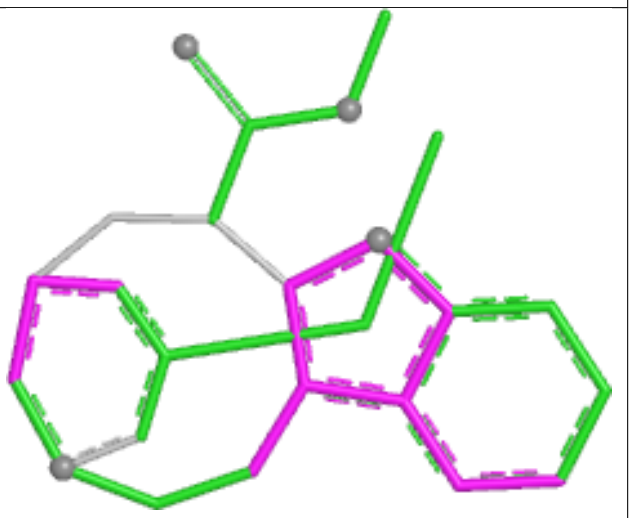
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

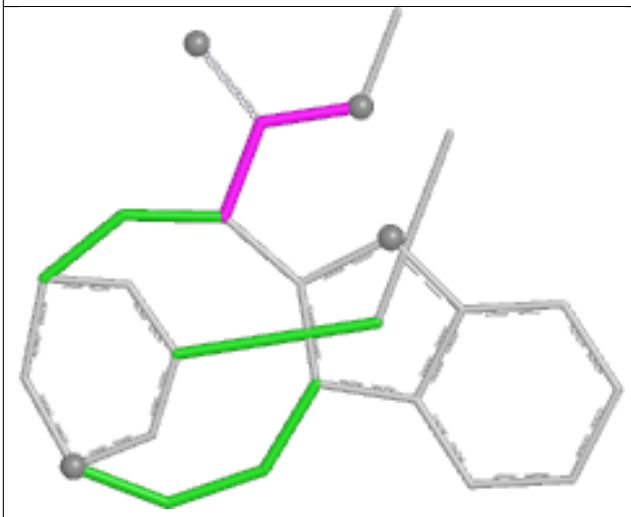
Ligand KJE F 401



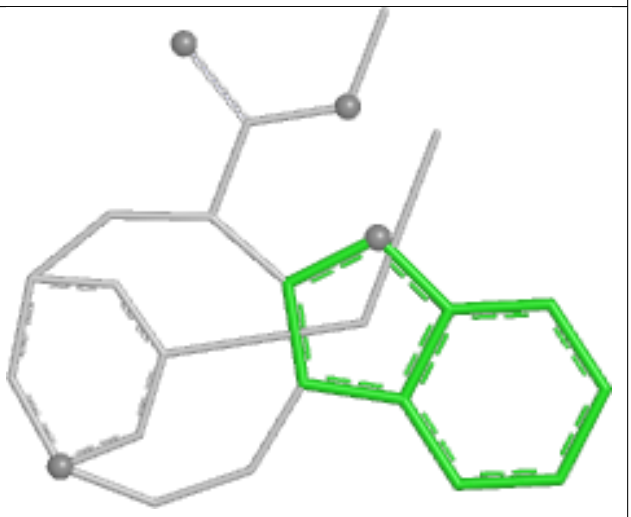
Bond lengths



Bond angles

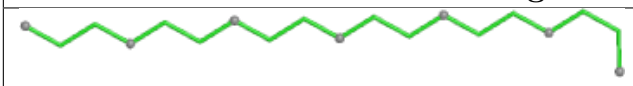


Torsions



Rings

Ligand P6G E 402



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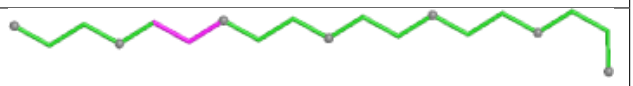
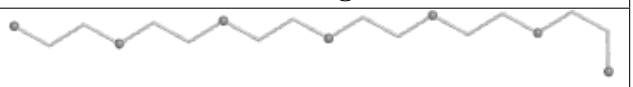


Bond angles

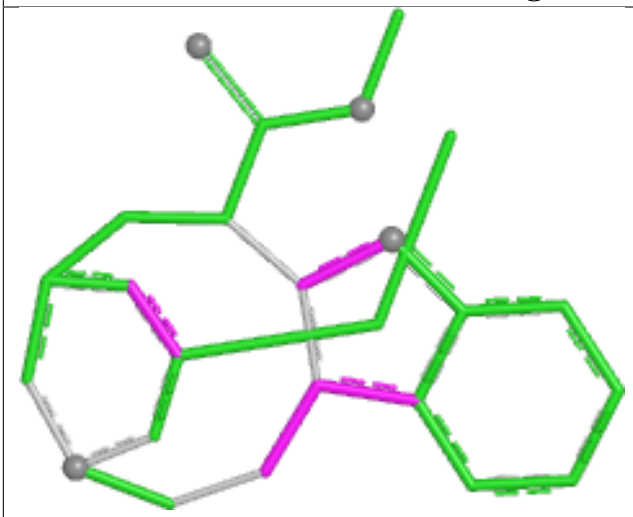


Torsions



Rings

Ligand KJE G 401



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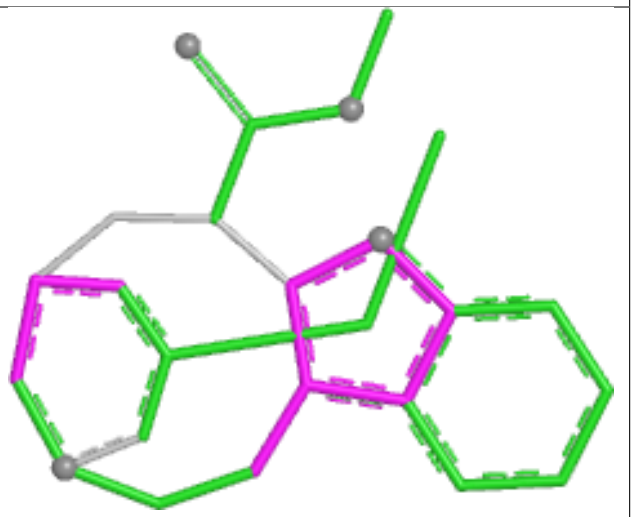
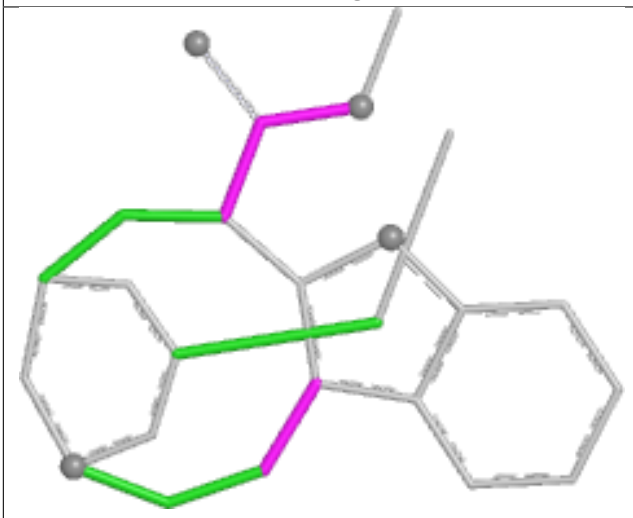


Bond angles



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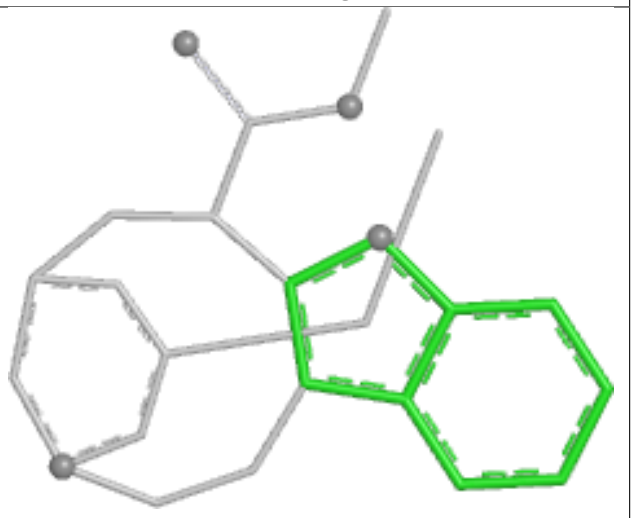
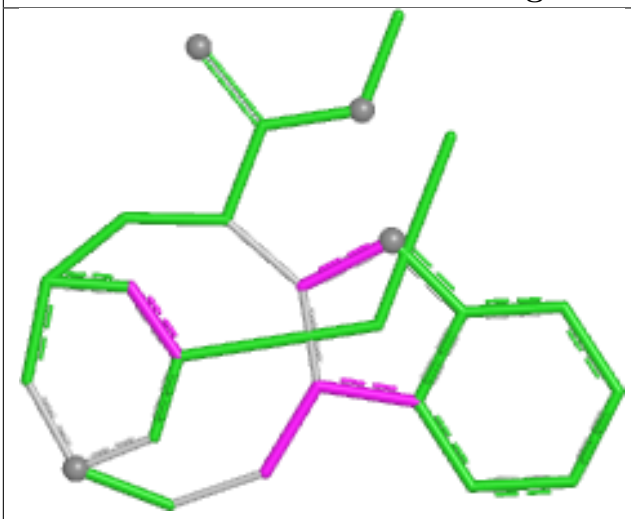


Rings

Ligand KJE A 401



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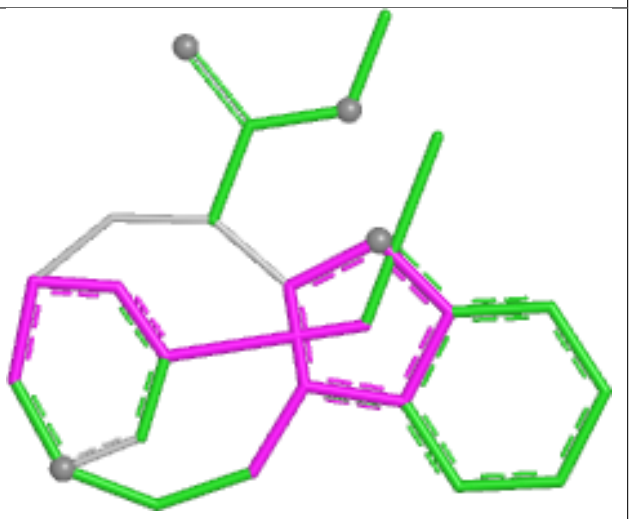

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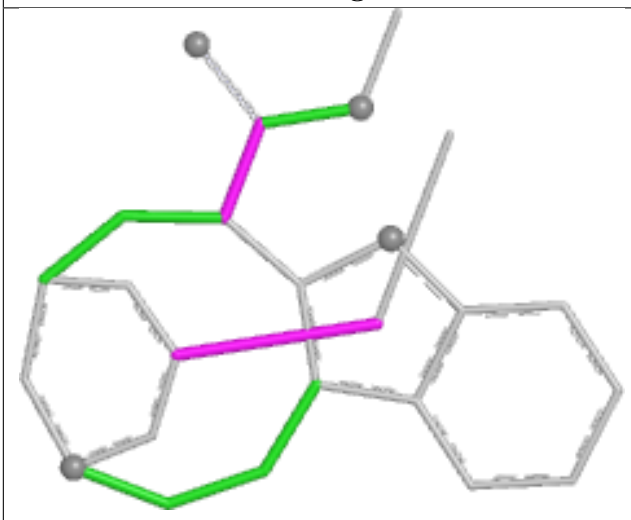

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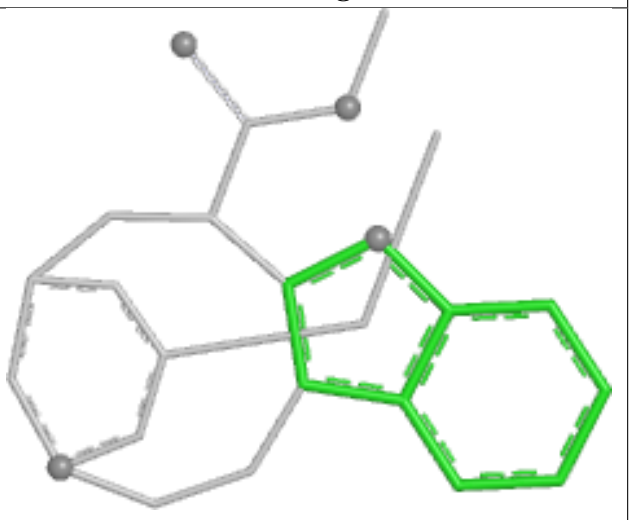
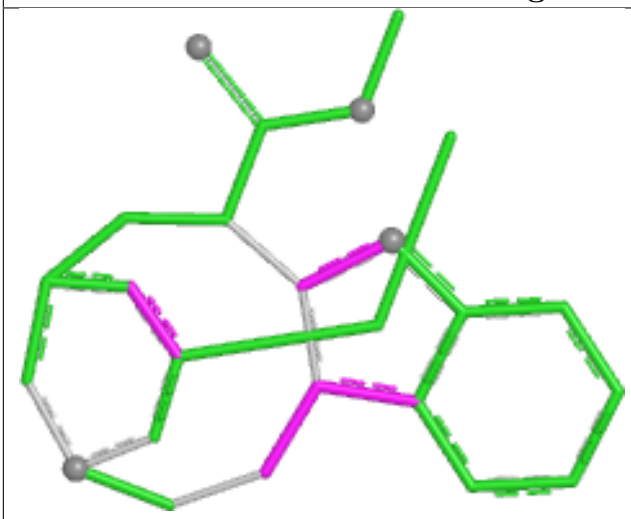


Rings

Ligand KJE E 401



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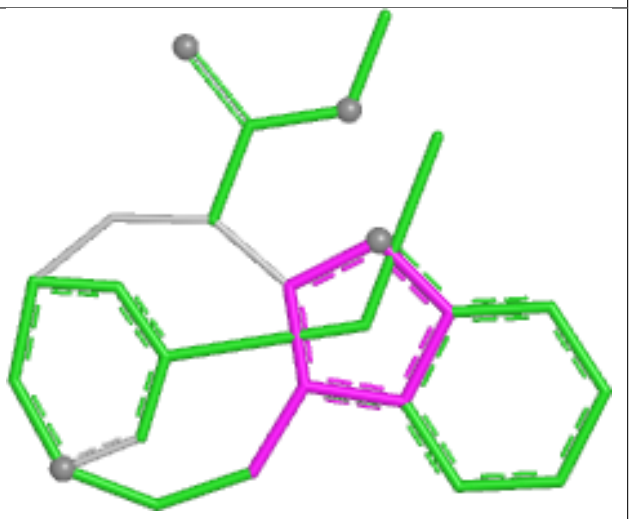

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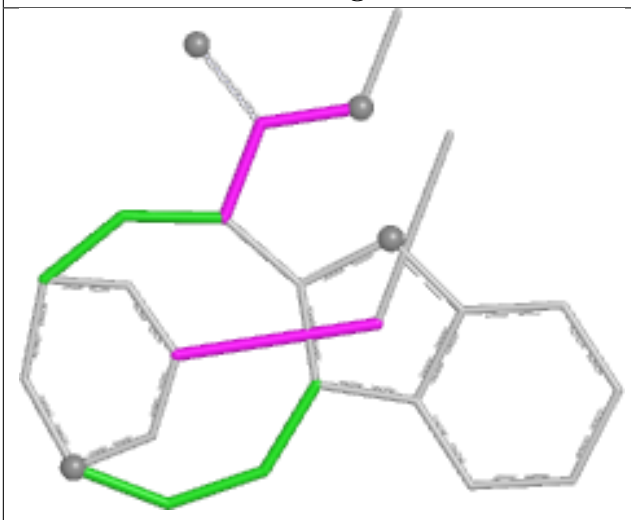

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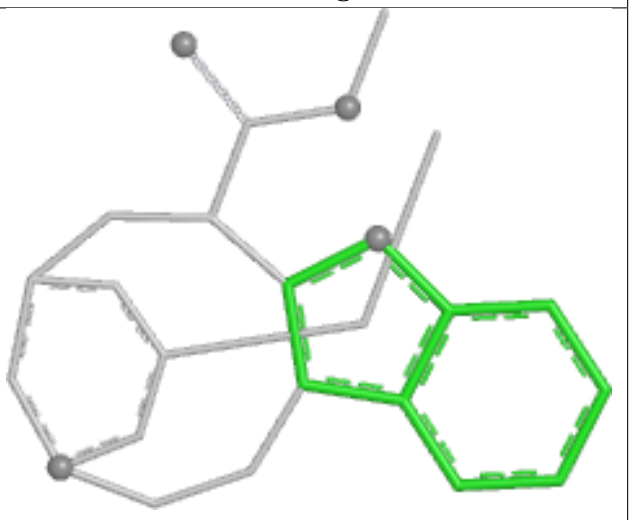

Rings

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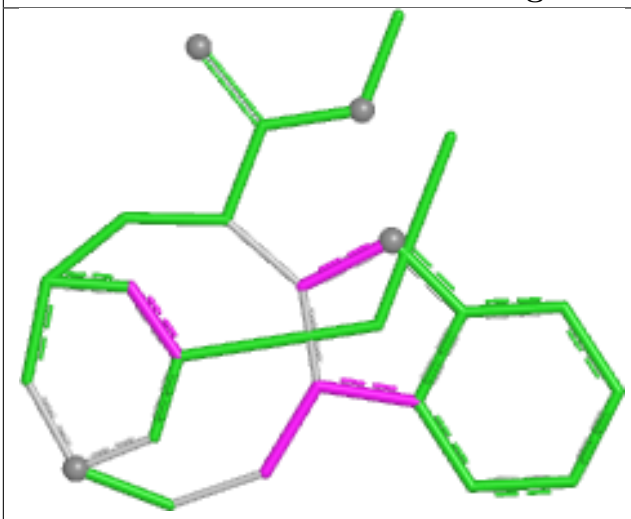

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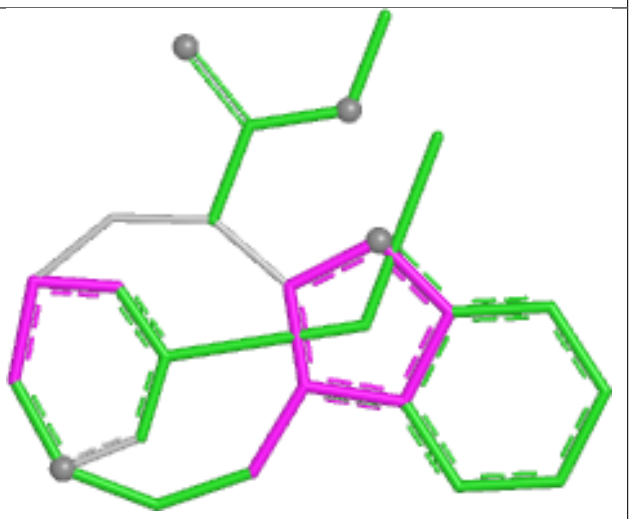

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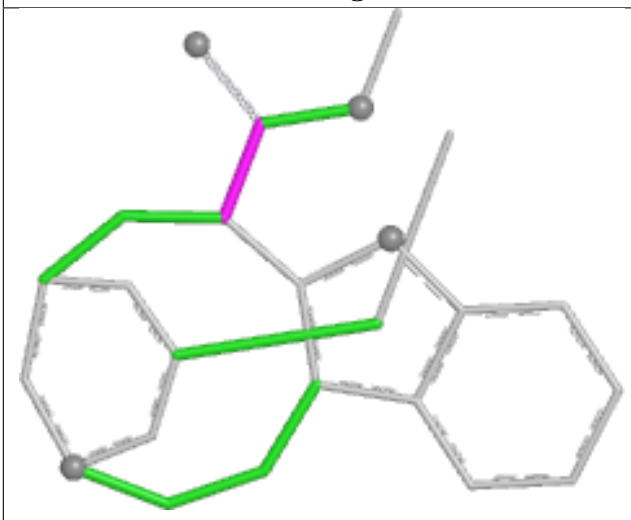

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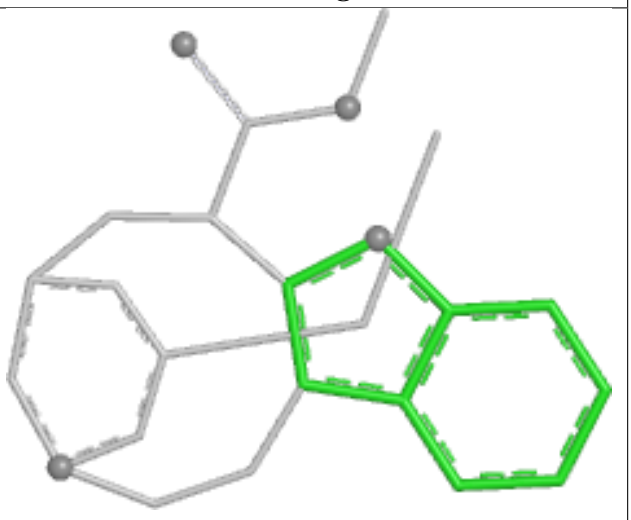

Rings

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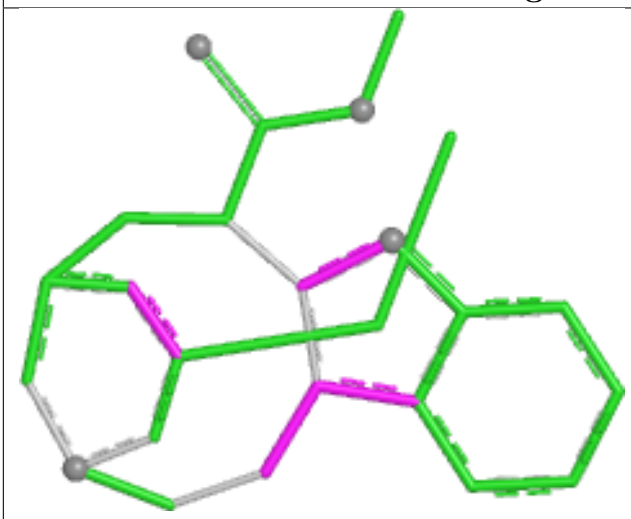

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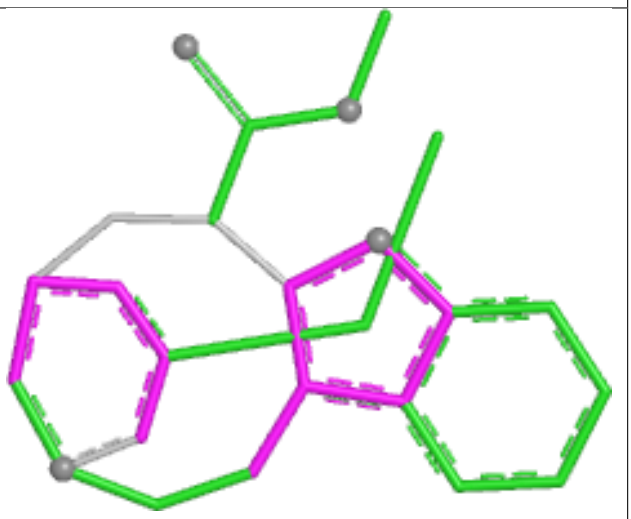

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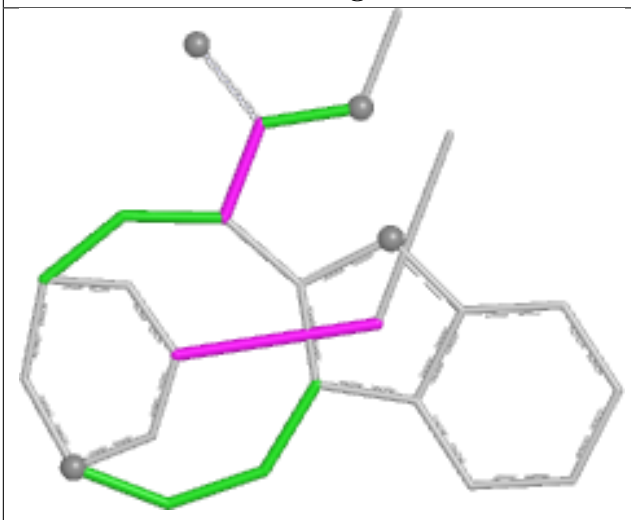

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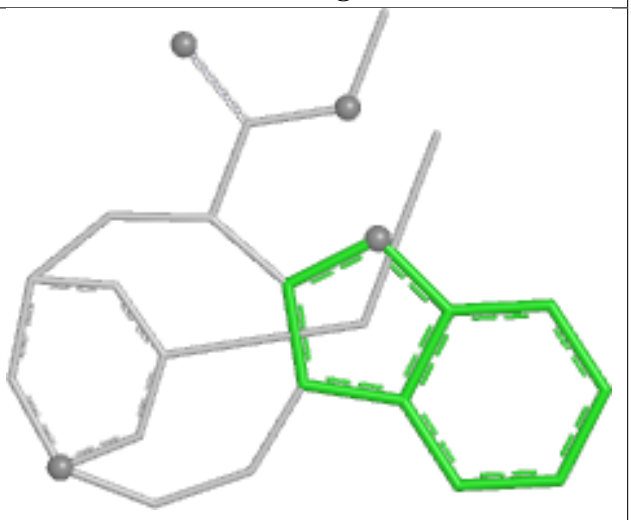
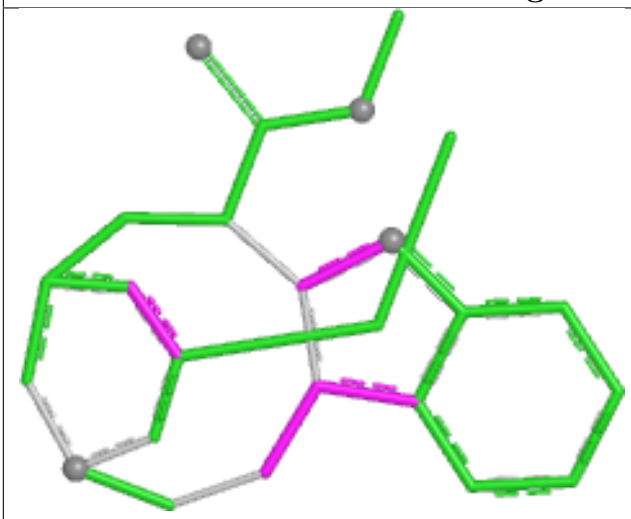


Rings

Ligand KJE B 401



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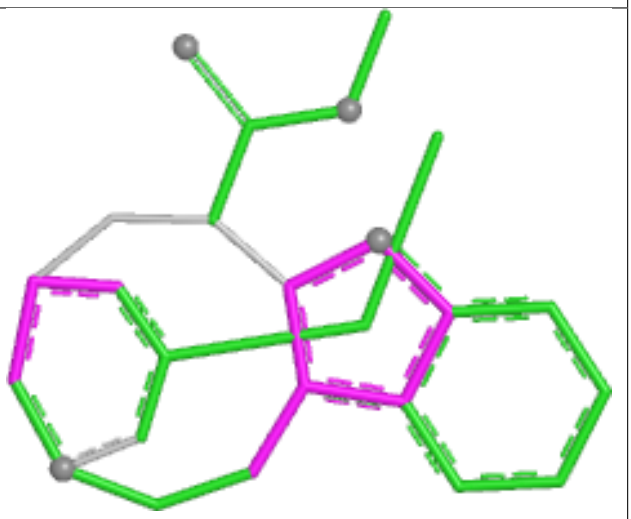

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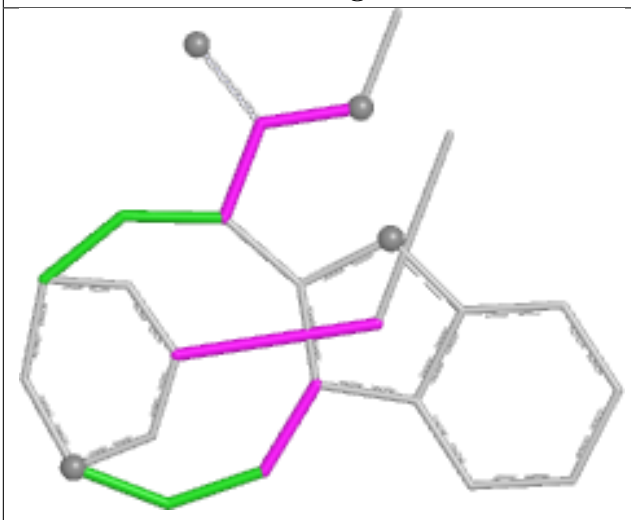

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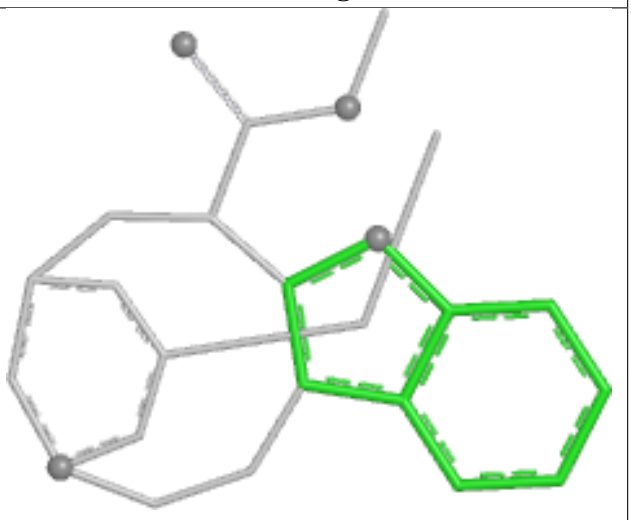
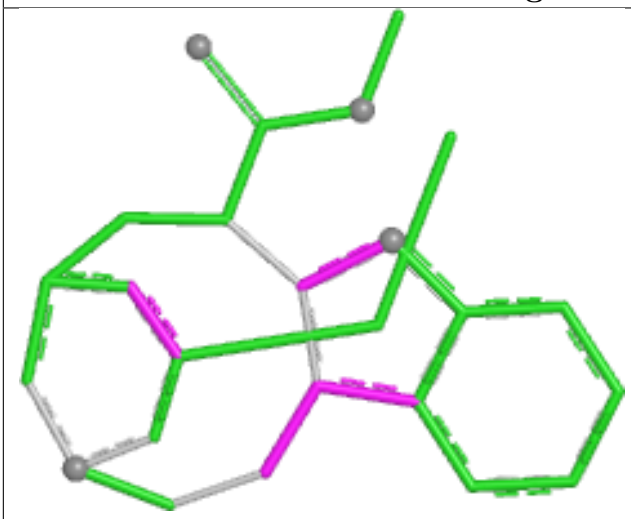


Rings

Ligand KJE D 401



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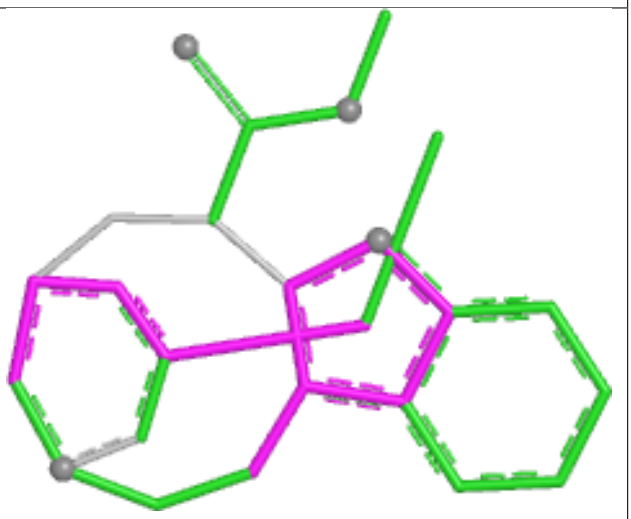

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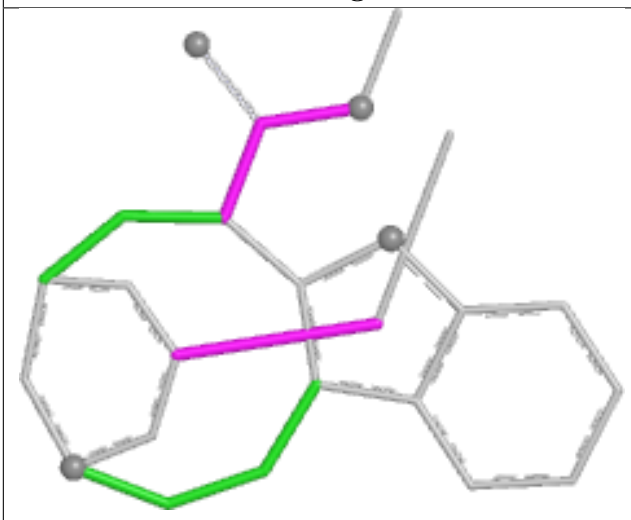

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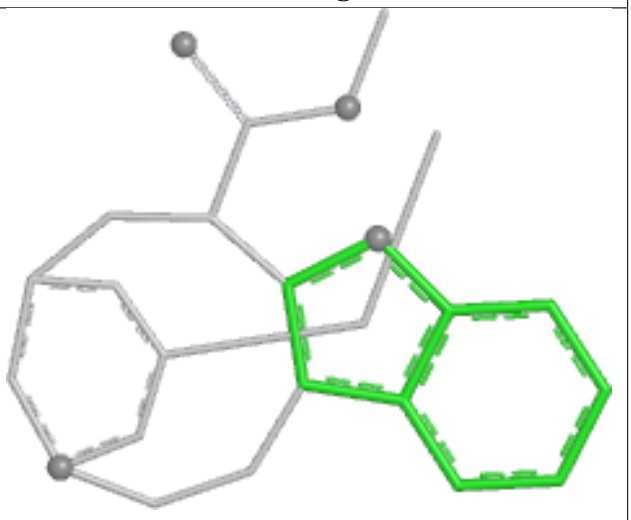
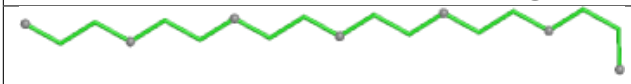
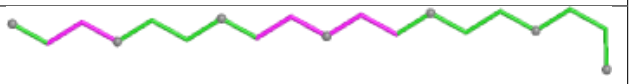


Rings

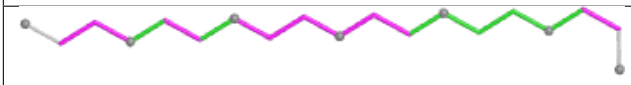
Ligand P6G C 402



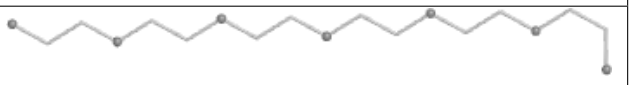
Bond lengths



Bond angles

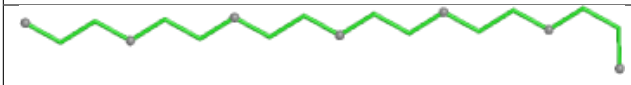


Torsions

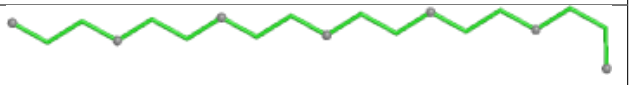


Rings

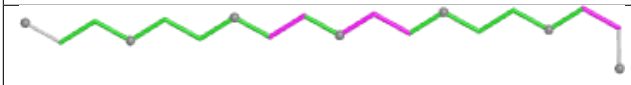
Ligand P6G A 402



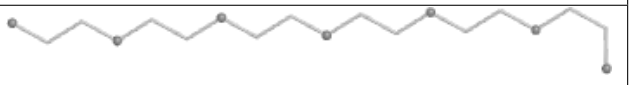
Bond lengths



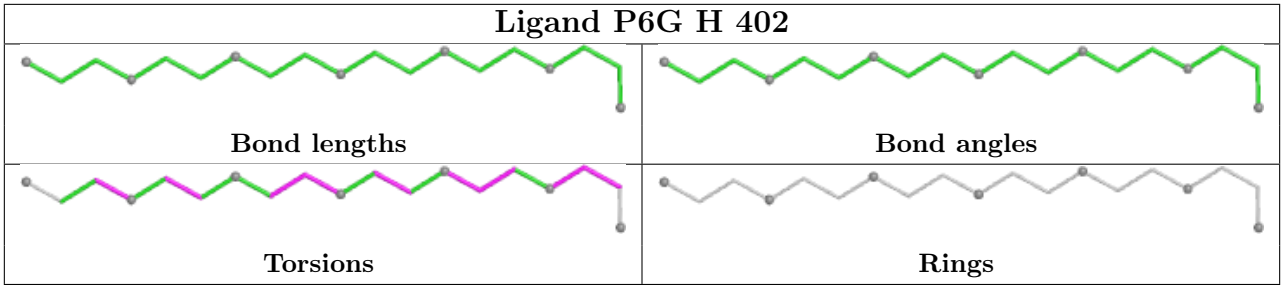
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	314/330 (95%)	-0.04	4 (1%) 75 73	43, 56, 86, 130	0
1	B	314/330 (95%)	0.10	6 (1%) 66 63	46, 62, 95, 128	0
1	C	314/330 (95%)	0.04	7 (2%) 62 59	45, 61, 95, 122	0
1	D	314/330 (95%)	0.06	9 (2%) 53 50	44, 61, 102, 135	0
1	E	305/330 (92%)	0.75	37 (12%) 8 6	47, 88, 124, 167	0
1	F	313/330 (94%)	0.21	11 (3%) 47 44	40, 70, 104, 128	0
1	G	313/330 (94%)	0.06	3 (0%) 79 77	46, 65, 94, 118	0
1	H	314/330 (95%)	0.44	23 (7%) 21 18	45, 66, 121, 157	0
All	All	2501/2640 (94%)	0.20	100 (3%) 42 39	40, 64, 111, 167	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	242	ILE	5.2
1	H	149	THR	4.3
1	C	76	PHE	4.2
1	A	149	THR	4.1
1	H	30	LEU	4.1
1	B	70	HIS	4.0
1	F	143	ASP	3.8
1	G	280	ALA	3.8
1	B	149	THR	3.8
1	E	149	THR	3.8
1	E	257	CYS	3.7
1	H	282	TYR	3.7
1	D	10	GLU	3.5
1	A	327	LYS	3.4
1	B	9	ASP	3.4
1	E	261	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	291	TRP	3.4
1	H	10	GLU	3.4
1	H	31	HIS	3.3
1	C	149	THR	3.2
1	E	25	GLY	3.2
1	H	70	HIS	3.2
1	E	291	TRP	3.1
1	B	69	ASP	3.1
1	E	201	LEU	3.1
1	E	71	GLU	3.1
1	F	70	HIS	3.1
1	D	68	SER	3.1
1	D	69	ASP	3.0
1	C	70	HIS	3.0
1	F	283	ILE	3.0
1	H	21	ILE	3.0
1	D	282	TYR	3.0
1	E	279	ASN	3.0
1	C	69	ASP	2.9
1	E	208	ILE	2.9
1	D	67	ILE	2.9
1	E	19	ILE	2.9
1	E	214	LEU	2.8
1	E	260	LEU	2.8
1	D	149	THR	2.8
1	G	327	LYS	2.8
1	E	248	ASN	2.8
1	H	142	LEU	2.8
1	H	214	LEU	2.8
1	E	167	TYR	2.7
1	E	13	TRP	2.7
1	E	304	TYR	2.7
1	B	10	GLU	2.6
1	D	327	LYS	2.6
1	E	143	ASP	2.6
1	H	283	ILE	2.6
1	H	84	PHE	2.5
1	H	18	TYR	2.5
1	C	21	ILE	2.5
1	H	309	THR	2.5
1	A	248	ASN	2.5
1	H	69	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	310	LEU	2.5
1	B	327	LYS	2.4
1	E	197	LEU	2.4
1	F	67	ILE	2.4
1	C	68	SER	2.4
1	E	314	MET	2.4
1	E	236	GLY	2.4
1	E	18	TYR	2.4
1	F	325	PHE	2.4
1	D	9	ASP	2.3
1	E	163	PHE	2.3
1	E	223	THR	2.3
1	H	207	ILE	2.3
1	H	278	ILE	2.3
1	E	252	LEU	2.3
1	A	292	LYS	2.3
1	E	283	ILE	2.2
1	E	142	LEU	2.2
1	G	282	TYR	2.2
1	H	71	GLU	2.2
1	C	327	LYS	2.2
1	H	12	ILE	2.2
1	E	54	ILE	2.1
1	E	325	PHE	2.1
1	F	297	VAL	2.1
1	H	25	GLY	2.1
1	F	292	LYS	2.1
1	H	143	ASP	2.1
1	E	268	ILE	2.1
1	E	265	VAL	2.1
1	E	213	LYS	2.1
1	F	310	LEU	2.1
1	E	294	GLU	2.1
1	E	282	TYR	2.1
1	H	19	ILE	2.1
1	E	166	LEU	2.1
1	E	10	GLU	2.1
1	D	70	HIS	2.1
1	F	296	GLU	2.0
1	E	157	ILE	2.0
1	F	286	LEU	2.0
1	E	204	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

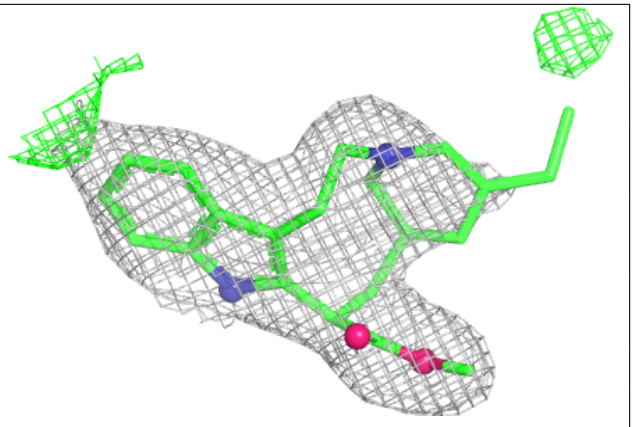
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

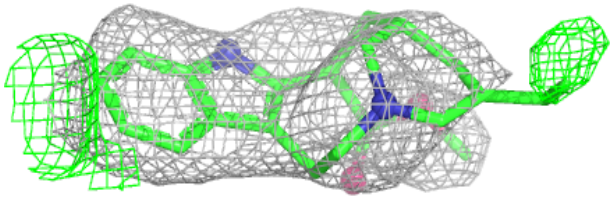
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KJE	H	401	25/25	0.88	0.15	64,88,113,168	0
3	P6G	E	402	19/19	0.88	0.15	52,78,104,119	0
3	P6G	H	402	19/19	0.92	0.12	56,82,127,135	0
3	P6G	A	402	19/19	0.93	0.12	48,67,102,107	0
3	P6G	C	402	19/19	0.93	0.10	48,64,78,88	0
2	KJE	E	401	25/25	0.95	0.10	57,80,97,102	0
2	KJE	F	401	25/25	0.96	0.08	44,54,63,76	0
2	KJE	C	401	25/25	0.96	0.08	42,58,64,69	0
2	KJE	A	401	25/25	0.96	0.09	38,45,57,81	0
2	KJE	G	401	25/25	0.97	0.07	50,65,75,94	0
2	KJE	B	401	25/25	0.97	0.07	41,52,62,65	0
2	KJE	D	401	25/25	0.97	0.07	45,52,69,74	0

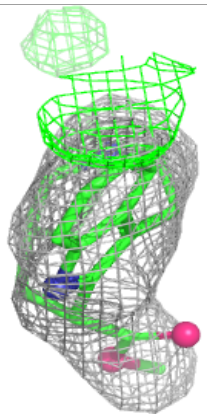
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KJE 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)

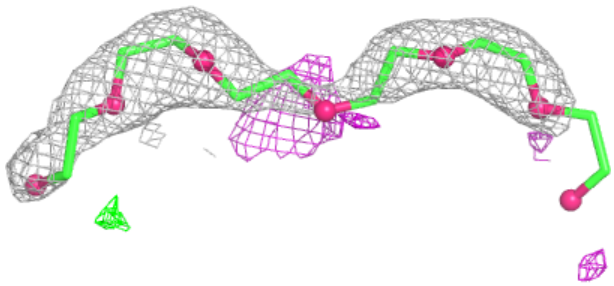


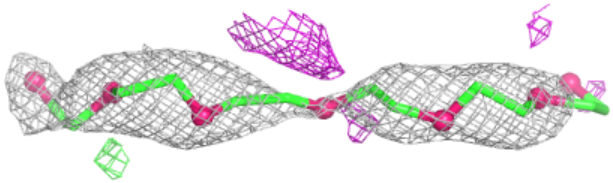


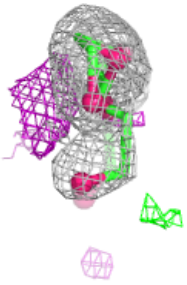


Electron density around P6G E 402:

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

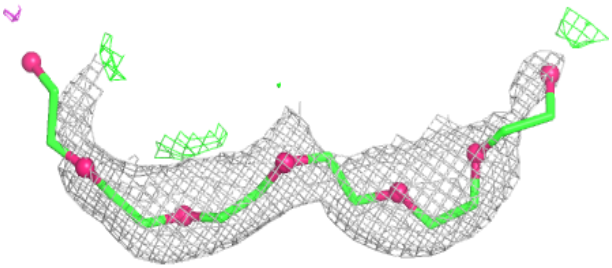


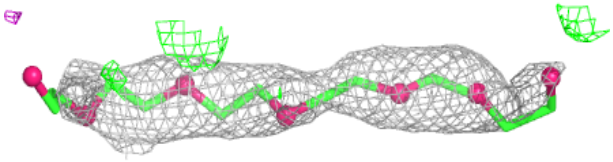


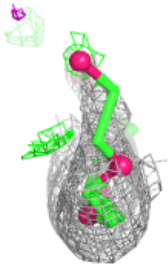


Electron density around P6G H 402:

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

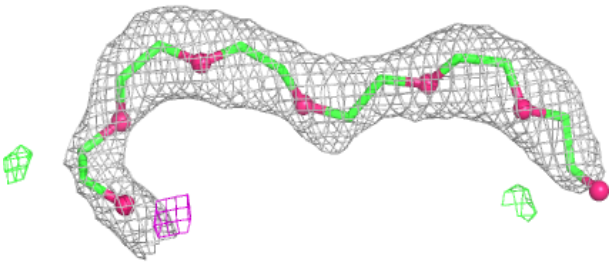


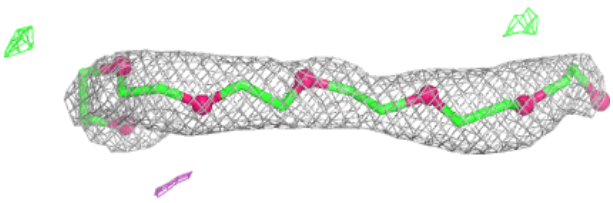


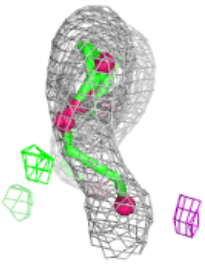


Electron density around P6G A 402:

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

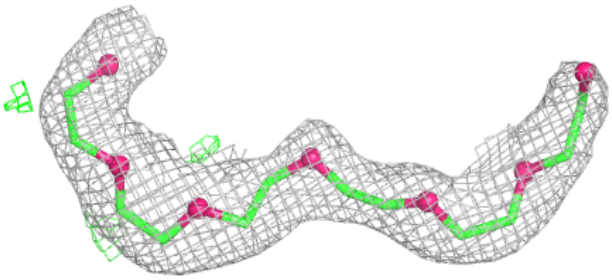


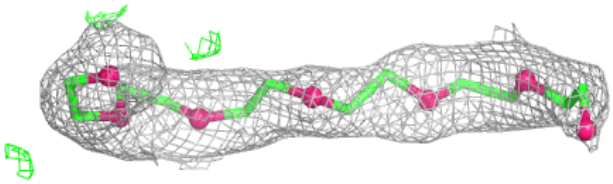


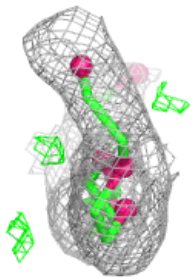


Electron density around P6G C 402:

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

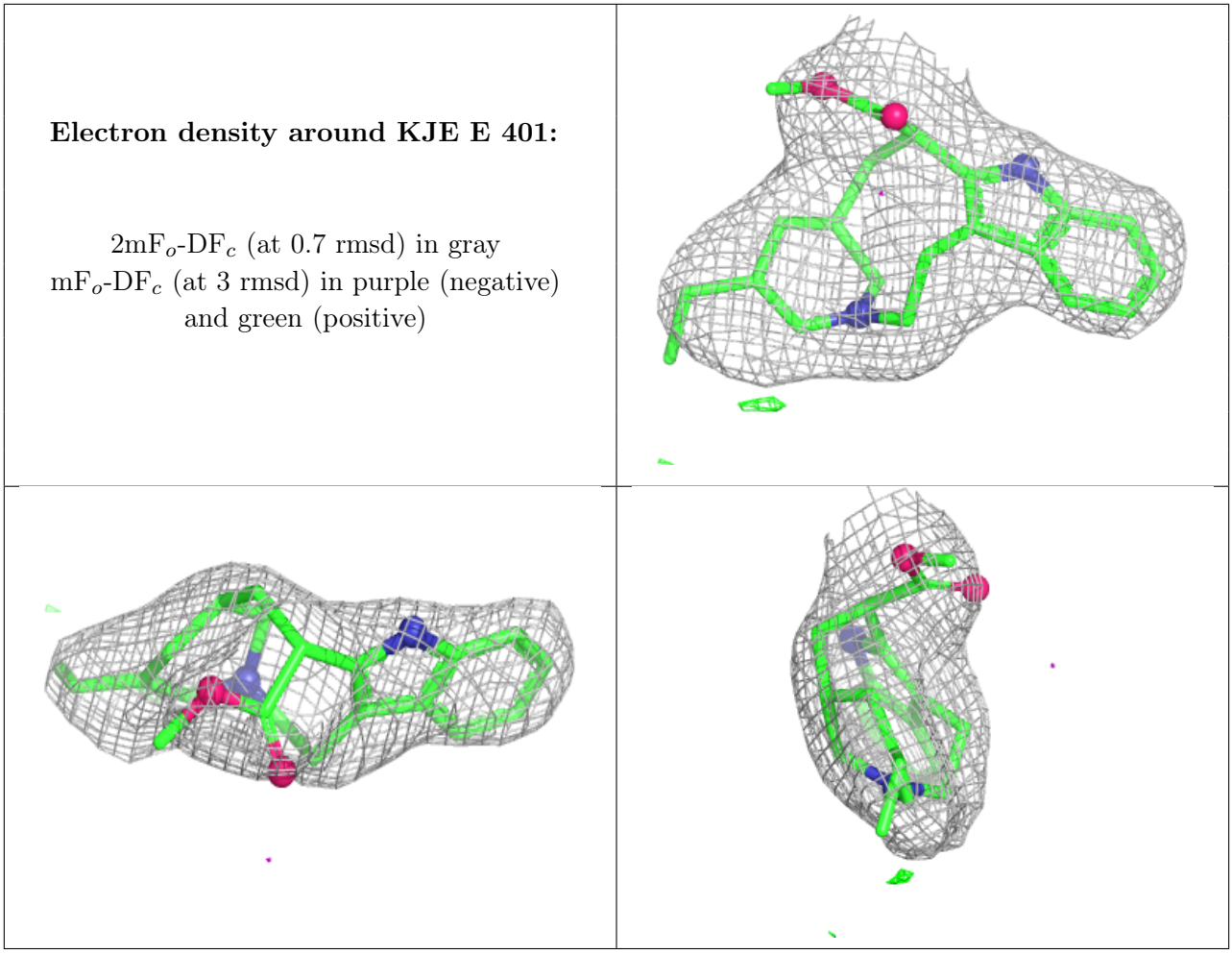






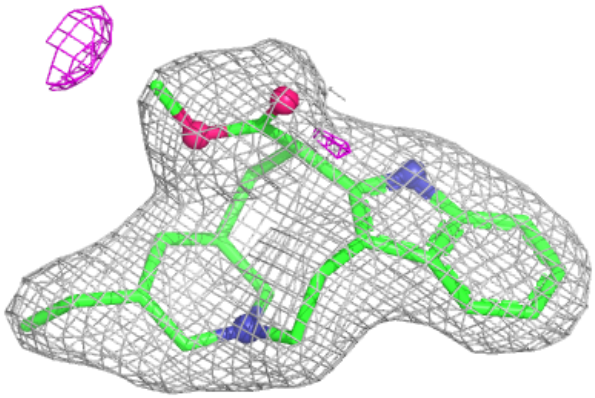
Electron density around KJE E 401:

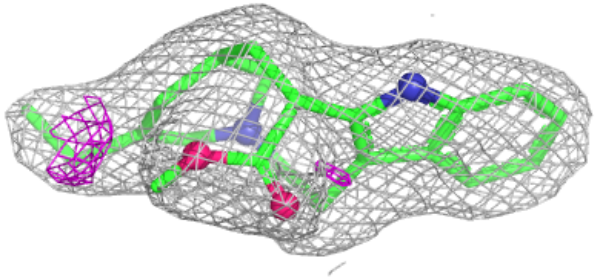
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

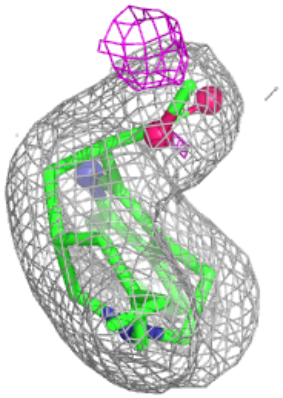


Electron density around KJE F 401:

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

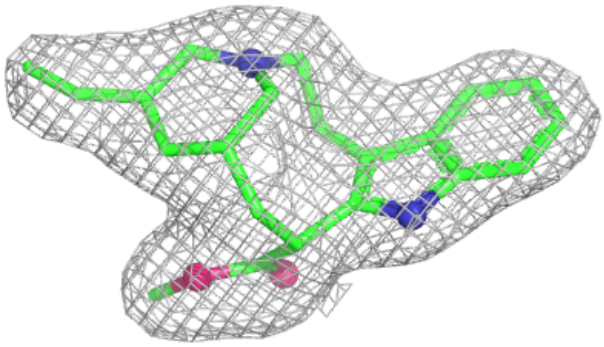


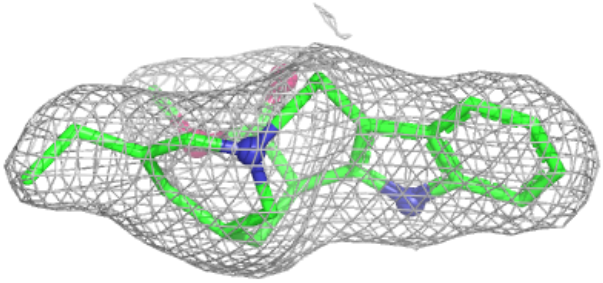


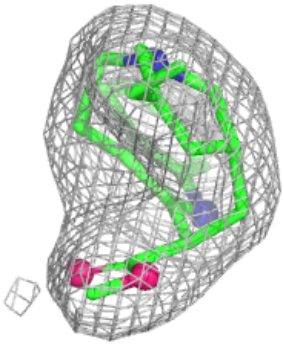


Electron density around KJE C 401:

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

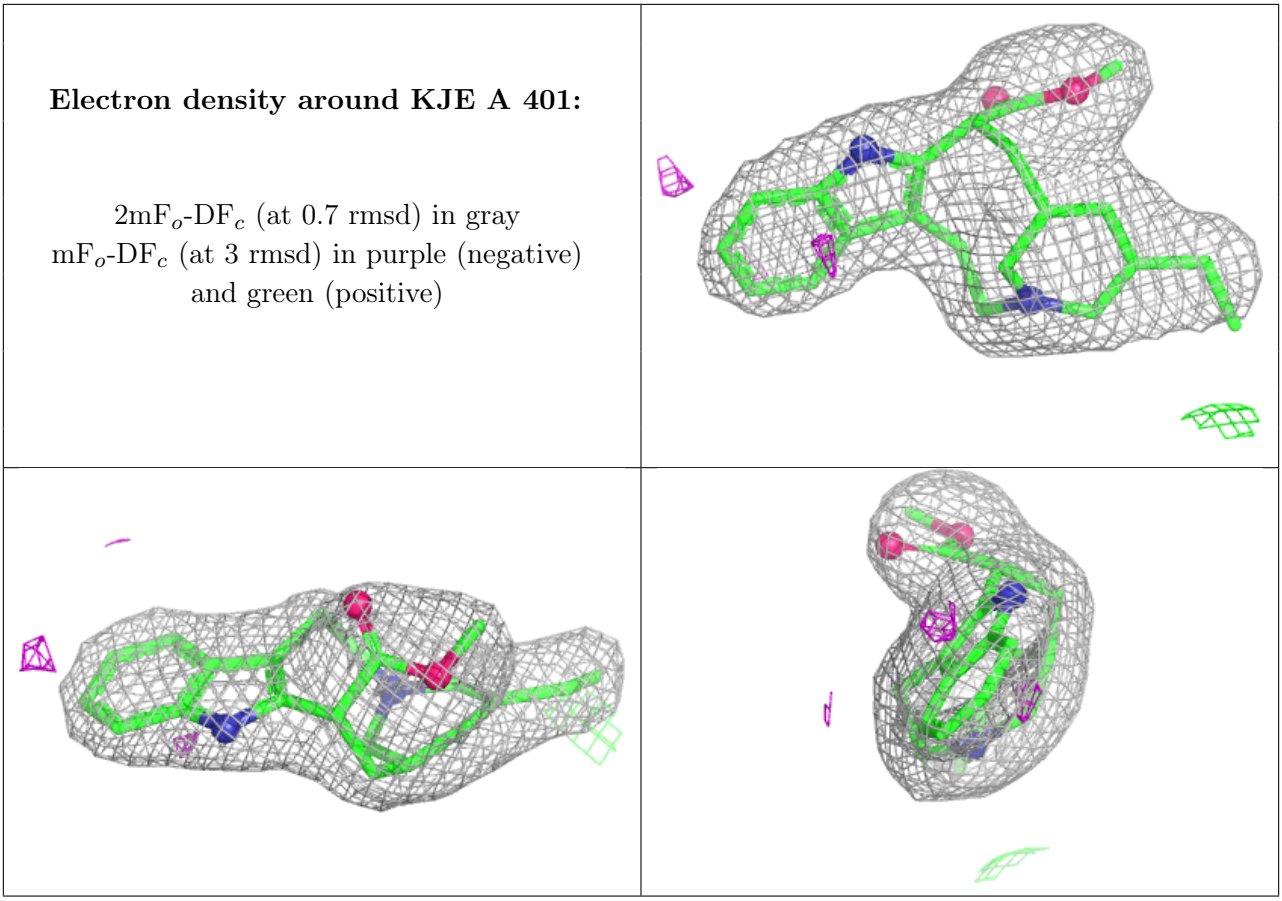






Electron density around KJE A 401:

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



Electron density around KJE G 401:

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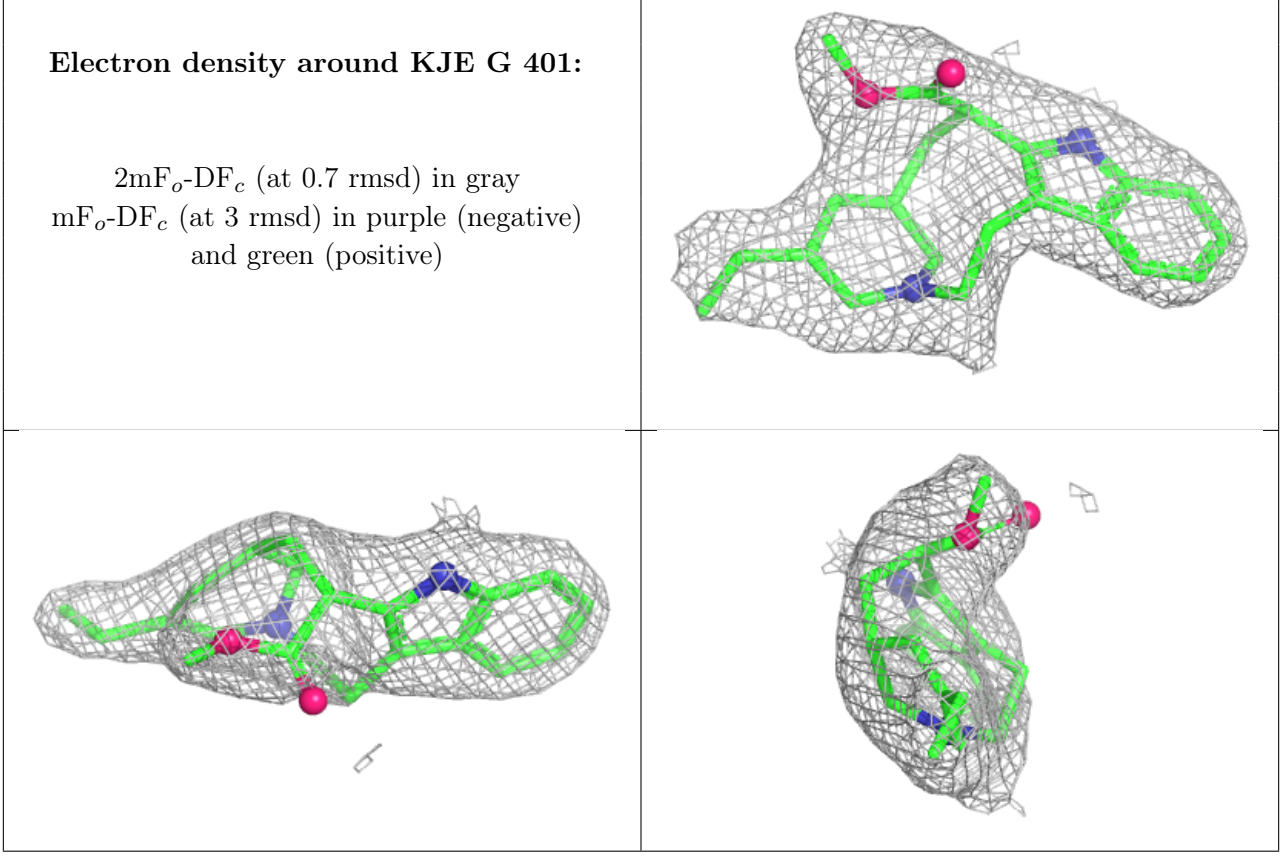
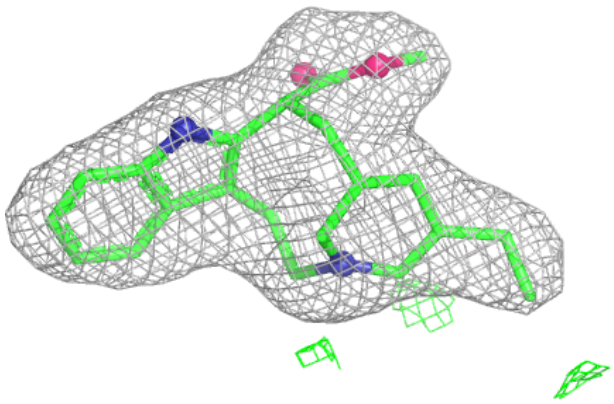
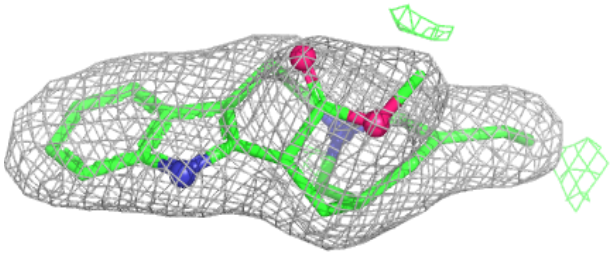
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

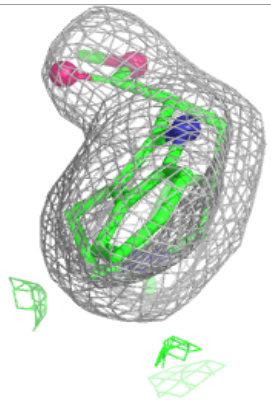


Electron density around KJE B 401:

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

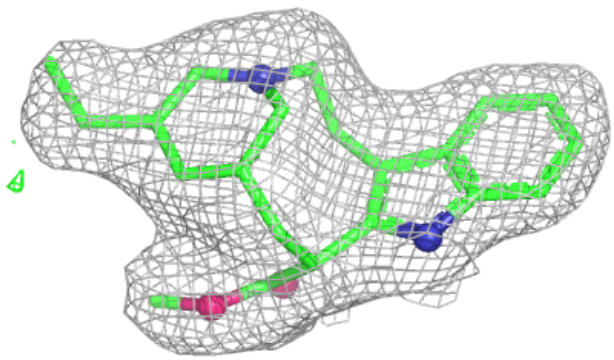


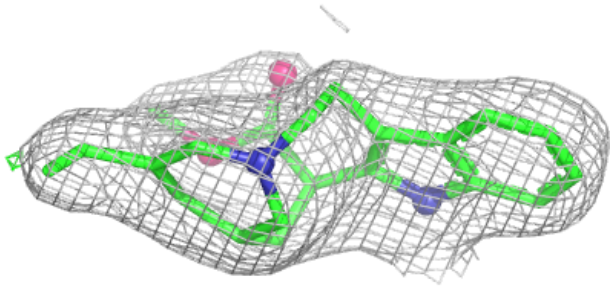


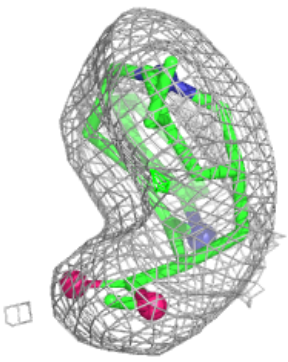


Electron density around KJE D 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.