Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 04:48 PM EDT

PDB ID	:	6RT8
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:

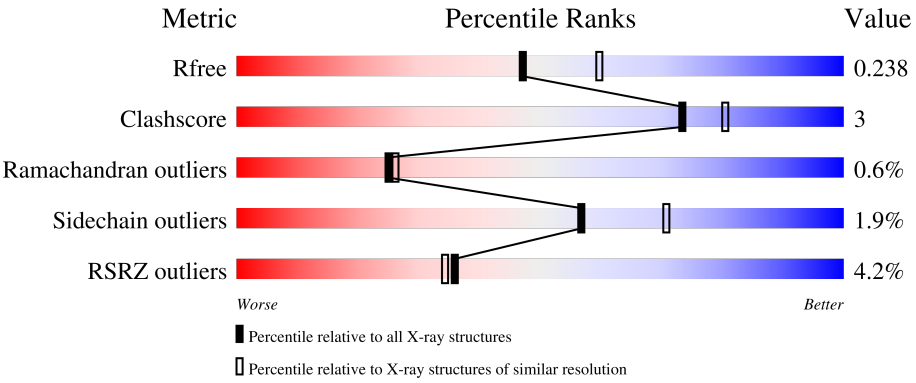
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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% 7% • 5%
1	C	330	% 88% 7% • 5%
1	D	330	% 88% 6% • 5%

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Mol	Chain	Length	Quality of chain
1	E	330	12% 85% 6% • 8%
1	F	330	4% 86% 8% • 5%
1	G	330	% 87% 7% • 5%
1	H	330	12% 88% 6% • 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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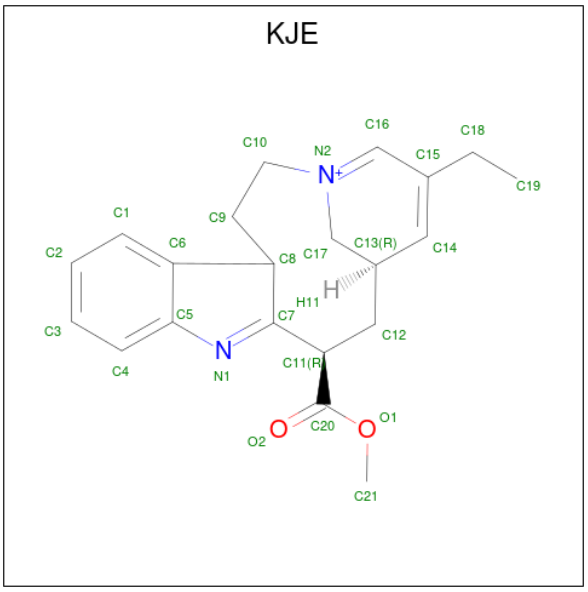
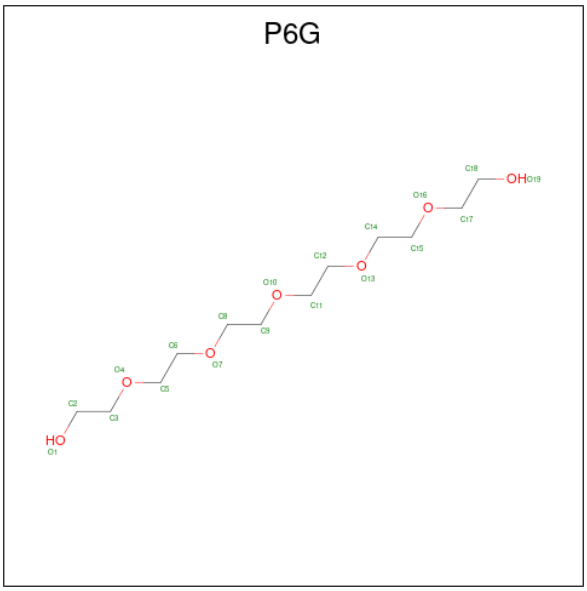
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	PRO	-	expression tag	UNP A0A2P1GIW2
C	2	ALA	-	expression tag	UNP A0A2P1GIW2
C	3	SER	-	expression tag	UNP A0A2P1GIW2
C	4	GLN	-	expression tag	UNP A0A2P1GIW2
C	5	THR	-	expression tag	UNP A0A2P1GIW2
D	0	GLY	-	expression tag	UNP A0A2P1GIW2
D	1	PRO	-	expression 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 (three-letter code: 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 (three-letter code: 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.

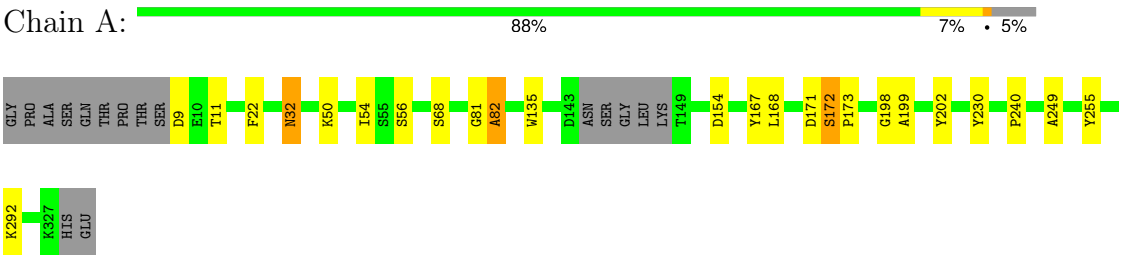
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	40	Total O 40 40	0	0
4	C	44	Total O 44 44	0	0
4	D	70	Total O 70 70	0	0
4	E	33	Total O 33 33	0	0
4	F	64	Total O 64 64	0	0
4	G	38	Total O 38 38	0	0
4	H	34	Total O 34 34	0	0

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.

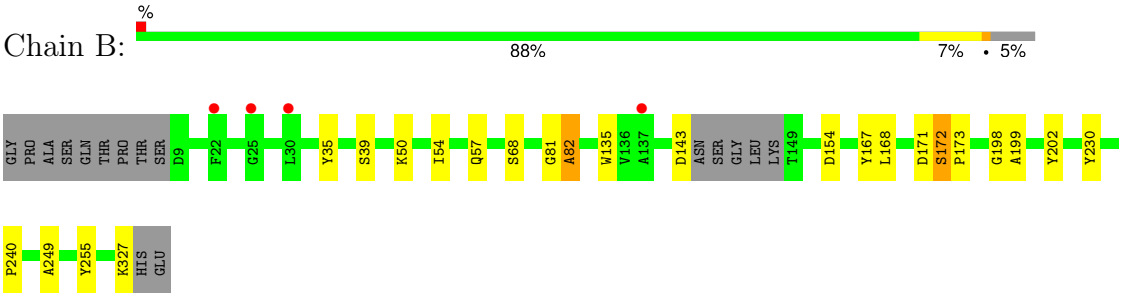
• Molecule 1: Catharanthine synthase

Chain A:



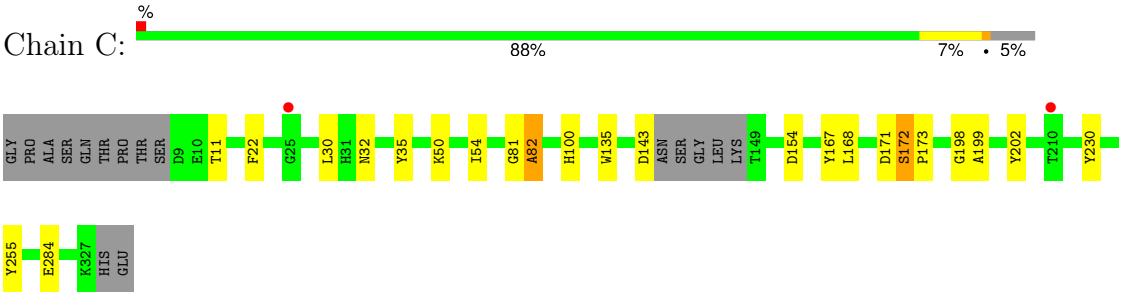
• Molecule 1: Catharanthine synthase

Chain B:



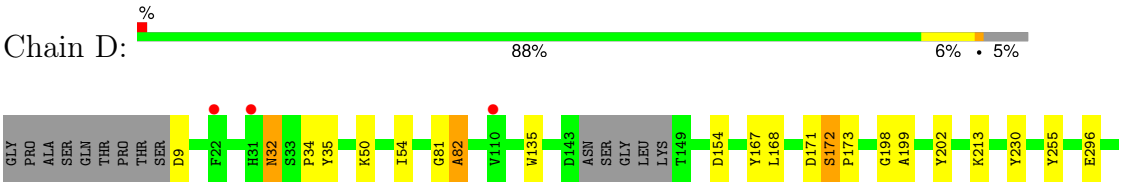
• Molecule 1: Catharanthine synthase

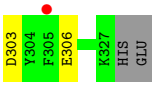
Chain C:



• Molecule 1: Catharanthine synthase

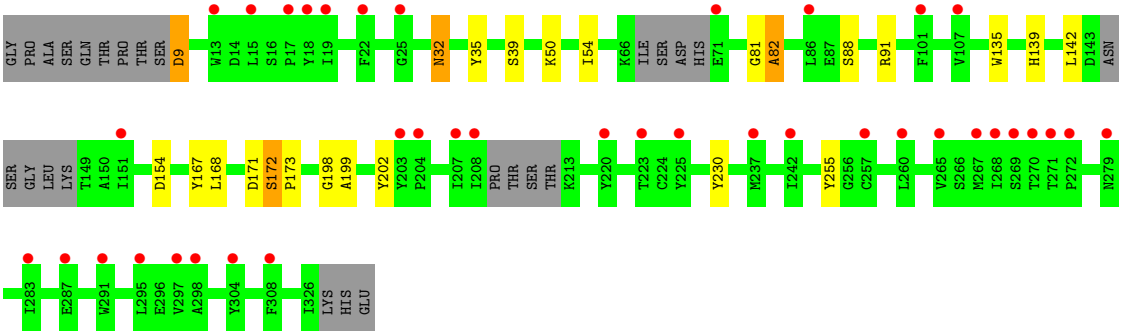
Chain D:





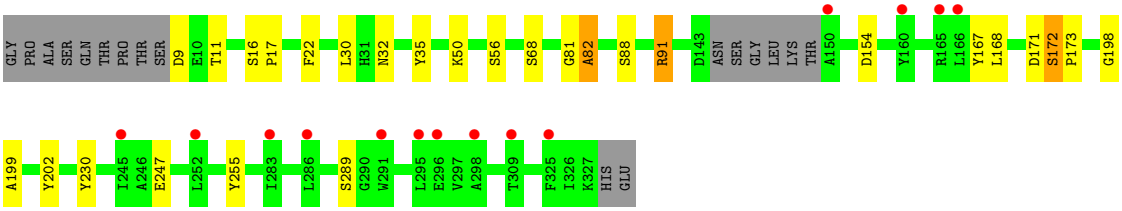
• Molecule 1: Catharanthine synthase

Chain E:



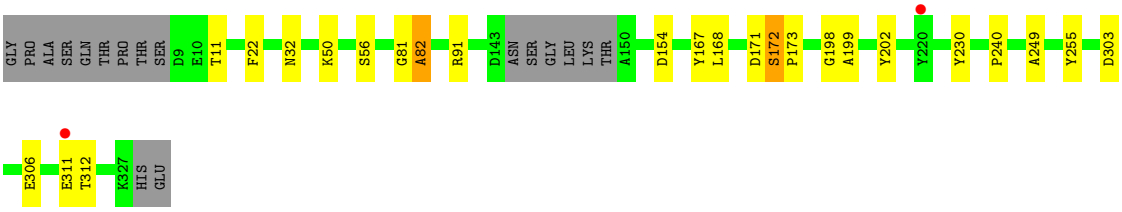
• Molecule 1: Catharanthine synthase

Chain F:



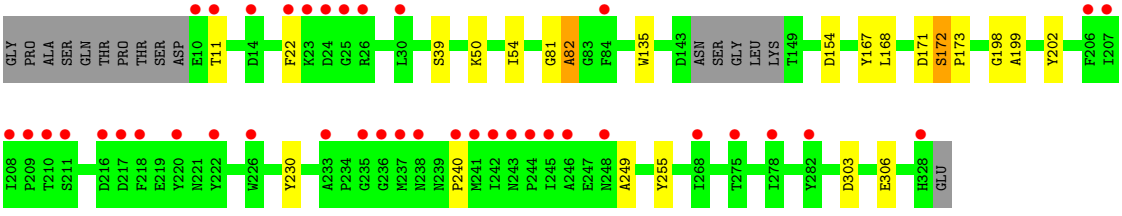
• Molecule 1: Catharanthine synthase

Chain G:



• Molecule 1: Catharanthine synthase

Chain H:



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 (4.97%)	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)	0.31 , 41.5	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	0.68	0/2534	0.82	0/3460
1	B	0.70	0/2530	0.81	0/3455
1	C	0.68	0/2537	0.81	0/3463
1	D	0.69	1/2534 (0.0%)	0.81	0/3459
1	E	0.70	0/2380	0.83	1/3256 (0.0%)
1	F	0.67	0/2511	0.80	1/3434 (0.0%)
1	G	0.68	0/2528	0.81	0/3452
1	H	0.68	0/2491	0.83	0/3406
All	All	0.69	1/20045 (0.0%)	0.81	2/27385 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	GLU	CD-OE2	5.36	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	32	ASN	N-CA-CB	-5.45	100.79	110.60
1	F	91	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	15	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
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	1	0
All	All	20132	0	18565	127	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 (127) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:50:LYS:NZ	4:H:501:HOH:O	2.45	0.49
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	25	26
1	B	310/330 (94%)	291 (94%)	17 (6%)	2 (1%)	25	26
1	C	310/330 (94%)	296 (96%)	12 (4%)	2 (1%)	25	26
1	D	310/330 (94%)	296 (96%)	12 (4%)	2 (1%)	25	26
1	E	297/330 (90%)	282 (95%)	13 (4%)	2 (1%)	22	22
1	F	309/330 (94%)	295 (96%)	12 (4%)	2 (1%)	25	26
1	G	309/330 (94%)	296 (96%)	11 (4%)	2 (1%)	25	26
1	H	310/330 (94%)	296 (96%)	12 (4%)	2 (1%)	25	26
All	All	2465/2640 (93%)	2347 (95%)	102 (4%)	16 (1%)	25	26

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

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Mol	Chain	Res	Type
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%)	250 (98%)	6 (2%)	50	63
1	B	256/283 (90%)	250 (98%)	6 (2%)	50	63
1	C	254/283 (90%)	249 (98%)	5 (2%)	55	69
1	D	255/283 (90%)	249 (98%)	6 (2%)	49	62
1	E	228/283 (81%)	225 (99%)	3 (1%)	69	81
1	F	252/283 (89%)	245 (97%)	7 (3%)	43	56
1	G	254/283 (90%)	251 (99%)	3 (1%)	71	83
1	H	245/283 (87%)	243 (99%)	2 (1%)	81	90
All	All	2000/2264 (88%)	1962 (98%)	38 (2%)	57	71

All (38) 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	230	TYR
1	A	255	TYR
1	A	292	LYS
1	B	57	GLN
1	B	68	SER
1	B	143	ASP
1	B	230	TYR
1	B	255	TYR
1	B	327	LYS
1	C	32	ASN

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Mol	Chain	Res	Type
1	C	143	ASP
1	C	230	TYR
1	C	255	TYR
1	C	284	GLU
1	D	9	ASP
1	D	32	ASN
1	D	34	PRO
1	D	213	LYS
1	D	230	TYR
1	D	255	TYR
1	E	9	ASP
1	E	230	TYR
1	E	255	TYR
1	F	9	ASP
1	F	32	ASN
1	F	68	SER
1	F	230	TYR
1	F	247	GLU
1	F	255	TYR
1	F	289	SER
1	G	32	ASN
1	G	230	TYR
1	G	255	TYR
1	H	230	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	32	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	H	401	-	23,28,28	4.24	4 (17%)	22,40,40	2.29	6 (27%)
3	P6G	H	402	-	18,18,18	0.66	0	17,17,17	0.92	0
2	KJE	E	401	-	23,28,28	4.18	4 (17%)	22,40,40	2.25	4 (18%)
3	P6G	A	402	-	18,18,18	0.85	0	17,17,17	0.93	0
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%)
3	P6G	C	402	-	18,18,18	0.82	0	17,17,17	1.21	3 (17%)
2	KJE	A	401	-	23,28,28	3.34	4 (17%)	22,40,40	2.21	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%)
2	KJE	C	401	-	23,28,28	3.52	4 (17%)	22,40,40	2.30	5 (22%)
2	KJE	G	401	-	23,28,28	4.00	4 (17%)	22,40,40	2.21	5 (22%)

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	H	401	-	2/2/7/9	2/11/45/45	0/2/4/4
3	P6G	H	402	-	-	9/16/16/16	-
2	KJE	E	401	-	2/2/7/9	4/11/45/45	0/2/4/4
3	P6G	A	402	-	-	4/16/16/16	-

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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	-
3	P6G	C	402	-	-	9/16/16/16	-
2	KJE	A	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
2	KJE	C	401	-	2/2/7/9	1/11/45/45	0/2/4/4
2	KJE	G	401	-	2/2/7/9	4/11/45/45	0/2/4/4

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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	N2
2	A	401	KJE	C8
2	B	401	KJE	N2
2	B	401	KJE	C8
2	C	401	KJE	N2
2	C	401	KJE	C8
2	D	401	KJE	N2
2	D	401	KJE	C8
2	E	401	KJE	N2
2	E	401	KJE	C8
2	F	401	KJE	N2
2	F	401	KJE	C8
2	G	401	KJE	N2
2	G	401	KJE	C8
2	H	401	KJE	N2
2	H	401	KJE	C8

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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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

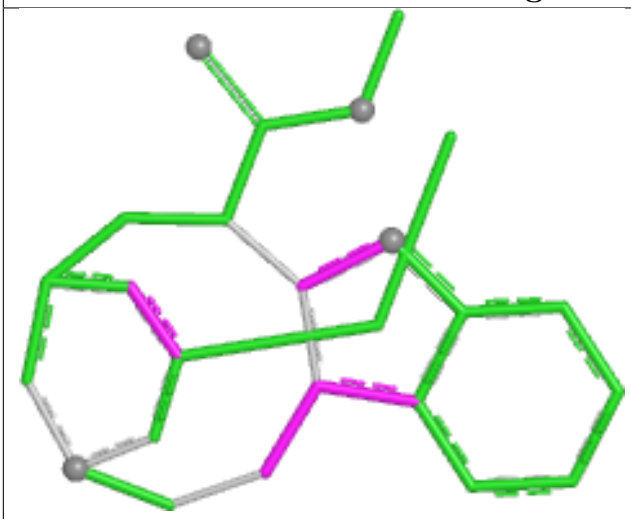
There are no ring outliers.

11 monomers are involved in 31 short contacts:

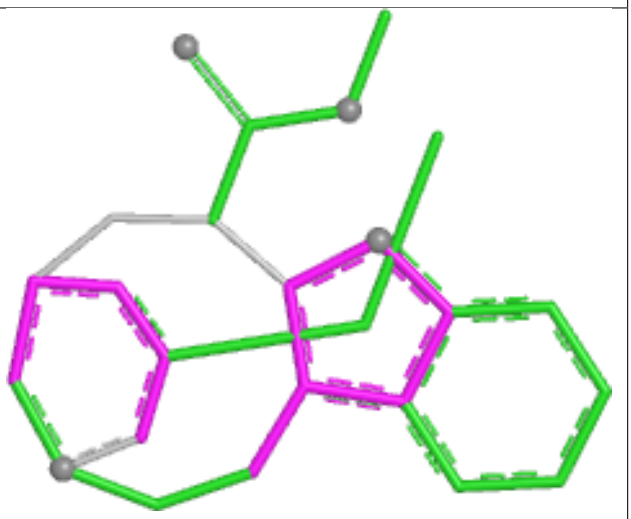
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	401	KJE	1	0
3	H	402	P6G	1	0
2	E	401	KJE	1	0
3	A	402	P6G	2	0
2	F	401	KJE	4	0
3	E	402	P6G	11	0
3	C	402	P6G	7	0
2	A	401	KJE	1	0
2	B	401	KJE	1	0
2	C	401	KJE	1	0
2	G	401	KJE	1	0

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.

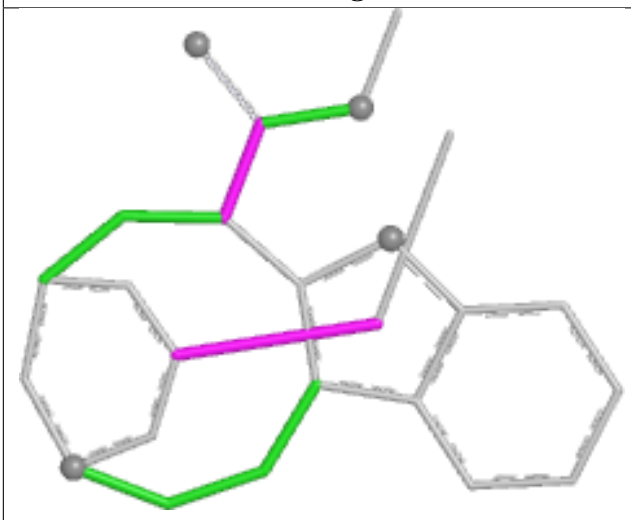
Ligand KJE H 401



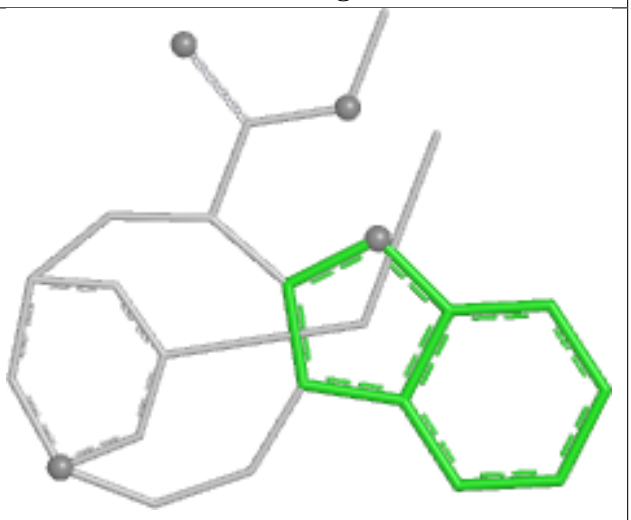
Bond lengths



Bond angles

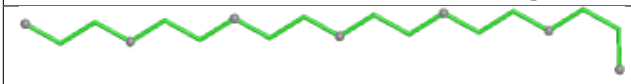


Torsions



Rings

Ligand P6G H 402



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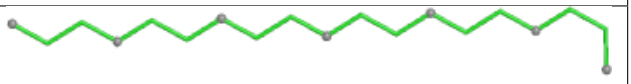

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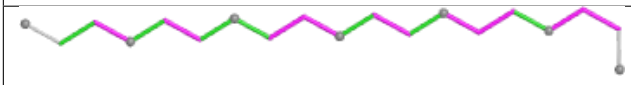

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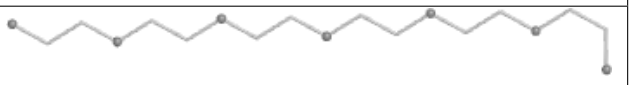
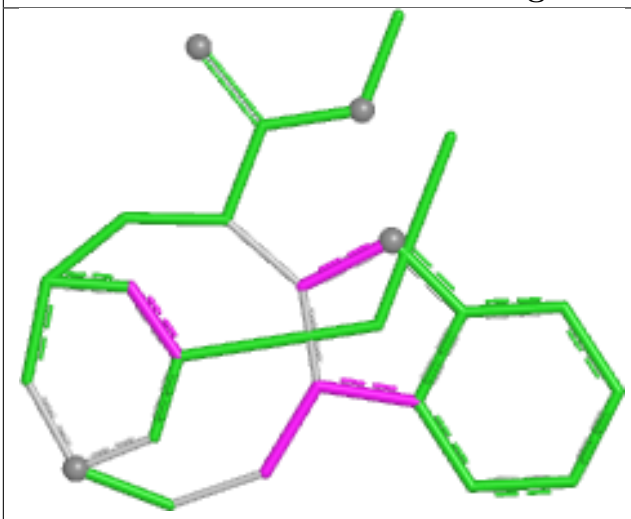


Rings

Ligand KJE E 401



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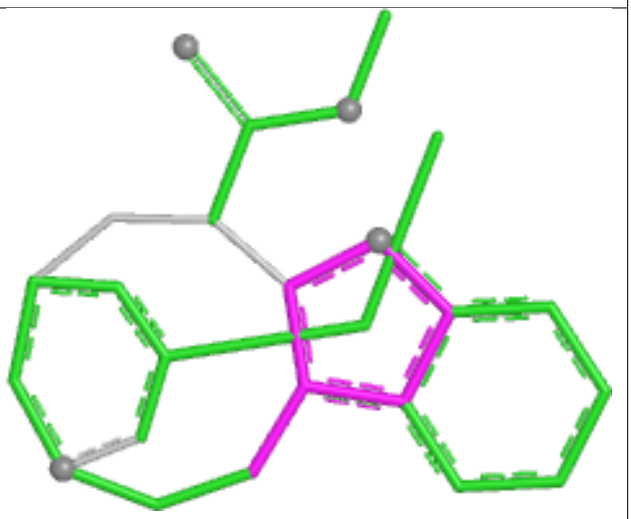

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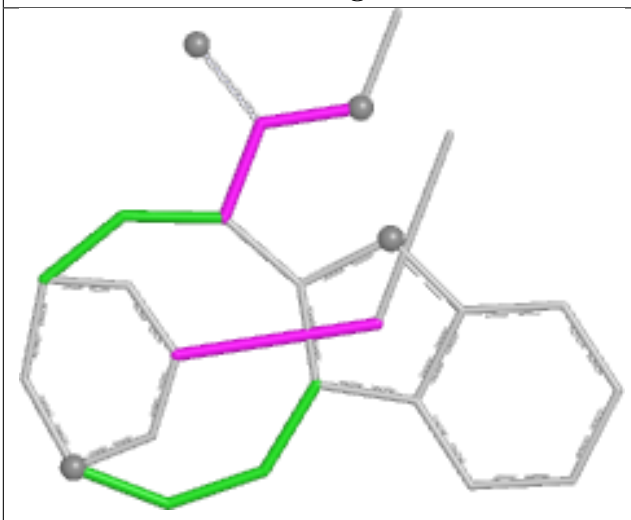

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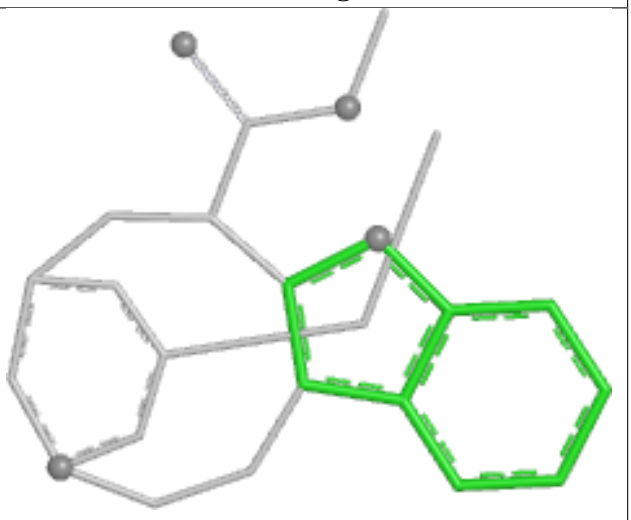
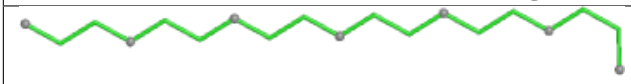


Rings

Ligand P6G A 402



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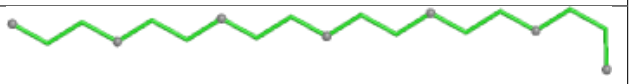

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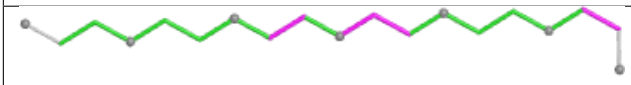

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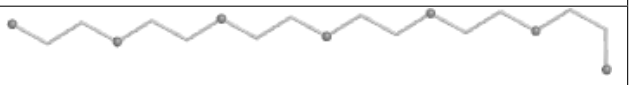
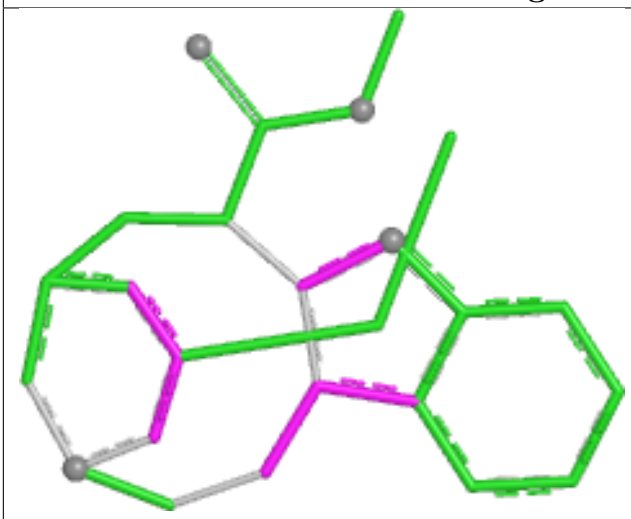


Rings

Ligand KJE F 401



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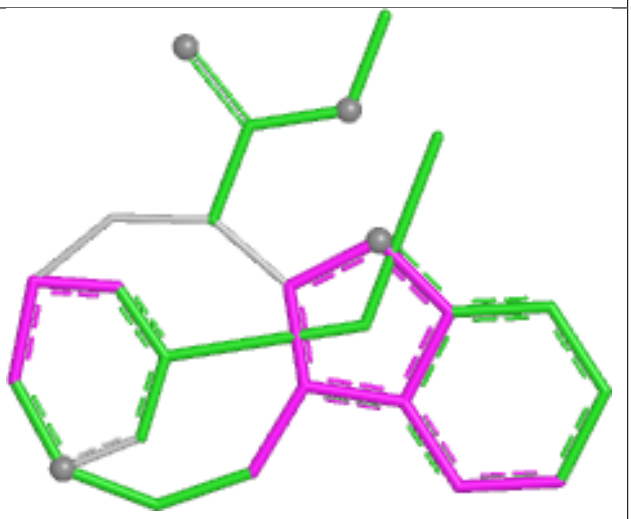

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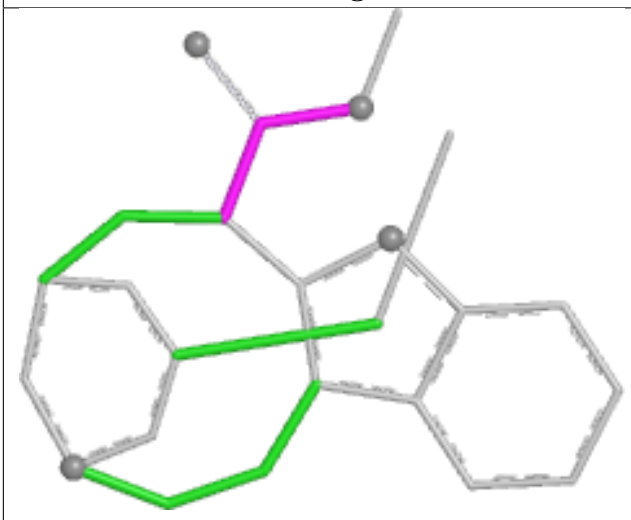

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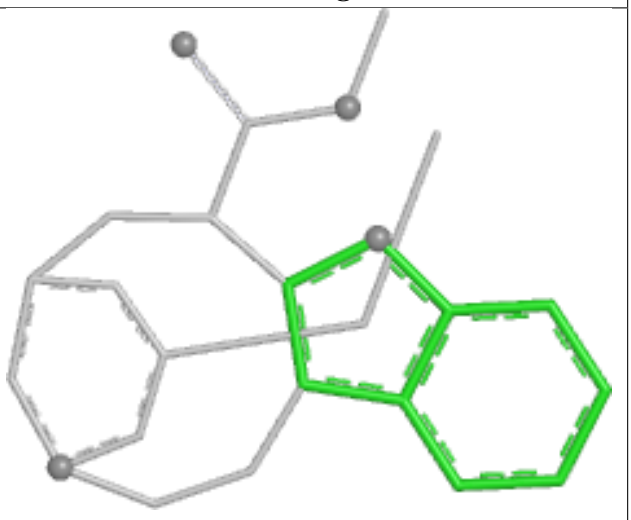
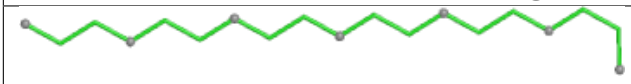


Rings

Ligand P6G E 402



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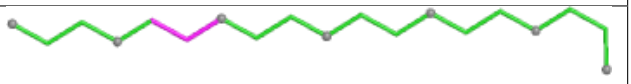

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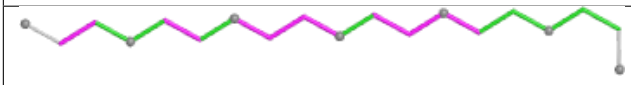

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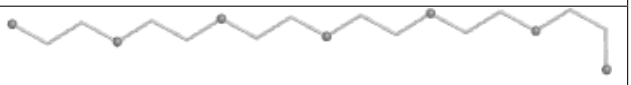
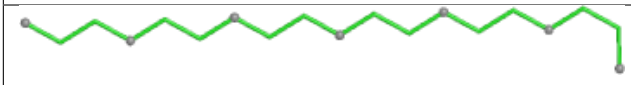


Rings

Ligand P6G C 402



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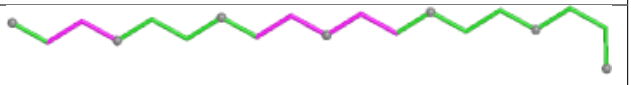

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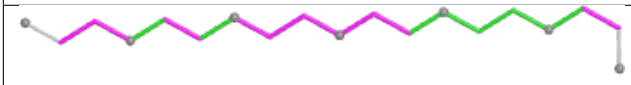

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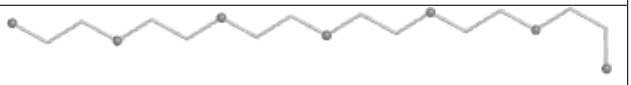
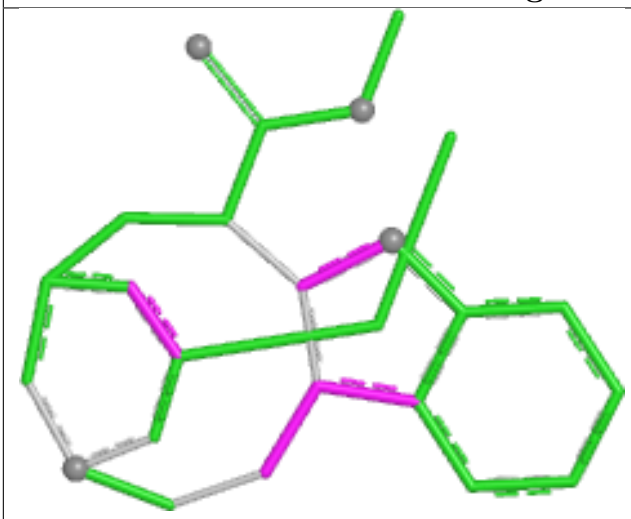


Rings

Ligand KJE A 401



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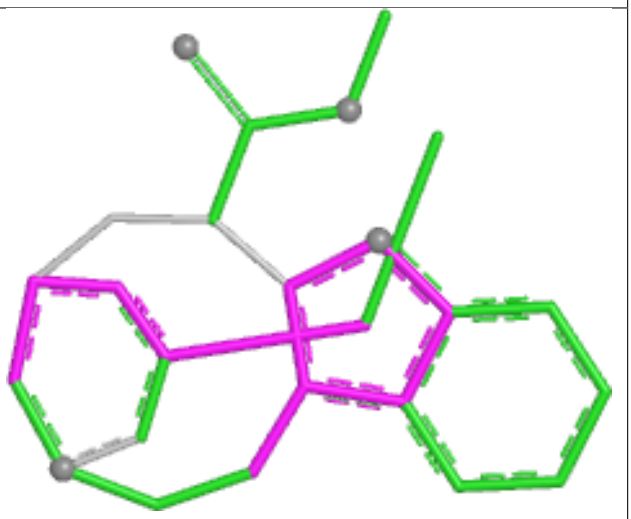
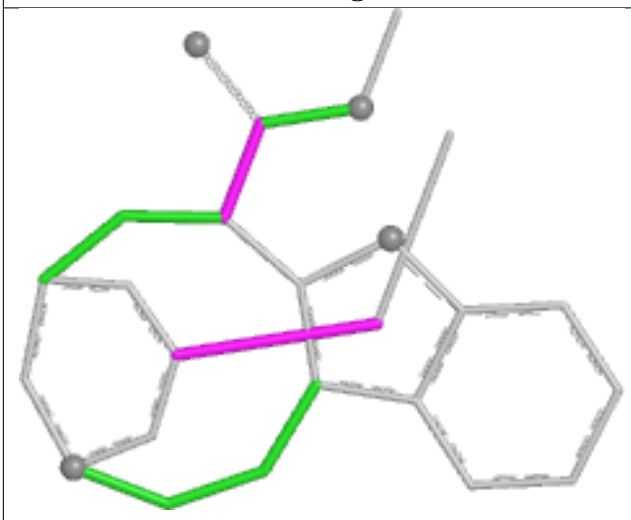


Bond angles



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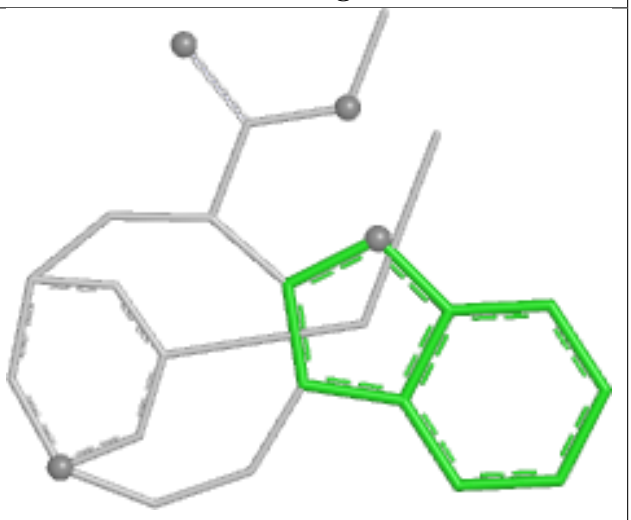
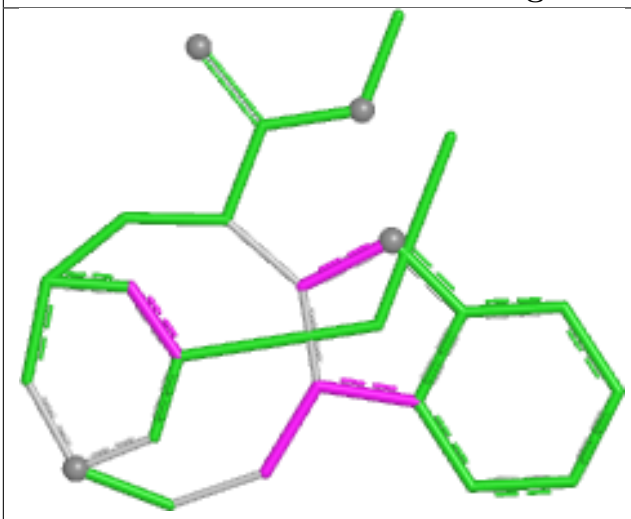


Rings

Ligand KJE B 401



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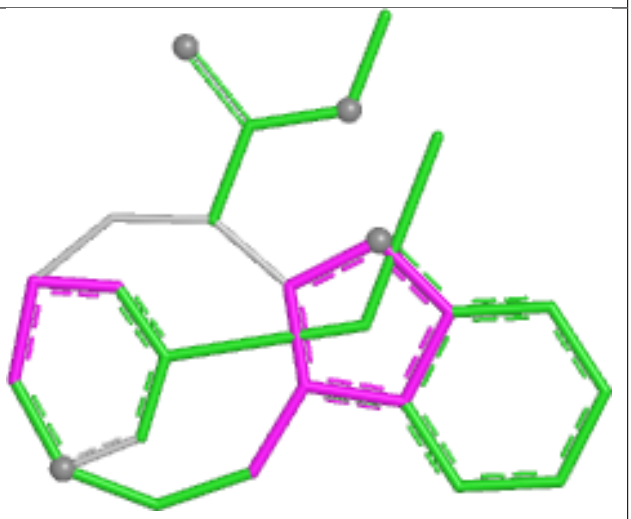

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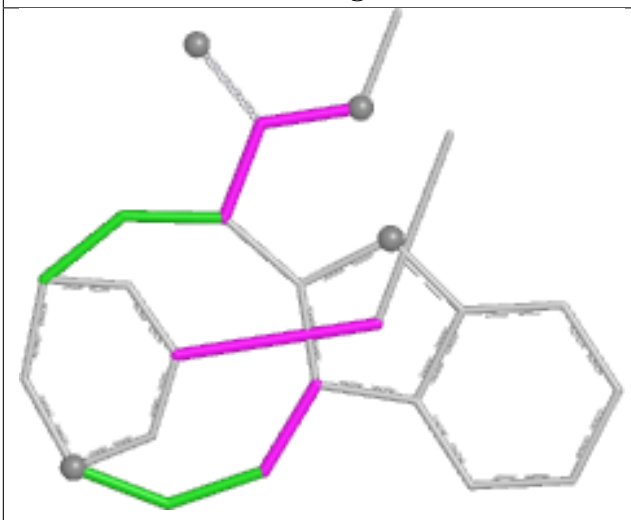

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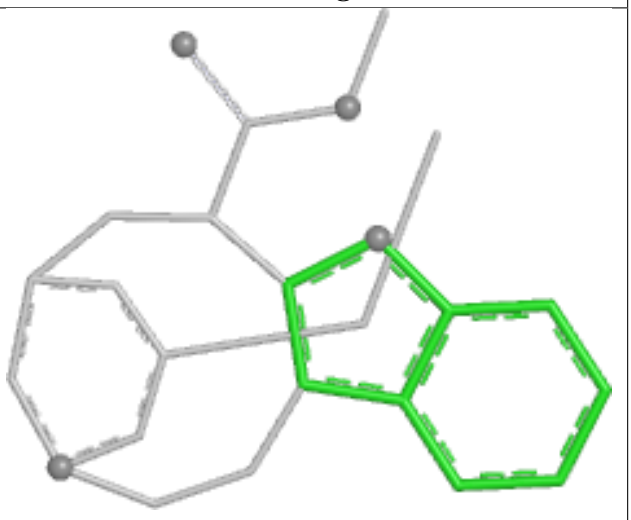
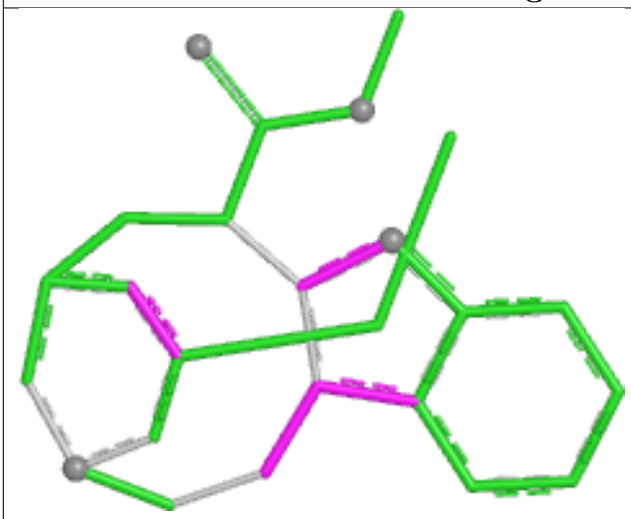


Rings

Ligand KJE D 401



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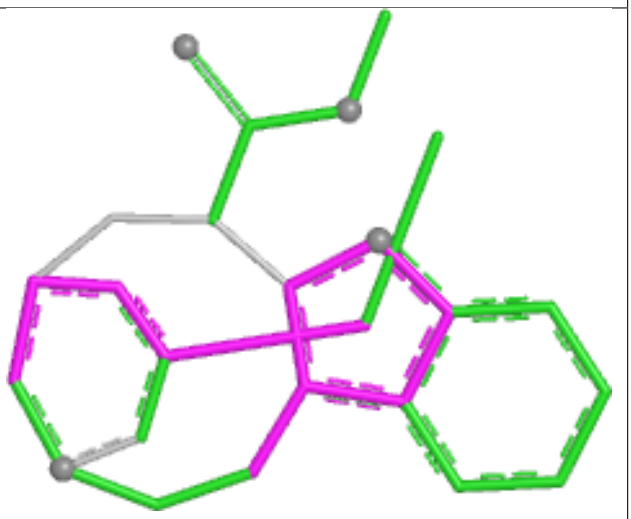

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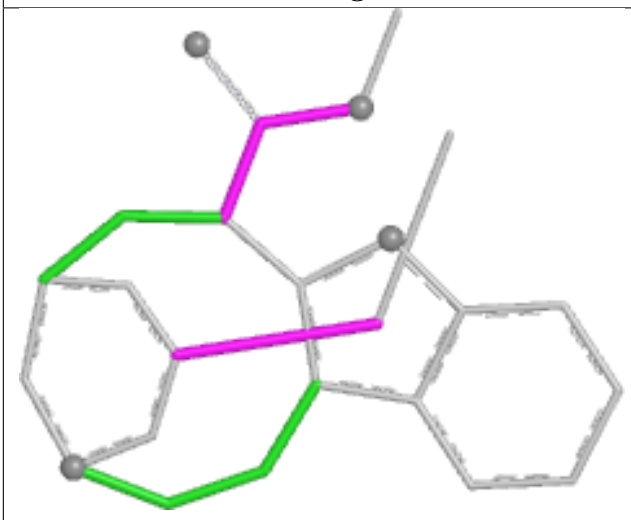

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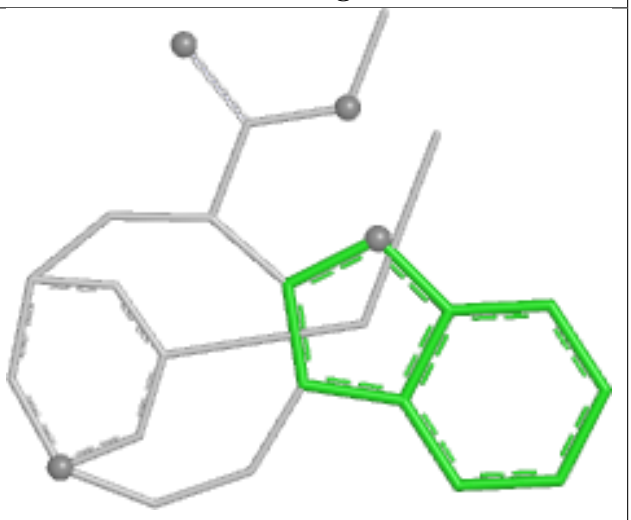
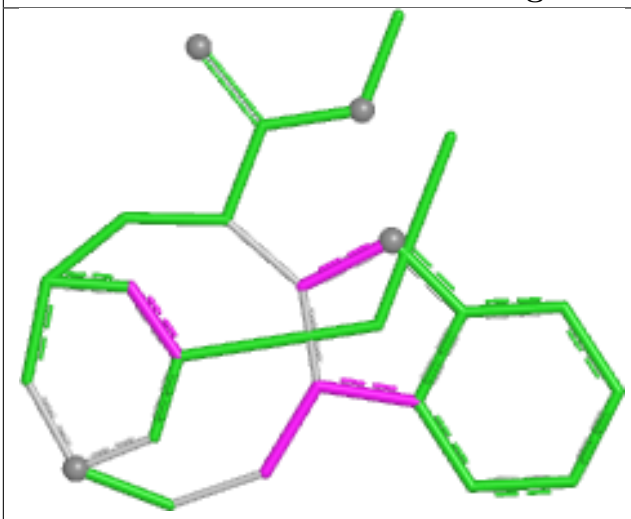
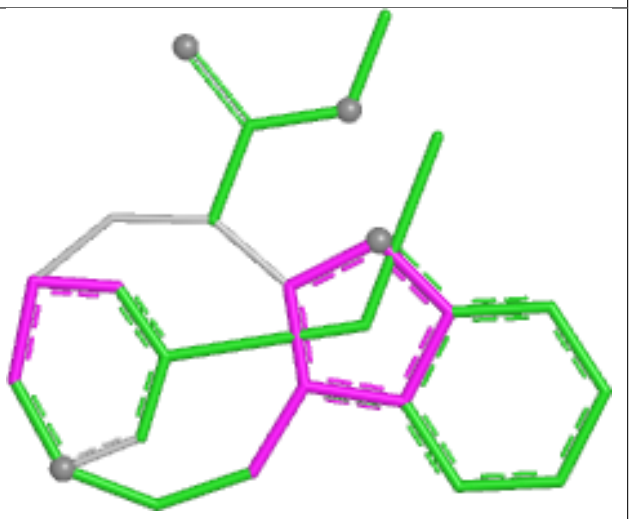


Rings

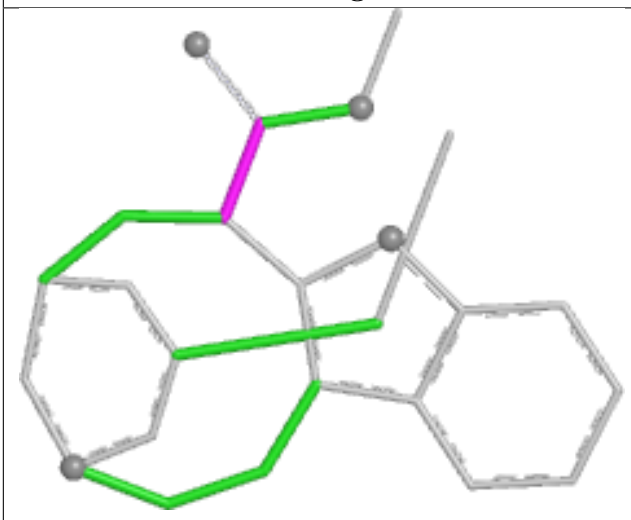
Ligand KJE C 401



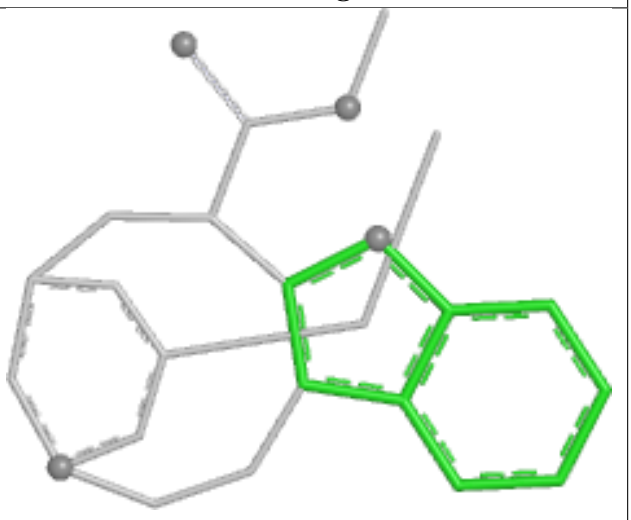
Bond lengths



Bond angles

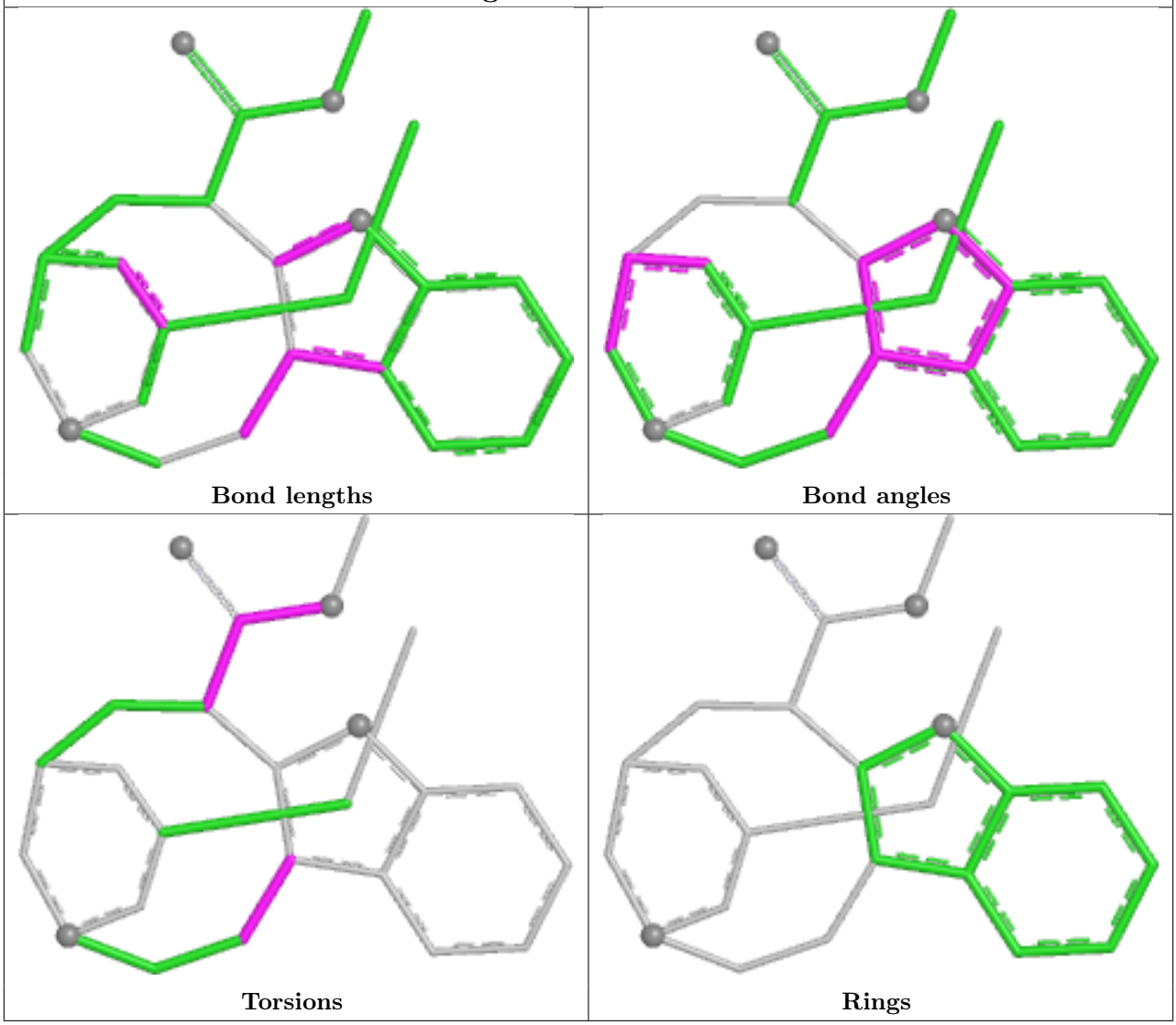


Torsions



Rings

Ligand KJE G 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	314/330 (95%)	0.05	0 100 100	43, 56, 86, 130	0
1	B	314/330 (95%)	0.18	4 (1%) 77 75	46, 62, 95, 128	0
1	C	314/330 (95%)	0.03	2 (0%) 89 88	45, 61, 95, 122	0
1	D	314/330 (95%)	0.21	4 (1%) 77 75	44, 61, 102, 135	0
1	E	305/330 (92%)	0.83	39 (12%) 3 3	47, 88, 124, 167	0
1	F	313/330 (94%)	0.33	14 (4%) 33 32	40, 70, 104, 128	0
1	G	313/330 (94%)	0.05	2 (0%) 89 88	46, 65, 94, 118	0
1	H	314/330 (95%)	0.64	40 (12%) 3 3	45, 66, 121, 157	0
All	All	2501/2640 (94%)	0.29	105 (4%) 36 34	40, 64, 111, 167	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	242	ILE	7.5
1	E	268	ILE	6.0
1	H	245	ILE	6.0
1	H	22	PHE	5.7
1	E	18	TYR	5.5
1	H	208	ILE	5.4
1	E	223	THR	5.0
1	H	207	ILE	4.9
1	E	15	LEU	4.6
1	E	304	TYR	4.6
1	H	278	ILE	4.4
1	H	10	GLU	4.4
1	E	265	VAL	4.4
1	H	24	ASP	4.3
1	E	283	ILE	4.3
1	F	283	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	248	ASN	4.2
1	H	235	GLY	4.2
1	H	282	TYR	4.2
1	H	25	GLY	4.2
1	F	325	PHE	4.2
1	H	210	THR	4.1
1	H	11	THR	4.1
1	H	209	PRO	4.1
1	E	13	TRP	4.1
1	H	211	SER	4.1
1	E	257	CYS	4.0
1	H	220	TYR	3.8
1	H	218	PHE	3.8
1	H	206	PHE	3.7
1	E	19	ILE	3.7
1	E	225	TYR	3.6
1	E	71	GLU	3.6
1	H	238	ASN	3.5
1	H	328	HIS	3.4
1	F	286	LEU	3.4
1	H	243	ASN	3.3
1	H	246	ALA	3.3
1	H	84	PHE	3.3
1	E	207	ILE	3.3
1	H	237	MET	3.3
1	E	271	THR	3.2
1	E	17	PRO	3.2
1	H	268	ILE	3.2
1	H	241	MET	3.2
1	F	245	ILE	3.2
1	D	31	HIS	3.1
1	G	311	GLU	3.1
1	F	295	LEU	3.1
1	E	203	TYR	3.0
1	H	236	GLY	3.0
1	E	298	ALA	3.0
1	H	216	ASP	3.0
1	E	25	GLY	2.9
1	E	220	TYR	2.9
1	E	242	ILE	2.9
1	E	237	MET	2.9
1	E	291	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	291	TRP	2.8
1	F	160	TYR	2.8
1	E	279	ASN	2.8
1	F	166	LEU	2.8
1	H	30	LEU	2.8
1	E	260	LEU	2.8
1	D	22	PHE	2.7
1	H	217	ASP	2.7
1	E	204	PRO	2.6
1	H	240	PRO	2.6
1	H	222	TYR	2.6
1	H	233	ALA	2.5
1	F	165	ARG	2.5
1	E	308	PHE	2.5
1	F	309	THR	2.5
1	E	151	ILE	2.4
1	D	110	VAL	2.4
1	E	270	THR	2.4
1	E	208	ILE	2.4
1	H	226	TRP	2.4
1	H	14	ASP	2.3
1	B	22	PHE	2.3
1	E	107	VAL	2.3
1	B	137	ALA	2.3
1	E	269	SER	2.3
1	H	275	THR	2.3
1	E	267	MET	2.2
1	F	296	GLU	2.2
1	H	244	PRO	2.2
1	B	25	GLY	2.2
1	B	30	LEU	2.2
1	E	22	PHE	2.2
1	E	101	PHE	2.2
1	E	86	LEU	2.1
1	E	295	LEU	2.1
1	C	25	GLY	2.1
1	F	150	ALA	2.1
1	E	272	PRO	2.1
1	H	23	LYS	2.1
1	E	297	VAL	2.1
1	C	210	THR	2.1
1	F	252	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	305	PHE	2.1
1	H	26	ARG	2.1
1	E	287	GLU	2.0
1	F	298	ALA	2.0
1	G	220	TYR	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)

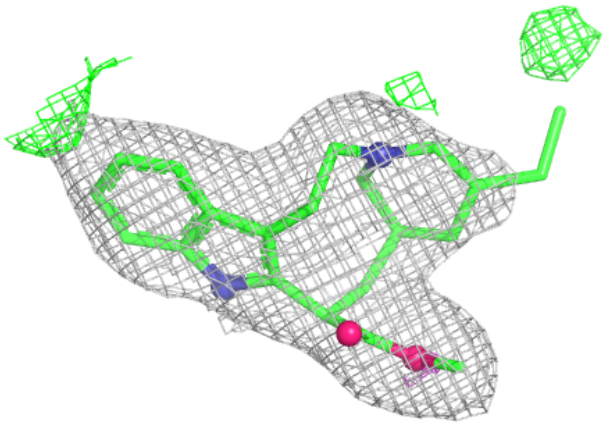
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

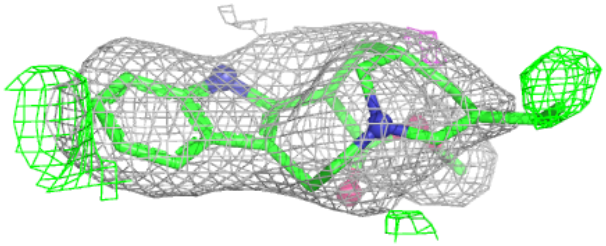
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KJE	H	401	25/25	0.91	0.19	64,88,113,168	0
3	P6G	E	402	19/19	0.91	0.36	52,78,104,119	0
3	P6G	C	402	19/19	0.92	0.15	48,64,78,88	0
3	P6G	A	402	19/19	0.94	0.20	48,67,102,107	0
2	KJE	A	401	25/25	0.96	0.13	38,45,57,81	0
2	KJE	F	401	25/25	0.96	0.14	44,54,63,76	0
3	P6G	H	402	19/19	0.96	0.20	56,82,127,135	0
2	KJE	B	401	25/25	0.97	0.11	41,52,62,65	0
2	KJE	D	401	25/25	0.97	0.11	45,52,69,74	0
2	KJE	E	401	25/25	0.97	0.24	57,80,97,102	0
2	KJE	G	401	25/25	0.98	0.15	50,65,75,94	0
2	KJE	C	401	25/25	0.98	0.13	42,58,64,69	0

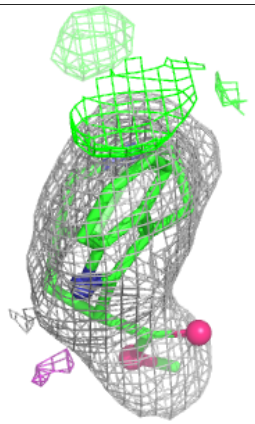
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

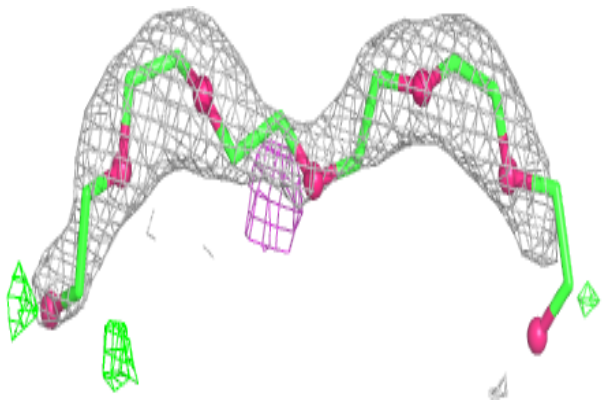


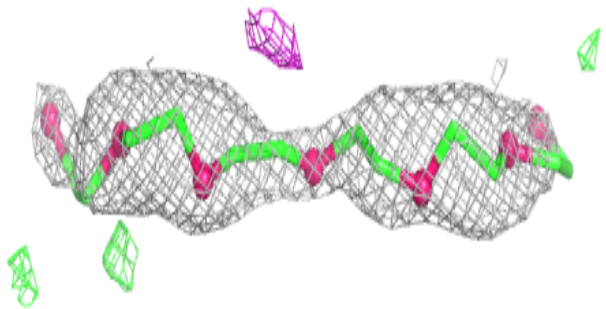


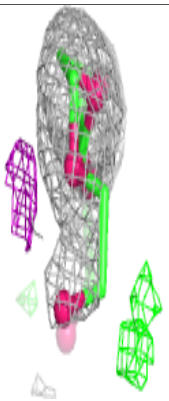


Electron density around P6G E 402:

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

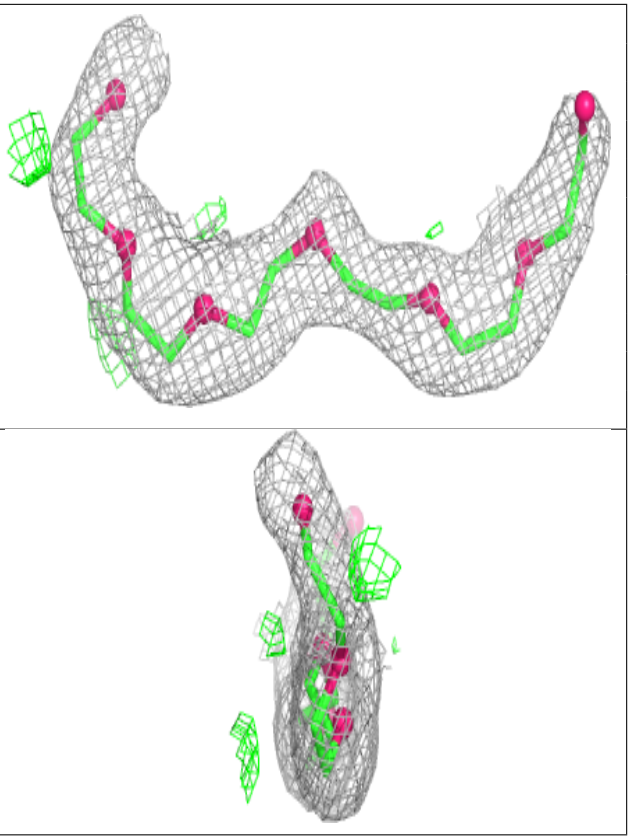






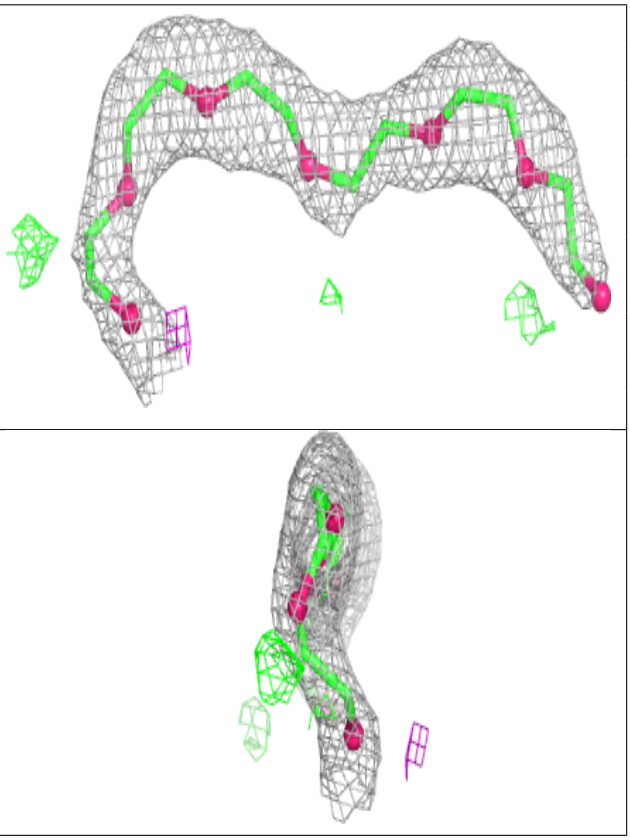
Electron density around P6G C 402:

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



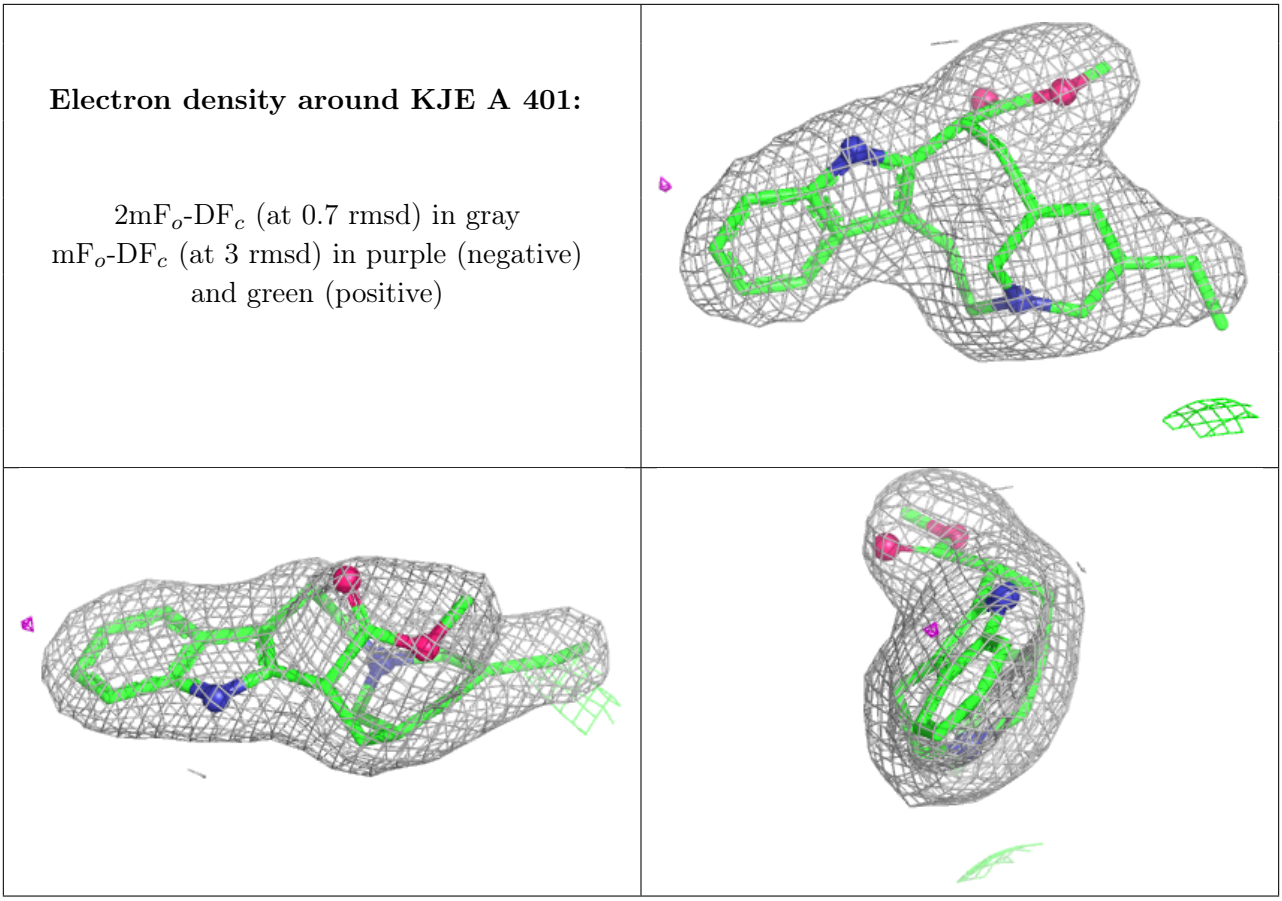
Electron density around P6G A 402:

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



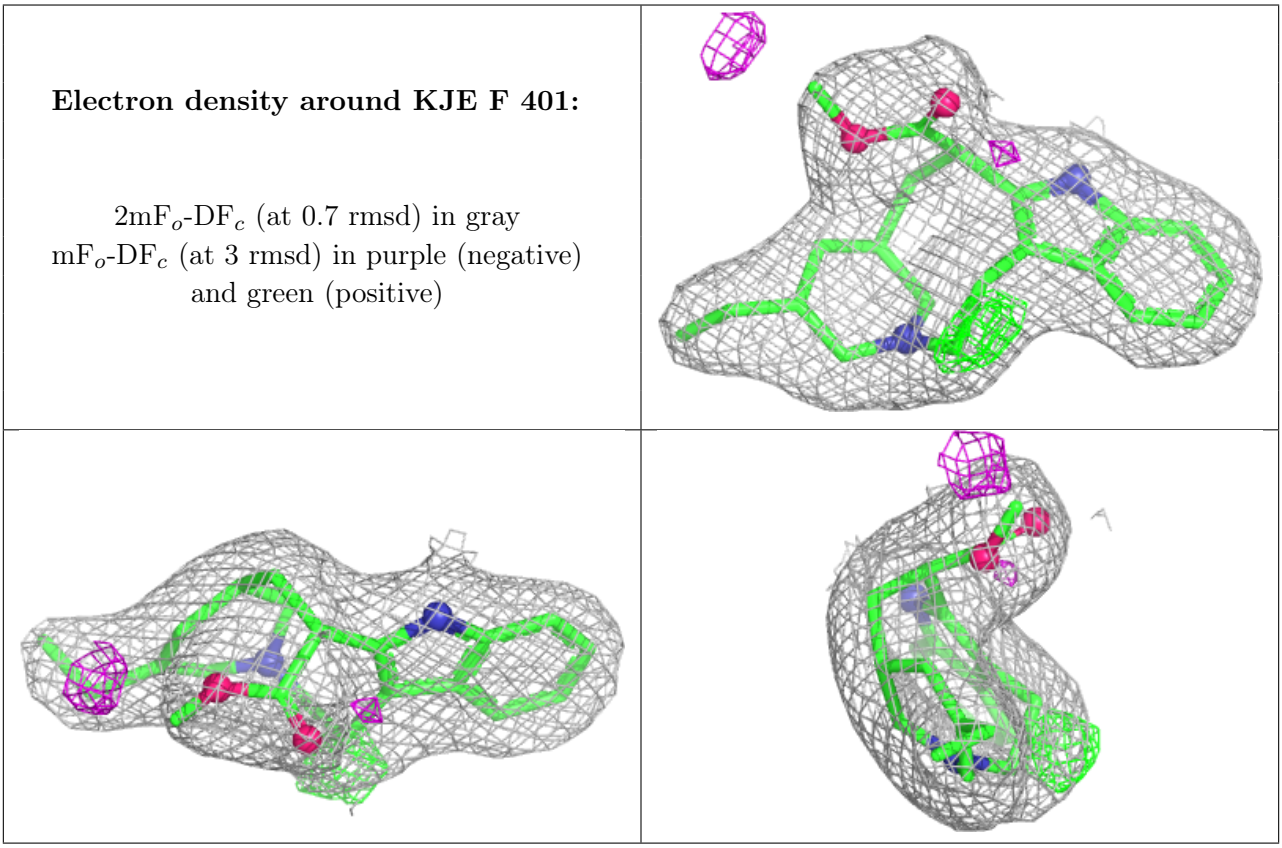
Electron density around KJE A 401:

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



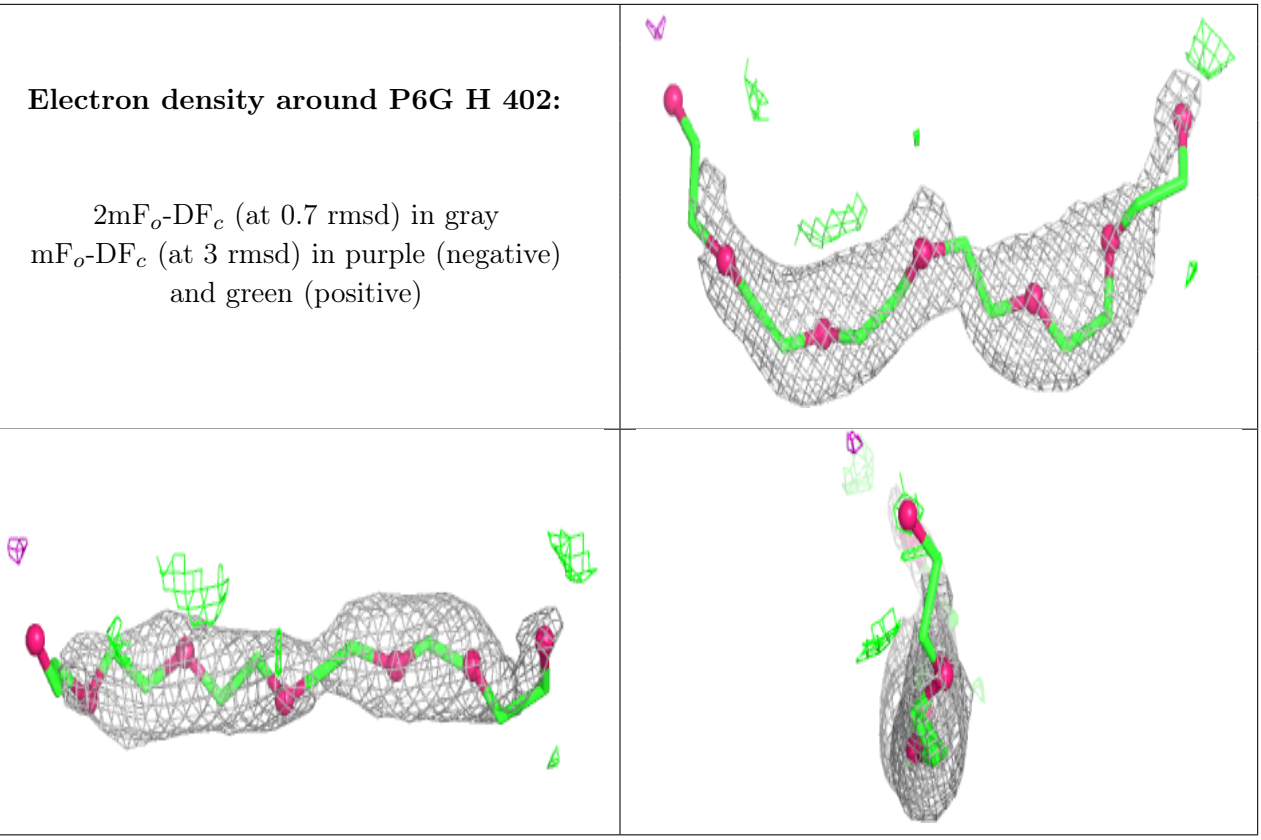
Electron density around KJE F 401:

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



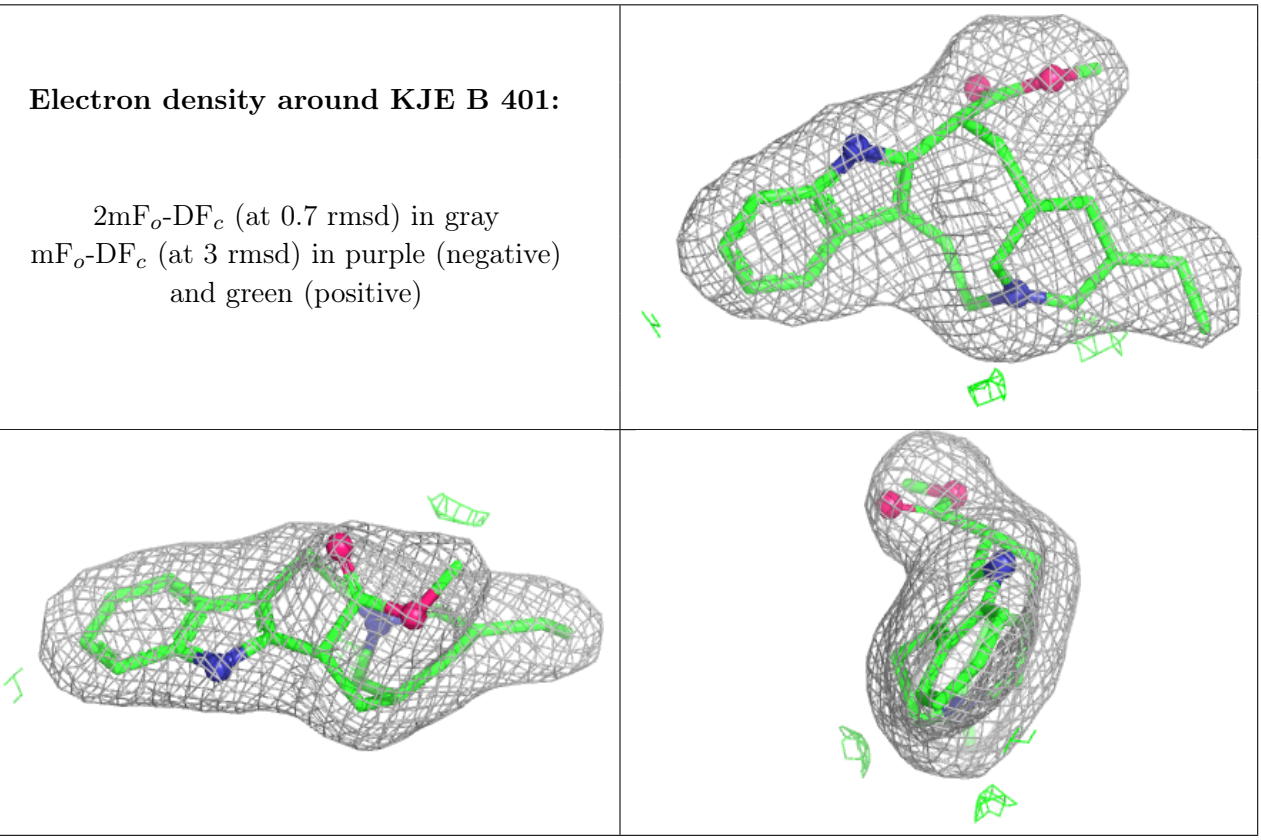
Electron density around P6G H 402:

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



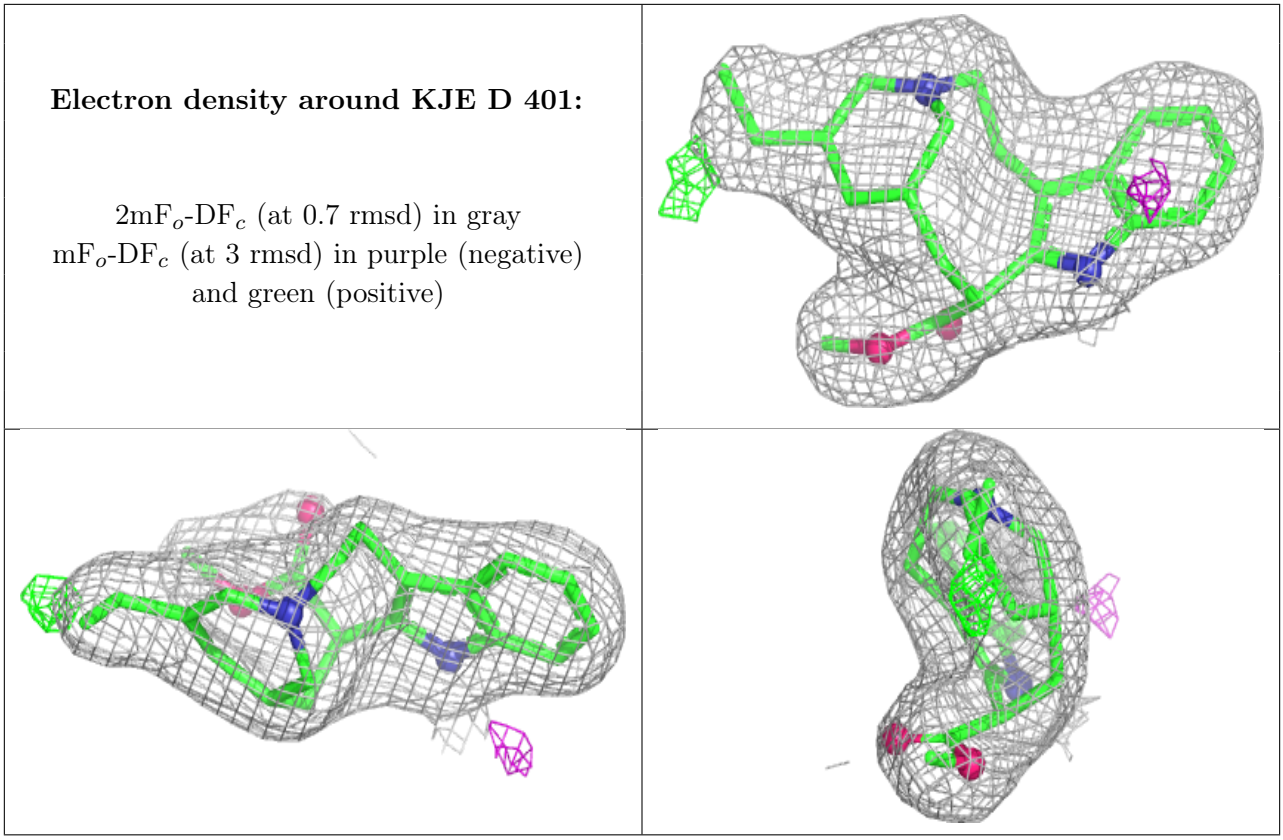
Electron density around KJE B 401:

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



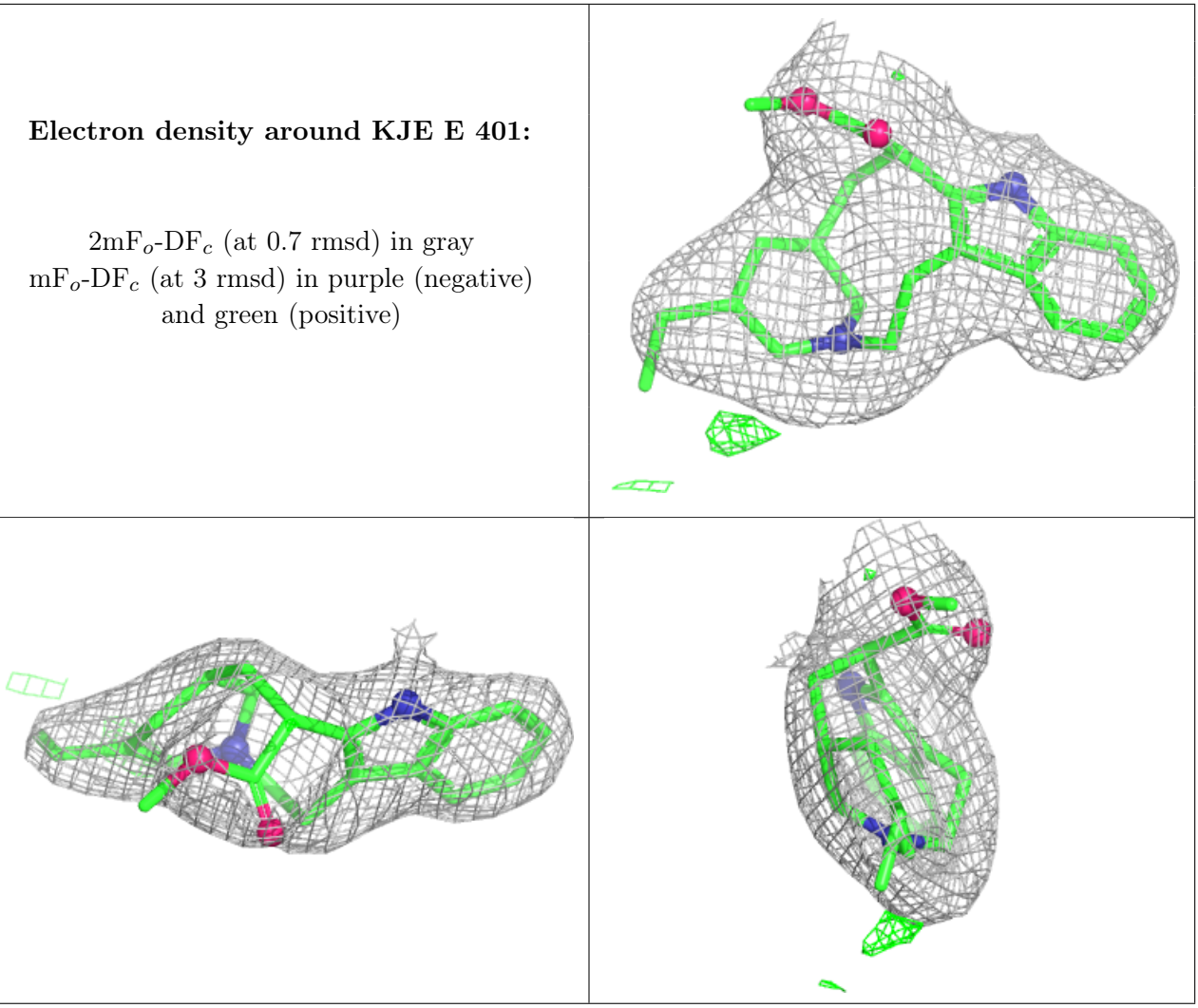
Electron density around KJE D 401:

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



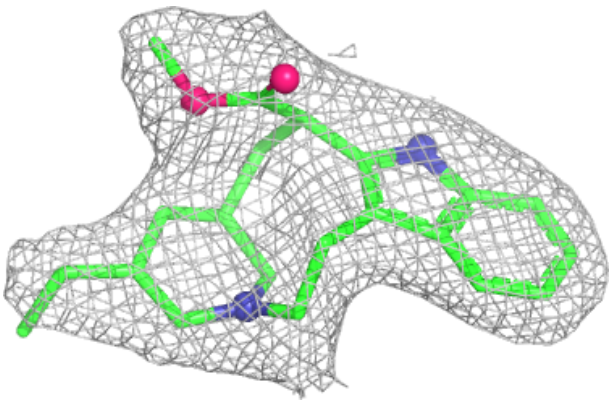
Electron density around KJE E 401:

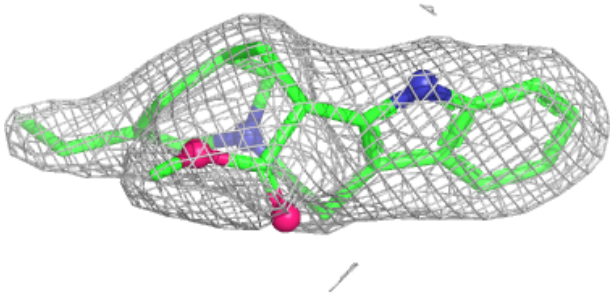
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

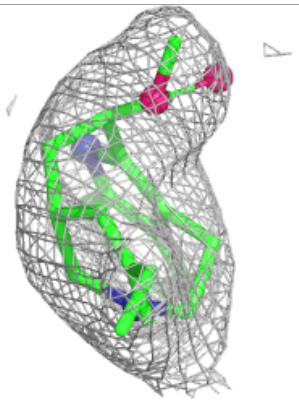


Electron density around KJE G 401:

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

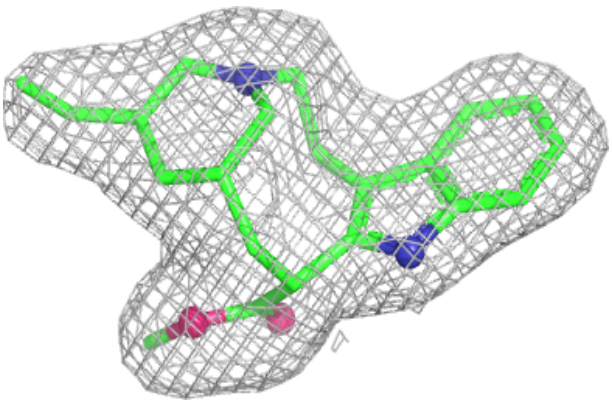


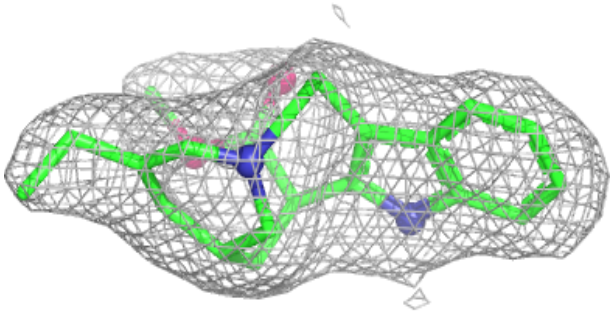


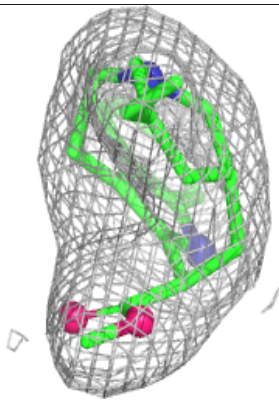


Electron density around KJE C 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.