



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 09:39 PM EDT

PDB ID : 6N94
Title : Methylmalonyl-CoA decarboxylase in complex with 2-nitronate-propionyl-amino(dethia)-CoA
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on : 2018-11-30
Resolution : 1.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

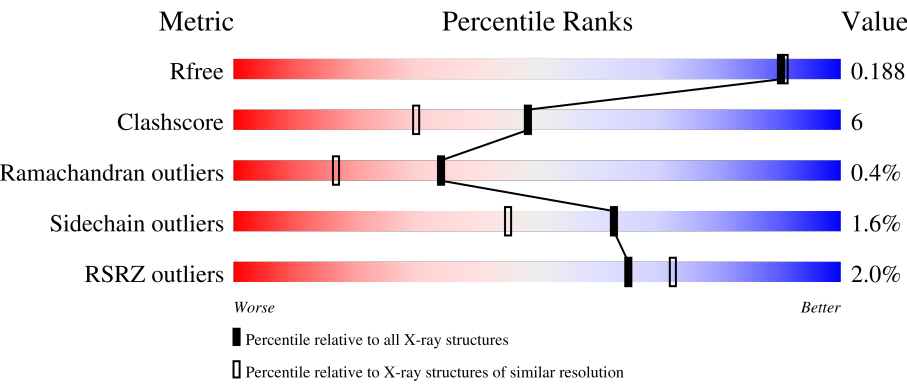
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



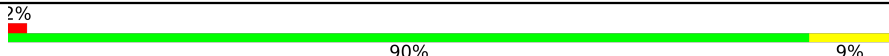
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	261	<div><div>92%8%</div></div>
1	B	261	<div><div>88%11%</div></div>
1	C	261	<div><div>91%8%</div></div>
1	D	261	<div><div>91%8%</div></div>
1	E	261	<div><div>90%9%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	261	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '90%', and a small yellow segment at the end labeled '9%'.

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15267 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.

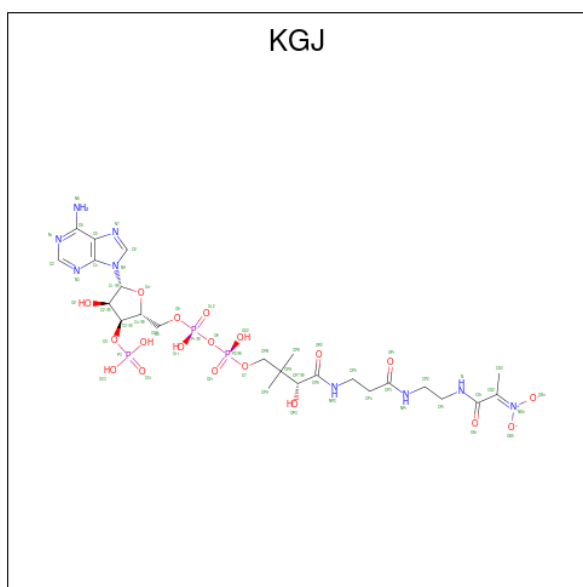
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	20	0
			2153	1379	366	395	13			
1	B	260	Total	C	N	O	S	0	18	0
			2139	1377	361	389	12			
1	C	260	Total	C	N	O	S	0	16	0
			2136	1369	363	392	12			
1	D	260	Total	C	N	O	S	0	15	0
			2110	1351	355	391	13			
1	E	260	Total	C	N	O	S	0	17	0
			2135	1368	360	395	12			
1	F	260	Total	C	N	O	S	0	19	0
			2150	1381	365	392	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is [1-[2-[3-[[[(2 {R})-4-[[[(2 {R}),3 {S},4 {R}),5 {R}]-5-(6-aminopurin-9-yl)-4-oxidan-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethylamino]-1-oxidanylidene-prop-2-ylidene]-bis(oxidanidyl)azanum (three-letter code: KGJ) (formula: C₂₄H₃₉N₉O₁₉P₃).

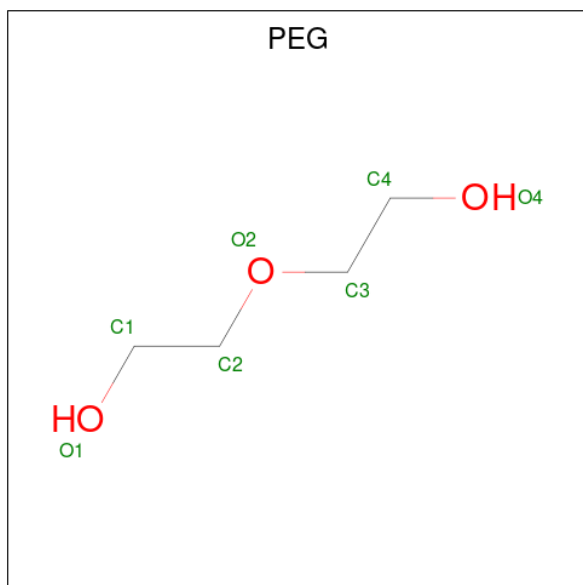


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			55	24	9	19	3		
2	B	1	Total	C	N	O	P	0	0
			55	24	9	19	3		
2	C	1	Total	C	N	O	P	0	0
			55	24	9	19	3		
2	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	1
			82	34	14	29	5		
2	E	1	Total	C	N	O	P	0	1
			82	34	14	29	5		
2	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	1
			82	34	14	29	5		
2	F	1	Total	C	N	O	P	0	1
			31	10	5	13	3		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

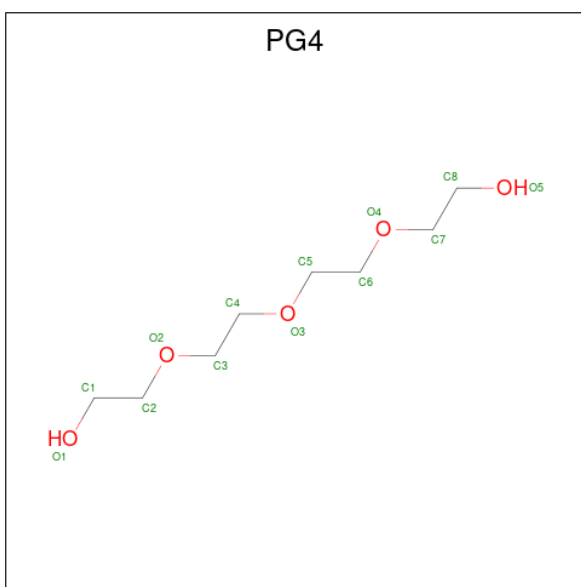


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

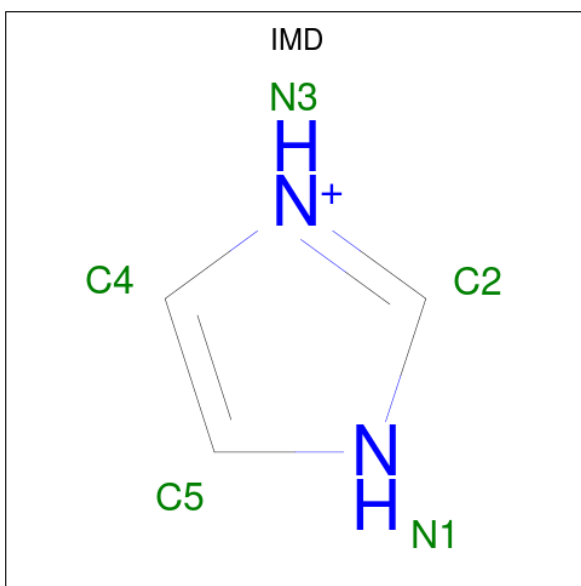
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		
5	F	1	Total	K	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



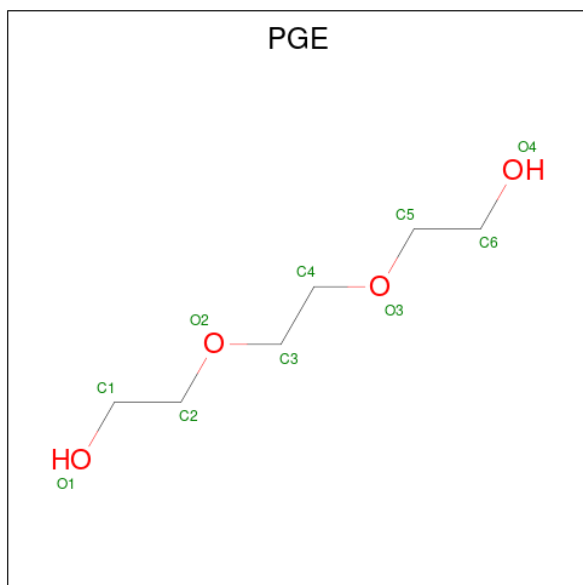
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	337	Total	O	0	14
			349	349		
9	B	280	Total	O	0	9
			286	286		
9	C	308	Total	O	0	17
			321	321		
9	D	300	Total	O	0	12
			309	309		
9	E	311	Total	O	0	18
			322	322		
9	F	299	Total	O	0	12
			307	307		

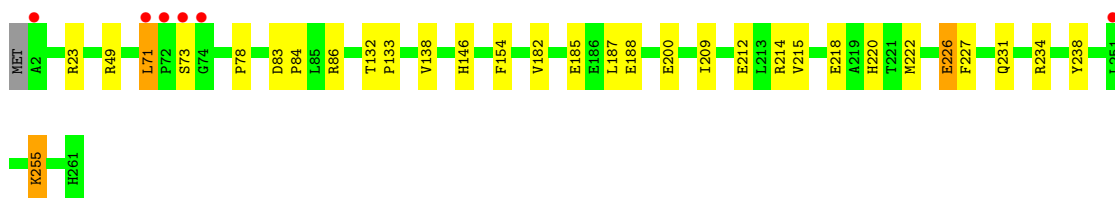
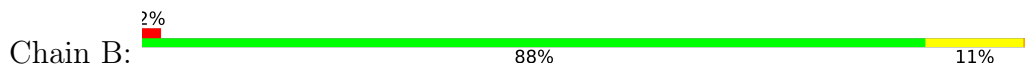
3 Residue-property plots

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

- Molecule 1: Methylmalonyl-CoA decarboxylase



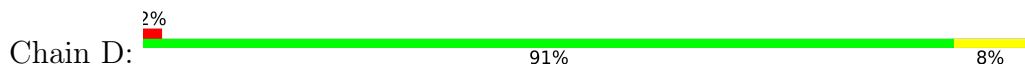
- Molecule 1: Methylmalonyl-CoA decarboxylase



- Molecule 1: Methylmalonyl-CoA decarboxylase



- Molecule 1: Methylmalonyl-CoA decarboxylase

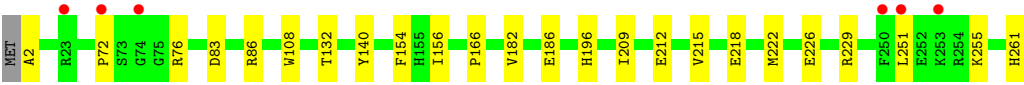
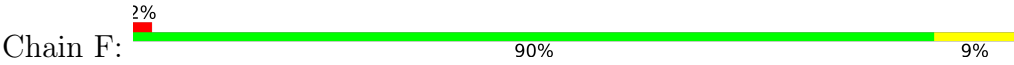


- Molecule 1: Methylmalonyl-CoA decarboxylase





● Molecule 1: Methylmalonyl-CoA decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.05Å 114.82Å 193.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.29 – 1.75 29.27 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.29-1.75) 94.1 (29.27-1.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.146 , 0.178 0.158 , 0.188	Depositor DCC
R_{free} test set	9164 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15267	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PG4, NI, PGE, IMD, KGJ, PEG

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	0.82	0/2250	0.85	1/3041 (0.0%)
1	B	0.83	4/2237 (0.2%)	0.85	2/3027 (0.1%)
1	C	0.83	0/2228	0.85	2/3013 (0.1%)
1	D	0.88	3/2195 (0.1%)	0.88	3/2969 (0.1%)
1	E	0.83	3/2228 (0.1%)	0.86	3/3016 (0.1%)
1	F	0.84	2/2251 (0.1%)	0.86	4/3046 (0.1%)
All	All	0.84	12/13389 (0.1%)	0.86	15/18112 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	226	GLU	CD-OE1	-11.99	1.12	1.25
1	F	226	GLU	CD-OE1	-11.68	1.12	1.25
1	D	226	GLU	CD-OE2	-9.64	1.15	1.25
1	F	212	GLU	CD-OE2	-7.13	1.17	1.25
1	D	185	GLU	CD-OE2	5.89	1.32	1.25
1	B	212	GLU	CD-OE2	-5.74	1.19	1.25
1	B	226[A]	GLU	CD-OE2	-5.57	1.19	1.25
1	B	226[B]	GLU	CD-OE2	-5.57	1.19	1.25
1	E	212	GLU	CD-OE2	-5.39	1.19	1.25
1	D	226	GLU	CD-OE1	5.31	1.31	1.25
1	B	200	GLU	CD-OE2	5.17	1.31	1.25
1	E	200	GLU	CD-OE2	5.09	1.31	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	86	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	C	86	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	86	ARG	NE-CZ-NH2	-6.78	116.91	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	86	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	86	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	150	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	86	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	86	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	F	229	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	238	TYR	CB-CA-C	5.43	121.27	110.40
1	E	82[A]	ASP	CB-CA-C	5.24	120.88	110.40
1	E	82[B]	ASP	CB-CA-C	5.24	120.88	110.40
1	D	82	ASP	CB-CA-C	5.07	120.53	110.40
1	F	83[A]	ASP	CB-CA-C	5.05	120.51	110.40
1	F	83[B]	ASP	CB-CA-C	5.05	120.51	110.40

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	2153	0	2202	39	0
1	B	2139	0	2200	31	0
1	C	2136	0	2176	31	0
1	D	2110	0	2143	25	0
1	E	2135	0	2164	32	0
1	F	2150	0	2192	30	0
2	A	55	0	0	1	0
2	B	55	0	0	1	0
2	C	86	0	0	4	0
2	D	82	0	0	0	0
2	E	113	0	0	9	0
2	F	113	0	0	9	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	B	7	0	10	0	0
4	C	7	0	10	1	0
5	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1	0	0	0	0
6	C	13	0	18	0	0
7	D	5	0	5	2	0
8	F	10	0	14	0	0
9	A	349	0	0	5	0
9	B	286	0	0	9	0
9	C	321	0	0	7	0
9	D	309	0	0	1	0
9	E	322	0	0	4	0
9	F	307	0	0	4	0
All	All	15267	0	13134	156	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 6.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222[A]:MET:CE	1:A:226[A]:GLU:HG2	1.11	1.54
1:A:222[A]:MET:CE	1:A:226[A]:GLU:CG	2.04	1.34
1:E:215[A]:VAL:CG1	1:F:222[A]:MET:SD	2.24	1.25
1:B:215[B]:VAL:CG1	1:C:222[B]:MET:HE1	1.69	1.22
1:C:49[B]:ARG:NH1	9:C:401:HOH:O	1.69	1.19
1:D:222[B]:MET:HE1	1:F:215[B]:VAL:CG1	1.75	1.17
1:A:222[A]:MET:HE2	1:A:226[A]:GLU:HG2	1.18	1.16
1:A:222[A]:MET:HE1	1:A:226[A]:GLU:CG	1.72	1.15
1:E:130[A]:SER:OG	2:E:302[A]:KGJ:N7	1.79	1.15
1:D:222[B]:MET:CE	1:F:215[B]:VAL:CG1	2.25	1.14
1:D:222[B]:MET:HE1	1:F:215[B]:VAL:HG11	1.17	1.11
1:C:231[B]:GLN:CD	1:D:231[B]:GLN:HE22	1.55	1.08
1:A:222[A]:MET:HE1	1:A:226[A]:GLU:HG2	1.12	1.07
1:B:215[B]:VAL:HG11	1:C:222[B]:MET:HE1	1.15	1.06
1:A:222[A]:MET:HE3	1:A:226[A]:GLU:HG2	1.31	1.06
1:B:215[B]:VAL:CG1	1:C:222[B]:MET:CE	2.35	1.04
1:B:188:GLU:OE2	9:B:401:HOH:O	1.82	0.97
1:E:215[A]:VAL:HG12	1:F:222[A]:MET:SD	2.03	0.94
1:E:215[A]:VAL:HG13	1:F:222[A]:MET:SD	2.03	0.94
1:D:222[B]:MET:CE	1:F:215[B]:VAL:HG13	1.94	0.94
1:D:222[B]:MET:CE	1:F:215[B]:VAL:HG11	1.96	0.93
1:A:222[B]:MET:HG2	1:A:227[B]:PHE:CZ	2.04	0.91
1:C:231[B]:GLN:CD	1:D:231[B]:GLN:NE2	2.23	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222[B]:MET:SD	1:F:215[B]:VAL:CG1	2.63	0.86
1:A:196[B]:HIS:HD2	9:A:581:HOH:O	1.57	0.86
1:A:222[B]:MET:HG2	1:A:227[B]:PHE:CE2	2.11	0.85
1:E:130[A]:SER:OG	2:E:302[A]:KGJ:C5	2.25	0.84
1:A:36:LEU:HD23	1:A:88[B]:ILE:CD1	2.07	0.84
1:A:222[B]:MET:CG	1:A:227[B]:PHE:CE2	2.62	0.82
1:D:222[B]:MET:SD	1:F:215[B]:VAL:HG12	2.21	0.81
1:E:226:GLU:OE2	9:E:401[A]:HOH:O	1.99	0.79
1:F:108:TRP:CH2	2:F:302[A]:KGJ:C4	2.69	0.75
1:B:182[B]:VAL:HG21	1:B:187:LEU:HA	1.68	0.74
1:D:222[B]:MET:HE3	1:F:215[B]:VAL:HG13	1.69	0.73
1:E:130[A]:SER:CB	2:E:302[A]:KGJ:N7	2.51	0.73
1:A:222[B]:MET:CG	1:A:227[B]:PHE:CZ	2.73	0.72
1:A:222[B]:MET:SD	1:A:227[B]:PHE:CE1	2.83	0.72
1:F:108:TRP:CZ3	2:F:302[A]:KGJ:N7	2.57	0.71
1:F:108:TRP:CH2	2:F:302[A]:KGJ:C5	2.72	0.71
1:F:108:TRP:CZ3	2:F:302[A]:KGJ:C8	2.73	0.71
1:E:222[B]:MET:HE3	1:E:226:GLU:HB3	1.72	0.71
1:E:215[A]:VAL:HG11	1:F:222[A]:MET:SD	2.31	0.69
1:A:222[A]:MET:HE3	1:C:215[A]:VAL:HB	1.75	0.69
1:E:108:TRP:CH2	2:E:302[A]:KGJ:C4	2.75	0.69
1:F:218[A]:GLU:CD	9:F:407:HOH:O	2.31	0.68
1:F:196[B]:HIS:HD2	9:F:575:HOH:O	1.76	0.68
1:C:231[B]:GLN:OE1	1:D:231[B]:GLN:NE2	2.18	0.68
1:A:36:LEU:CD2	1:A:88[B]:ILE:HD11	2.23	0.68
1:A:36:LEU:HD23	1:A:88[B]:ILE:HD13	1.77	0.64
1:C:257:ASN:HB2	9:C:619:HOH:O	1.97	0.63
1:E:108:TRP:CZ3	2:E:302[A]:KGJ:C8	2.81	0.63
1:B:133:PRO:CB	1:B:138[B]:VAL:HG22	2.29	0.62
4:C:304:PEG:H41	9:C:462:HOH:O	1.98	0.62
1:E:74:GLY:H	1:E:244:GLN:HE22	1.48	0.61
1:B:214:ARG:O	1:B:218[B]:GLU:HG3	1.99	0.61
1:C:108:TRP:CZ3	2:C:302[A]:KGJ:C8	2.84	0.61
1:A:36:LEU:CD2	1:A:88[B]:ILE:CD1	2.76	0.61
1:D:76:ARG:HG3	9:D:618:HOH:O	2.01	0.61
1:A:222[A]:MET:HE1	1:A:226[A]:GLU:CB	2.31	0.61
1:A:222[B]:MET:HG3	1:A:227[B]:PHE:CE2	2.35	0.60
1:B:215[B]:VAL:CG1	1:C:222[B]:MET:HE3	2.28	0.60
1:A:222[A]:MET:HE3	1:A:226[A]:GLU:CG	2.05	0.60
1:E:66[A]:HIS:CE1	1:E:71:LEU:CD1	2.85	0.59
1:D:54:ARG:HH12	1:D:188[B]:GLU:CD	2.06	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68[B]:ILE:HD12	1:E:250:PHE:CZ	2.38	0.58
1:B:133:PRO:HB3	1:B:138[B]:VAL:HG22	1.84	0.58
1:A:13[A]:LYS:NZ	1:A:200[A]:GLU:OE2	2.35	0.57
1:A:200[B]:GLU:CD	9:A:438:HOH:O	2.42	0.57
1:D:231[A]:GLN:HE22	1:D:234:ARG:HH11	1.52	0.57
1:B:215[B]:VAL:HG13	1:C:222[B]:MET:CE	2.30	0.57
1:B:49:ARG:NH1	9:B:402:HOH:O	1.93	0.56
1:B:23:ARG:NH2	9:B:473[B]:HOH:O	2.37	0.56
1:D:196[B]:HIS:HE1	7:D:303:IMD:HN3	1.51	0.56
1:A:222[A]:MET:HE2	1:A:226[A]:GLU:CG	2.08	0.55
1:B:83:ASP:HB3	9:B:417[B]:HOH:O	2.05	0.55
1:A:222[B]:MET:SD	1:A:227[B]:PHE:CD1	3.00	0.55
1:B:182[B]:VAL:CG2	1:B:187:LEU:HA	2.37	0.54
1:C:7:ASN:ND2	9:C:553[B]:HOH:O	2.41	0.53
1:B:231:GLN:NE2	9:B:406:HOH:O	2.30	0.53
1:B:218[A]:GLU:CD	9:B:412:HOH:O	2.47	0.53
1:C:231[A]:GLN:CG	1:D:227[A]:PHE:HE2	2.22	0.53
1:A:222[B]:MET:HG3	1:A:227[B]:PHE:CD2	2.44	0.53
1:E:196[B]:HIS:HD2	9:E:560:HOH:O	1.92	0.53
1:E:68[B]:ILE:HD12	1:E:250:PHE:CE1	2.44	0.52
1:F:182[B]:VAL:HG12	1:F:186:GLU:HB2	1.91	0.51
2:A:301:KGJ:N	2:A:301:KGJ:OS4	2.44	0.51
1:B:215[B]:VAL:HG12	1:C:222[B]:MET:CE	2.32	0.51
1:F:261:HIS:HD2	9:F:517:HOH:O	1.94	0.51
1:B:226[B]:GLU:HG2	9:B:494:HOH:O	2.11	0.51
1:E:108:TRP:CZ3	2:E:302[A]:KGJ:N7	2.79	0.50
1:E:66[A]:HIS:CE1	1:E:71:LEU:HD12	2.46	0.50
1:E:108:TRP:CH2	2:E:302[A]:KGJ:C5	2.95	0.50
1:C:222[A]:MET:HE3	1:C:227[A]:PHE:CE1	2.47	0.49
1:A:257[A]:ASN:OD1	9:A:401:HOH:O	2.20	0.49
1:B:227[B]:PHE:CE2	1:E:231[B]:GLN:HG2	2.48	0.49
1:C:196[B]:HIS:HD2	9:C:506:HOH:O	1.94	0.49
1:C:45[B]:ARG:NH2	1:C:47:GLU:OE2	2.45	0.49
1:E:66[A]:HIS:CE1	1:E:71:LEU:HD13	2.48	0.48
1:E:136:LEU:HB3	1:E:247:MET:CE	2.42	0.48
1:B:227[B]:PHE:HE2	1:E:231[B]:GLN:HG2	1.79	0.48
1:E:215[A]:VAL:HG11	1:F:222[A]:MET:CE	2.44	0.48
1:A:161:ILE:HG21	1:C:209:ILE:HG21	1.96	0.48
1:B:227[B]:PHE:HE2	1:E:231[B]:GLN:CG	2.27	0.47
1:B:255:LYS:HG3	9:B:579:HOH:O	2.14	0.47
1:D:196[B]:HIS:CE1	7:D:303:IMD:HN3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:KGJ:N	2:B:301:KGJ:OS4	2.48	0.47
1:F:182[B]:VAL:CG1	1:F:186:GLU:HB2	2.44	0.46
1:A:182[B]:VAL:HG12	1:A:186:GLU:HB2	1.97	0.46
1:B:215[B]:VAL:HG12	1:C:222[B]:MET:HE3	1.92	0.46
1:D:237:VAL:O	1:D:240[B]:SER:HB2	2.15	0.46
1:C:136:LEU:HD12	2:C:301:KGJ:OS4	2.16	0.46
1:A:215[B]:VAL:HG12	1:B:222[B]:MET:CE	2.46	0.46
1:A:13[A]:LYS:CE	1:A:200[A]:GLU:OE2	2.63	0.46
1:C:49[B]:ARG:CZ	9:C:401:HOH:O	2.34	0.45
1:B:185[A]:GLU:HG3	9:B:650:HOH:O	2.17	0.45
1:E:196[B]:HIS:HE1	9:E:586:HOH:O	2.00	0.45
1:F:108:TRP:CZ3	2:F:302[A]:KGJ:C5	2.96	0.45
1:D:222[B]:MET:HE2	1:D:226:GLU:HB3	1.99	0.45
1:D:243:TYR:O	1:D:247[B]:MET:HG2	2.17	0.45
1:D:222[B]:MET:CE	1:D:226:GLU:HG2	2.47	0.45
1:F:108:TRP:HZ3	2:F:302[A]:KGJ:C8	2.28	0.44
1:E:108:TRP:CH2	2:E:302[A]:KGJ:N9	2.86	0.43
1:F:222[A]:MET:HB2	1:F:222[A]:MET:HE2	1.95	0.43
1:B:146:HIS:HE2	1:B:220:HIS:HD1	1.67	0.43
1:A:233[B]:MET:HE1	1:C:211:GLU:HG2	2.01	0.43
1:B:231:GLN:HE22	1:B:234:ARG:HH11	1.65	0.43
1:C:45[B]:ARG:NH1	9:C:414:HOH:O	2.50	0.42
9:E:470:HOH:O	1:F:156[B]:ILE:HD12	2.18	0.42
1:A:222[B]:MET:SD	1:A:227[B]:PHE:CZ	3.12	0.42
1:A:166:PRO:HD3	9:A:503:HOH:O	2.19	0.42
1:C:128:THR:OG1	2:C:302[A]:KGJ:N1	2.53	0.42
1:C:222[A]:MET:CE	1:C:227[A]:PHE:CE1	3.02	0.42
1:E:166:PRO:HB3	2:E:302[A]:KGJ:C5	2.49	0.42
1:F:72:PRO:HB2	1:F:76:ARG:HB2	2.02	0.42
1:A:36:LEU:HG	1:A:88[B]:ILE:HD11	2.02	0.42
1:B:209:ILE:HG21	1:C:161:ILE:HG21	2.02	0.42
1:E:66[A]:HIS:ND1	1:E:71:LEU:HD13	2.35	0.42
1:C:231[A]:GLN:HG2	1:D:227[A]:PHE:CE2	2.55	0.42
1:C:231[B]:GLN:CG	1:D:231[B]:GLN:NE2	2.83	0.41
1:A:215[B]:VAL:HG12	1:B:222[B]:MET:HE2	2.01	0.41
1:B:71:LEU:HD12	1:B:78:PRO:HB2	2.02	0.41
1:F:166:PRO:HB3	2:F:302[A]:KGJ:C5	2.51	0.41
1:C:108:TRP:CZ3	2:C:302[A]:KGJ:N7	2.89	0.41
1:F:2:ALA:HB1	9:F:625:HOH:O	2.21	0.41
1:B:83:ASP:HA	1:B:84:PRO:HD3	1.98	0.41
1:C:231[A]:GLN:CG	1:D:227[A]:PHE:CE2	3.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ILE:HG21	1:F:209:ILE:HG21	2.03	0.41
1:A:36:LEU:CG	1:A:88[B]:ILE:HD11	2.51	0.40
1:E:255:LYS:HD3	1:E:255:LYS:HA	1.89	0.40
1:A:23:ARG:H	1:A:23:ARG:HD3	1.87	0.40
1:A:66:HIS:CE1	9:A:436:HOH:O	2.74	0.40
1:A:222[A]:MET:HE1	1:A:226[A]:GLU:HB3	2.02	0.40
1:E:136:LEU:HB3	1:E:247:MET:HE3	2.03	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	278/261 (106%)	267 (96%)	10 (4%)	1 (0%)	34	17
1	B	276/261 (106%)	266 (96%)	9 (3%)	1 (0%)	34	17
1	C	274/261 (105%)	266 (97%)	7 (3%)	1 (0%)	34	17
1	D	272/261 (104%)	264 (97%)	7 (3%)	1 (0%)	34	17
1	E	275/261 (105%)	266 (97%)	8 (3%)	1 (0%)	34	17
1	F	277/261 (106%)	269 (97%)	7 (2%)	1 (0%)	34	17
All	All	1652/1566 (106%)	1598 (97%)	48 (3%)	6 (0%)	34	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	132	THR
1	A	132	THR
1	B	132	THR
1	D	132	THR
1	F	132	THR
1	C	132	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/224 (108%)	239 (99%)	3 (1%)	71	56
1	B	241/224 (108%)	237 (98%)	4 (2%)	60	42
1	C	239/224 (107%)	235 (98%)	4 (2%)	60	42
1	D	237/224 (106%)	233 (98%)	4 (2%)	60	42
1	E	240/224 (107%)	238 (99%)	2 (1%)	81	72
1	F	242/224 (108%)	238 (98%)	4 (2%)	60	42
All	All	1441/1344 (107%)	1420 (98%)	21 (2%)	62	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	140	TYR
1	A	154	PHE
1	B	71	LEU
1	B	73	SER
1	B	154	PHE
1	B	255	LYS
1	C	23	ARG
1	C	76	ARG
1	C	140	TYR
1	C	154	PHE
1	D	73	SER
1	D	140	TYR
1	D	154	PHE
1	D	235	ARG
1	E	23	ARG
1	E	154	PHE
1	F	140	TYR
1	F	154	PHE
1	F	251	LEU
1	F	255	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	ASN
1	B	69	HIS
1	C	7	ASN
1	C	244	GLN
1	D	66	HIS
1	E	244	GLN
1	F	261	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	KGJ	C	302[A]	-	28,33,57	1.07	2 (7%)	35,52,85	1.35	3 (8%)
2	KGJ	D	302[A]	-	45,57,57	1.67	3 (6%)	57,85,85	1.37	6 (10%)
2	KGJ	F	301[A]	-	45,57,57	1.43	3 (6%)	57,85,85	1.65	13 (22%)
2	KGJ	D	302[B]	-	45,57,57	1.69	3 (6%)	57,85,85	1.27	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KGJ	E	301[B]	-	45,57,57	1.56	5 (11%)	57,85,85	1.07	4 (7%)
2	KGJ	E	302[A]	-	28,33,57	1.11	1 (3%)	35,52,85	1.38	6 (17%)
8	PGE	F	304	5	9,9,9	0.29	0	8,8,8	0.24	0
2	KGJ	A	301	-	45,57,57	1.69	5 (11%)	57,85,85	1.62	13 (22%)
2	KGJ	F	301[B]	-	45,57,57	1.49	2 (4%)	57,85,85	1.48	10 (17%)
2	KGJ	F	302[A]	-	28,33,57	1.13	2 (7%)	35,52,85	1.60	6 (17%)
2	KGJ	C	301	-	45,57,57	1.56	4 (8%)	57,85,85	1.19	5 (8%)
4	PEG	C	304	-	6,6,6	0.17	0	5,5,5	0.16	0
6	PG4	C	305	5	12,12,12	0.29	0	11,11,11	0.25	0
7	IMD	D	303	-	3,5,5	0.27	0	4,5,5	0.67	0
4	PEG	B	302	-	6,6,6	0.19	0	5,5,5	0.12	0
2	KGJ	B	301	-	45,57,57	1.77	5 (11%)	57,85,85	3.07	18 (31%)
2	KGJ	E	301[A]	-	45,57,57	1.52	5 (11%)	57,85,85	1.52	7 (12%)

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	KGJ	C	302[A]	-	-	7/17/37/75	0/3/3/3
2	KGJ	D	302[A]	-	-	5/51/75/75	0/3/3/3
2	KGJ	F	301[A]	-	-	6/51/75/75	0/3/3/3
2	KGJ	D	302[B]	-	-	1/51/75/75	0/3/3/3
2	KGJ	E	301[B]	-	-	3/51/75/75	0/3/3/3
2	KGJ	E	302[A]	-	-	4/17/37/75	0/3/3/3
8	PGE	F	304	5	-	1/7/7/7	-
2	KGJ	A	301	-	-	1/51/75/75	0/3/3/3
2	KGJ	F	301[B]	-	-	6/51/75/75	0/3/3/3
2	KGJ	F	302[A]	-	-	4/17/37/75	0/3/3/3
2	KGJ	C	301	-	-	0/51/75/75	0/3/3/3
4	PEG	C	304	-	-	2/4/4/4	-
6	PG4	C	305	5	-	3/10/10/10	-
7	IMD	D	303	-	-	-	0/1/1/1
4	PEG	B	302	-	-	2/4/4/4	-
2	KGJ	B	301	-	-	9/51/75/75	0/3/3/3
2	KGJ	E	301[A]	-	-	4/51/75/75	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302[A]	KGJ	CS1-N	9.21	1.49	1.33
2	D	302[B]	KGJ	CS1-N	9.21	1.49	1.33
2	B	301	KGJ	CS1-N	9.18	1.49	1.33
2	C	301	KGJ	CS1-N	8.17	1.47	1.33
2	A	301	KGJ	CS1-N	8.12	1.47	1.33
2	E	301[A]	KGJ	CS1-N	8.10	1.47	1.33
2	E	301[B]	KGJ	CS1-N	8.10	1.47	1.33
2	F	301[A]	KGJ	CS1-N	7.78	1.47	1.33
2	F	301[B]	KGJ	CS1-N	7.78	1.47	1.33
2	A	301	KGJ	O4'-C1'	4.96	1.48	1.41
2	D	302[A]	KGJ	O4'-C1'	3.01	1.45	1.41
2	B	301	KGJ	O4'-C1'	2.99	1.45	1.41
2	A	301	KGJ	P3-O3'	2.93	1.64	1.59
2	E	302[A]	KGJ	C5-C4	2.77	1.48	1.40
2	D	302[B]	KGJ	O4'-C1'	2.77	1.44	1.41
2	F	301[B]	KGJ	C5-C4	2.75	1.48	1.40
2	C	301	KGJ	P3-O3'	2.63	1.64	1.59
2	F	302[A]	KGJ	C5-C4	2.62	1.47	1.40
2	A	301	KGJ	C5-C4	2.58	1.47	1.40
2	B	301	KGJ	CS3-CS2	2.54	1.54	1.49
2	F	302[A]	KGJ	P2-O7	2.52	1.64	1.54
2	C	302[A]	KGJ	C5-C4	2.49	1.47	1.40
2	B	301	KGJ	OS1-CS1	-2.39	1.19	1.23
2	E	301[A]	KGJ	C5-C4	2.33	1.47	1.40
2	C	301	KGJ	C5-C4	2.31	1.47	1.40
2	A	301	KGJ	C2-N1	2.28	1.38	1.33
2	E	301[B]	KGJ	C5-C4	2.25	1.46	1.40
2	E	301[A]	KGJ	OS1-CS1	-2.25	1.19	1.23
2	E	301[B]	KGJ	OS1-CS1	-2.25	1.19	1.23
2	C	302[A]	KGJ	C2-N3	2.24	1.35	1.32
2	C	301	KGJ	C5-N7	-2.15	1.31	1.39
2	F	301[A]	KGJ	C5-C4	2.11	1.46	1.40
2	D	302[A]	KGJ	P3-O33	-2.05	1.46	1.54
2	B	301	KGJ	CP8-CPA	2.05	1.58	1.53
2	D	302[B]	KGJ	C5-C4	2.04	1.46	1.40
2	E	301[A]	KGJ	CS3-CS2	2.04	1.53	1.49
2	E	301[B]	KGJ	CS3-CS2	2.04	1.53	1.49
2	F	301[A]	KGJ	C2'-C1'	-2.04	1.50	1.53
2	E	301[A]	KGJ	CP2-NP1	-2.01	1.41	1.46
2	E	301[B]	KGJ	CP2-NP1	-2.01	1.41	1.46

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	KGJ	CP8-CPA-CPB	-12.23	88.29	108.23
2	B	301	KGJ	CP9-CPA-CPB	9.82	124.26	108.23
2	B	301	KGJ	CP8-CPA-CP7	-9.67	92.06	108.82
2	B	301	KGJ	CP8-CPA-CP9	-7.25	94.39	109.17
2	E	301[A]	KGJ	P2-O6-P1	-5.77	113.03	132.83
2	F	301[A]	KGJ	P2-O6-P1	-5.21	114.94	132.83
2	D	302[A]	KGJ	P2-O6-P1	-4.81	116.34	132.83
2	F	301[B]	KGJ	O5'-C5'-C4'	4.39	124.10	108.99
2	A	301	KGJ	N3-C2-N1	-4.21	122.09	128.68
2	F	301[A]	KGJ	N3-C2-N1	-4.15	122.20	128.68
2	F	302[A]	KGJ	N3-C2-N1	-4.12	122.24	128.68
2	B	301	KGJ	N3-C2-N1	-4.09	122.28	128.68
2	C	302[A]	KGJ	N3-C2-N1	-3.98	122.46	128.68
2	D	302[A]	KGJ	CP9-CPA-CP7	3.92	115.61	108.82
2	D	302[B]	KGJ	CP9-CPA-CP7	3.92	115.61	108.82
2	E	301[A]	KGJ	N3-C2-N1	-3.88	122.62	128.68
2	B	301	KGJ	P2-O6-P1	-3.87	119.53	132.83
2	F	302[A]	KGJ	P1-O6-P2	-3.87	119.56	132.83
2	A	301	KGJ	O4'-C1'-C2'	3.86	112.57	106.93
2	A	301	KGJ	C1'-N9-C4	-3.75	120.05	126.64
2	D	302[A]	KGJ	N3-C2-N1	-3.72	122.87	128.68
2	F	302[A]	KGJ	C1'-N9-C4	-3.70	120.14	126.64
2	B	301	KGJ	OP3-CP7-CPA	-3.68	101.59	110.25
2	F	302[A]	KGJ	O22-P2-O6	3.60	116.70	104.64
2	E	302[A]	KGJ	N3-C2-N1	-3.51	123.19	128.68
2	B	301	KGJ	CP9-CPA-CP7	3.22	114.41	108.82
2	F	301[A]	KGJ	O7-P2-O21	-3.18	96.64	109.07
2	F	301[B]	KGJ	O7-P2-O21	-3.18	96.64	109.07
2	B	301	KGJ	CP5-CP4-CP3	-3.15	107.12	112.36
2	E	302[A]	KGJ	P1-O6-P2	-3.12	122.14	132.83
2	F	301[B]	KGJ	N3-C2-N1	-3.07	123.87	128.68
2	B	301	KGJ	C5-C6-N6	-3.04	115.72	120.35
2	E	301[B]	KGJ	N3-C2-N1	-2.99	124.00	128.68
2	E	301[A]	KGJ	CP5-CP4-CP3	-2.97	107.40	112.36
2	E	301[B]	KGJ	CP5-CP4-CP3	-2.97	107.40	112.36
2	A	301	KGJ	O5'-P1-O12	-2.91	97.71	109.07
2	E	301[A]	KGJ	C2-N1-C6	2.88	123.68	118.75
2	A	301	KGJ	C2-N1-C6	2.86	123.64	118.75
2	E	302[A]	KGJ	C4-C5-N7	-2.86	106.42	109.40
2	F	301[A]	KGJ	C1'-N9-C4	-2.85	121.64	126.64
2	F	302[A]	KGJ	C2-N1-C6	2.80	123.54	118.75
2	A	301	KGJ	O3'-P3-O31	-2.75	98.78	109.39
2	D	302[B]	KGJ	N3-C2-N1	-2.75	124.39	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301[A]	KGJ	OP1-CP3-CP4	-2.74	117.00	122.02
2	F	301[B]	KGJ	OP1-CP3-CP4	-2.74	117.00	122.02
2	C	301	KGJ	N3-C2-N1	-2.69	124.47	128.68
2	A	301	KGJ	N6-C6-N1	2.68	124.14	118.57
2	B	301	KGJ	O7-CPB-CPA	-2.67	106.25	110.55
2	D	302[B]	KGJ	O4'-C4'-C5'	2.64	118.06	109.37
2	E	301[A]	KGJ	O32-P3-O3'	2.63	117.76	105.99
2	D	302[A]	KGJ	N6-C6-N1	2.62	124.01	118.57
2	A	301	KGJ	O7-CPB-CPA	-2.61	106.35	110.55
2	D	302[B]	KGJ	N6-C6-N1	2.59	123.95	118.57
2	C	302[A]	KGJ	P1-O6-P2	-2.58	123.96	132.83
2	B	301	KGJ	C1'-N9-C4	-2.58	122.11	126.64
2	F	301[A]	KGJ	C2-N1-C6	2.56	123.13	118.75
2	C	301	KGJ	P2-O6-P1	-2.56	124.05	132.83
2	E	301[A]	KGJ	N6-C6-N1	2.52	123.81	118.57
2	D	302[A]	KGJ	CP2-CP1-N	-2.50	103.14	111.44
2	D	302[B]	KGJ	CP2-CP1-N	-2.50	103.14	111.44
2	F	302[A]	KGJ	C4-C5-N7	-2.49	106.81	109.40
2	B	301	KGJ	OS1-CS1-CS2	-2.47	117.29	120.41
2	F	301[A]	KGJ	CP5-CP4-CP3	-2.45	108.27	112.36
2	F	301[B]	KGJ	CP5-CP4-CP3	-2.45	108.27	112.36
2	C	301	KGJ	CP7-CP6-NP2	2.45	121.45	116.58
2	C	301	KGJ	C2-N1-C6	2.44	122.93	118.75
2	C	302[A]	KGJ	C2-N1-C6	2.44	122.92	118.75
2	B	301	KGJ	O5'-C5'-C4'	-2.41	100.68	108.99
2	F	301[A]	KGJ	C4-C5-N7	-2.35	106.95	109.40
2	F	301[B]	KGJ	C2-N1-C6	2.34	122.76	118.75
2	F	301[B]	KGJ	C4-C5-N7	-2.32	106.98	109.40
2	A	301	KGJ	O33-P3-O31	2.31	119.72	110.68
2	E	301[A]	KGJ	OS1-CS1-CS2	-2.30	117.51	120.41
2	E	301[B]	KGJ	OS1-CS1-CS2	-2.30	117.51	120.41
2	F	301[A]	KGJ	O4'-C4'-C5'	-2.28	101.87	109.37
2	A	301	KGJ	O2'-C2'-C3'	2.26	117.59	111.17
2	D	302[A]	KGJ	O3'-C3'-C2'	-2.24	103.57	111.68
2	F	301[A]	KGJ	CP8-CPA-CPB	-2.23	104.60	108.23
2	F	301[B]	KGJ	CP8-CPA-CPB	-2.23	104.60	108.23
2	B	301	KGJ	O3'-C3'-C2'	-2.23	103.62	111.68
2	D	302[B]	KGJ	C2'-C3'-C4'	2.20	107.13	103.22
2	A	301	KGJ	O33-P3-O32	2.19	116.00	107.64
2	C	301	KGJ	CP5-CP4-CP3	-2.17	108.73	112.36
2	F	301[A]	KGJ	O5'-P1-O12	-2.17	100.57	109.07
2	A	301	KGJ	CP5-CP4-CP3	-2.12	108.82	112.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301[A]	KGJ	O33-P3-O32	2.11	115.70	107.64
2	A	301	KGJ	CP2-CP1-N	-2.11	104.44	111.44
2	B	301	KGJ	CP7-CP6-NP2	-2.11	112.39	116.58
2	E	302[A]	KGJ	O7-P2-O21	-2.09	102.52	110.68
2	F	301[B]	KGJ	O4'-C1'-C2'	-2.07	103.90	106.93
2	F	301[A]	KGJ	CP8-CPA-CP7	2.07	112.41	108.82
2	F	301[B]	KGJ	CP8-CPA-CP7	2.07	112.41	108.82
2	E	302[A]	KGJ	O7-P2-O6	2.06	111.55	104.64
2	E	301[B]	KGJ	C4-C5-N7	-2.06	107.25	109.40
2	B	301	KGJ	C2'-C3'-C4'	2.06	106.87	103.22
2	B	301	KGJ	O33-P3-O31	2.05	118.70	110.68
2	E	302[A]	KGJ	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	KGJ	C3'-O3'-P3-O33
2	B	301	KGJ	C5'-O5'-P1-O12
2	B	301	KGJ	CP7-CPA-CPB-O7
2	B	301	KGJ	OP3-CP7-CPA-CP9
2	B	301	KGJ	CP6-CP7-CPA-CP9
2	D	302[A]	KGJ	C5'-O5'-P1-O12
2	D	302[A]	KGJ	C5'-O5'-P1-O6
2	E	301[A]	KGJ	C5'-O5'-P1-O12
2	E	301[B]	KGJ	P1-O6-P2-O7
2	F	301[A]	KGJ	C5'-O5'-P1-O6
2	F	301[B]	KGJ	C5'-O5'-P1-O11
2	F	301[B]	KGJ	C5'-O5'-P1-O12
2	F	302[A]	KGJ	C5'-O5'-P1-O11
2	F	302[A]	KGJ	C5'-O5'-P1-O12
4	C	304	PEG	O2-C3-C4-O4
2	F	301[B]	KGJ	O4'-C4'-C5'-O5'
4	B	302	PEG	O1-C1-C2-O2
2	C	302[A]	KGJ	C4'-C3'-O3'-P3
2	E	301[A]	KGJ	C4'-C3'-O3'-P3
2	D	302[A]	KGJ	CP4-CP5-NP2-CP6
2	D	302[B]	KGJ	CP4-CP5-NP2-CP6
2	C	302[A]	KGJ	C2'-C3'-O3'-P3
2	E	301[A]	KGJ	C2'-C3'-O3'-P3
4	B	302	PEG	O2-C3-C4-O4
4	C	304	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	302[A]	KGJ	O4'-C4'-C5'-O5'
2	D	302[A]	KGJ	C3'-C4'-C5'-O5'
2	E	301[A]	KGJ	P1-O6-P2-O7
2	B	301	KGJ	C5'-O5'-P1-O6
2	C	302[A]	KGJ	C3'-O3'-P3-O33
2	E	302[A]	KGJ	C5'-O5'-P1-O6
2	F	301[B]	KGJ	C5'-O5'-P1-O6
2	F	301[A]	KGJ	P2-O6-P1-O11
2	E	302[A]	KGJ	C5'-O5'-P1-O12
2	F	301[A]	KGJ	C5'-O5'-P1-O11
2	C	302[A]	KGJ	C3'-C4'-C5'-O5'
2	F	302[A]	KGJ	C4'-C5'-O5'-P1
2	F	301[B]	KGJ	C3'-C4'-C5'-O5'
2	B	301	KGJ	CP8-CPA-CPB-O7
2	C	302[A]	KGJ	O4'-C4'-C5'-O5'
2	A	301	KGJ	P2-O6-P1-O11
2	E	301[B]	KGJ	P2-O6-P1-O11
2	F	301[A]	KGJ	P1-O6-P2-O22
6	C	305	PG4	C4-C3-O2-C2
2	E	302[A]	KGJ	C4'-C3'-O3'-P3
8	F	304	PGE	O3-C5-C6-O4
2	B	301	KGJ	C3'-C4'-C5'-O5'
2	C	302[A]	KGJ	P1-O6-P2-O21
6	C	305	PG4	O1-C1-C2-O2
2	E	302[A]	KGJ	C2'-C3'-O3'-P3
2	F	301[A]	KGJ	CP4-CP5-NP2-CP6
2	F	301[B]	KGJ	CP4-CP5-NP2-CP6
6	C	305	PG4	C3-C4-O3-C5
2	B	301	KGJ	O4'-C4'-C5'-O5'
2	C	302[A]	KGJ	P1-O6-P2-O22
2	F	302[A]	KGJ	C5'-O5'-P1-O6
2	E	301[B]	KGJ	P2-O6-P1-O12
2	F	301[A]	KGJ	P1-O6-P2-O21

There are no ring outliers.

10 monomers are involved in 27 short contacts:

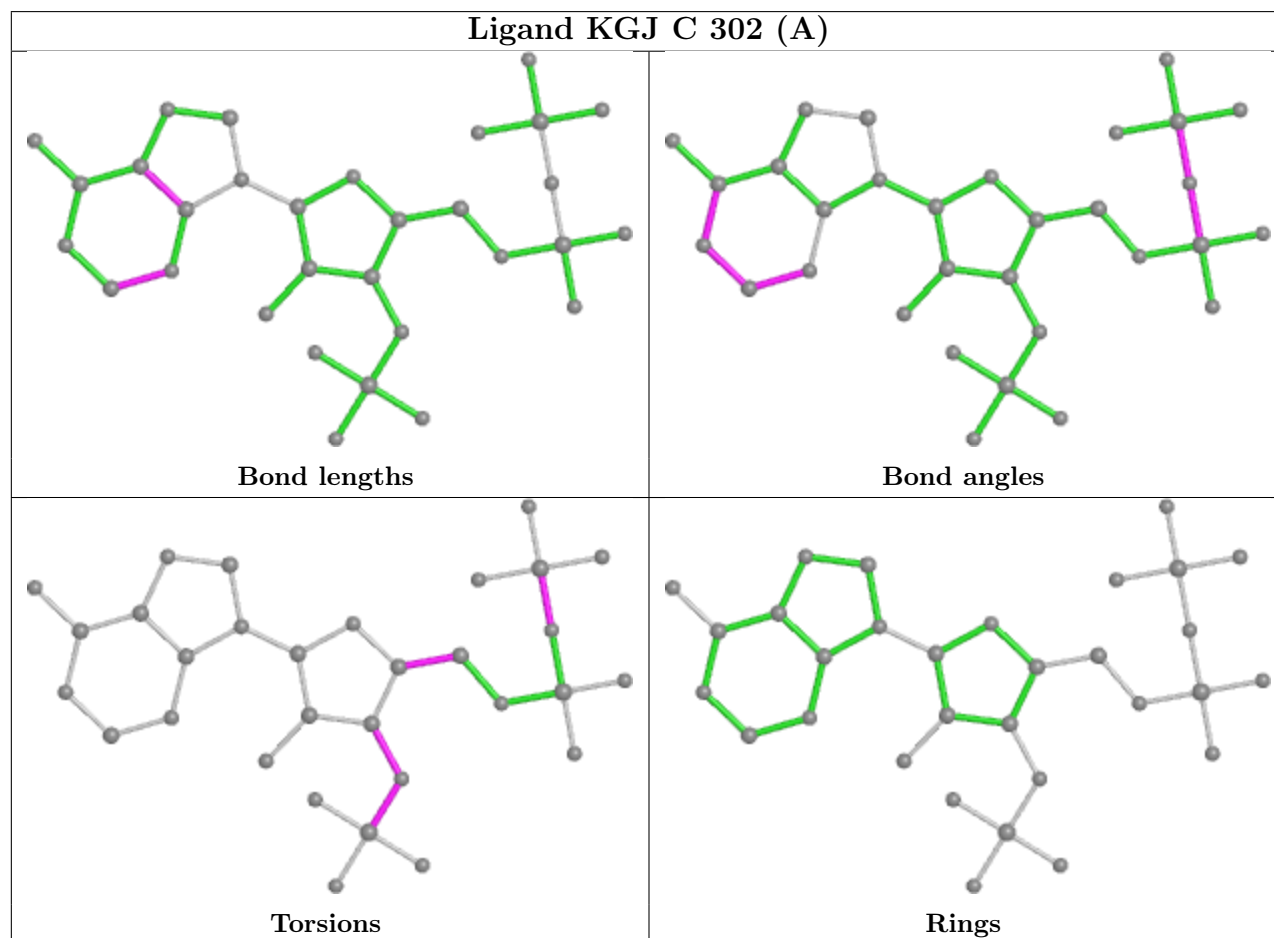
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	302[A]	KGJ	3	0
2	F	301[A]	KGJ	1	0
2	E	302[A]	KGJ	9	0
2	A	301	KGJ	1	0

Continued on next page...

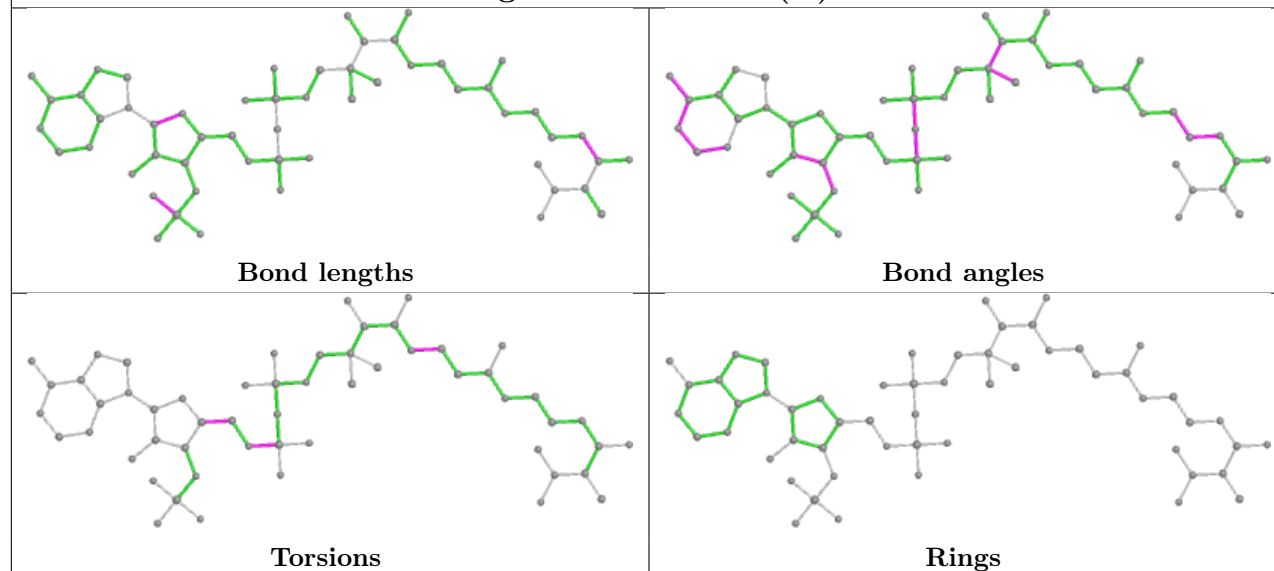
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301[B]	KGJ	1	0
2	F	302[A]	KGJ	7	0
2	C	301	KGJ	1	0
4	C	304	PEG	1	0
7	D	303	IMD	2	0
2	B	301	KGJ	1	0

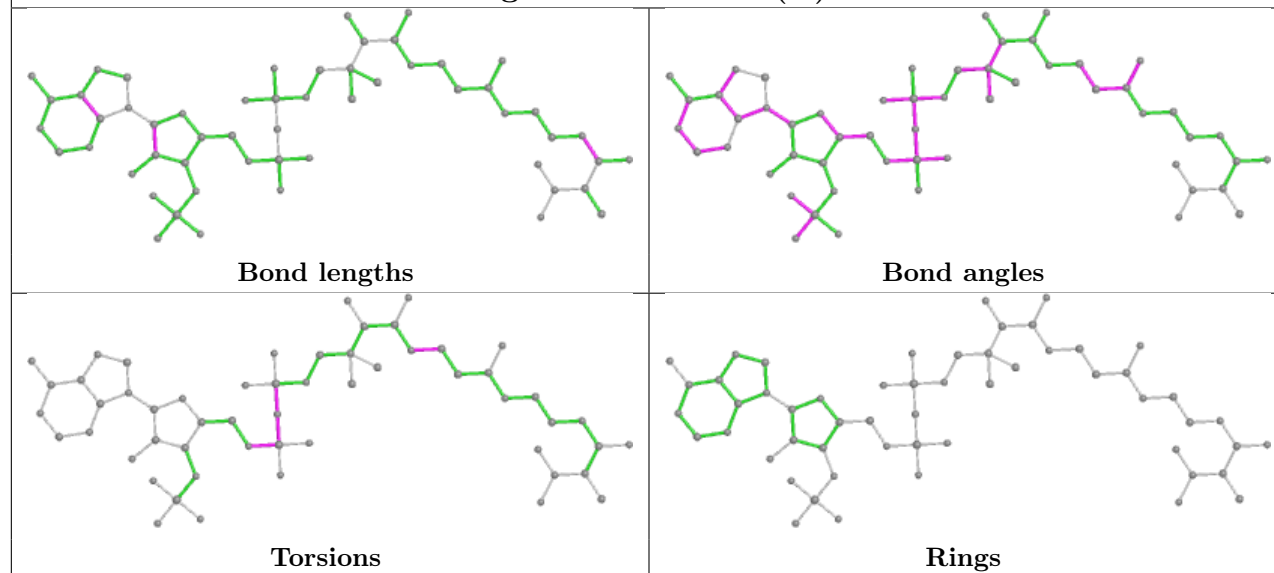
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



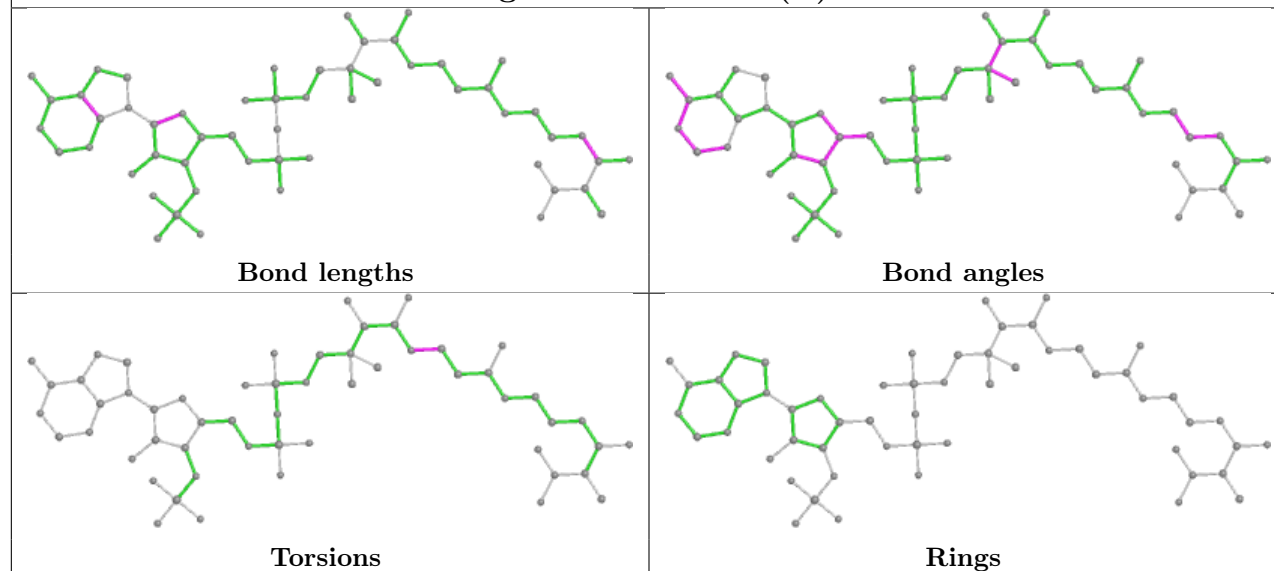
Ligand KGJ D 302 (A)



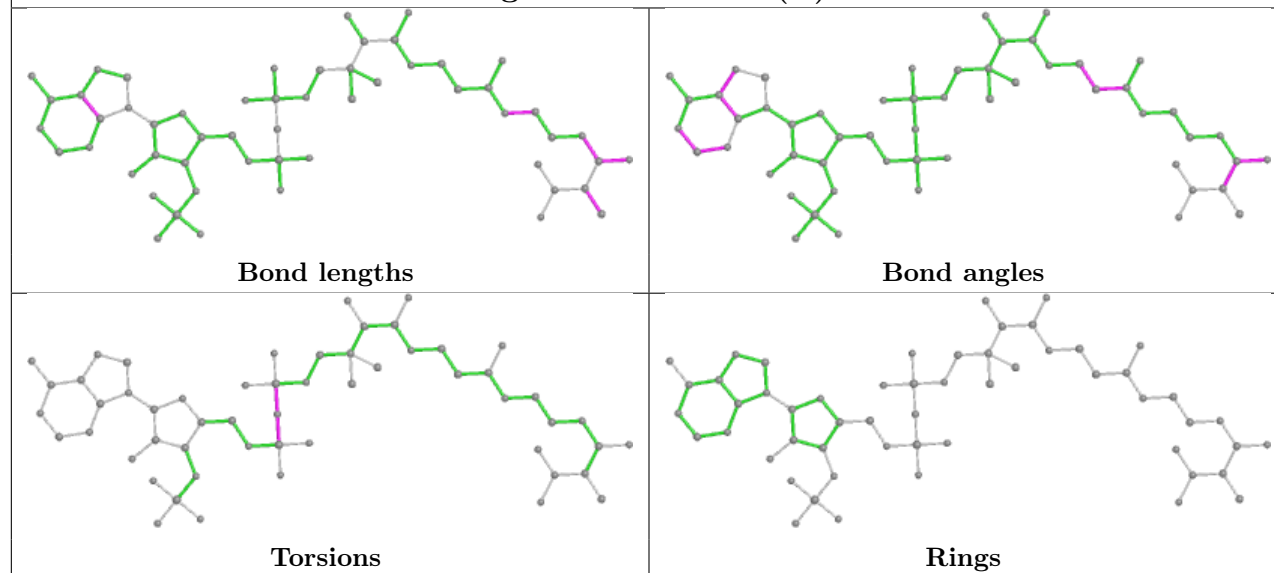
Ligand KGJ F 301 (A)



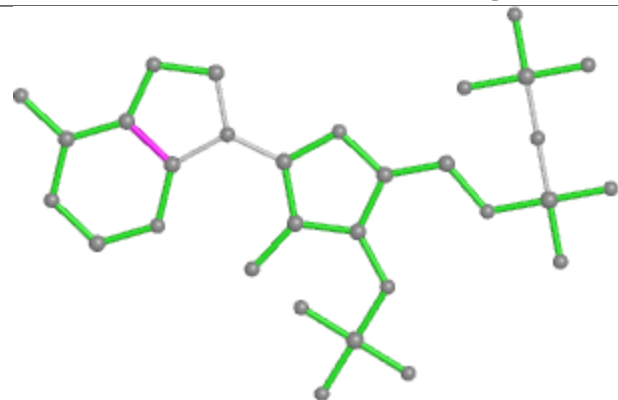
Ligand KGJ D 302 (B)



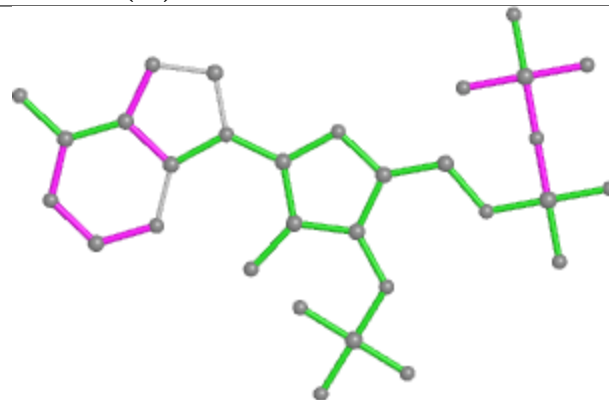
Ligand KGJ E 301 (B)



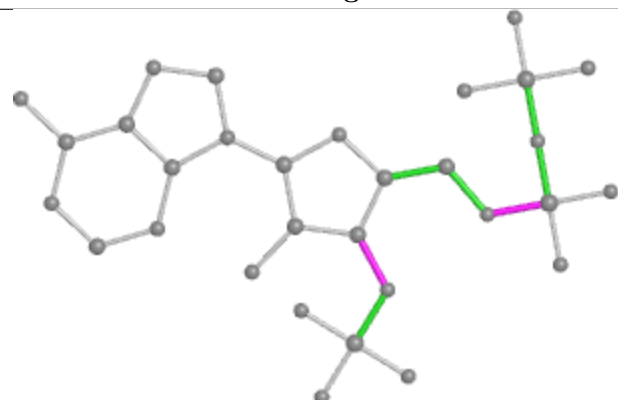
Ligand KGJ E 302 (A)



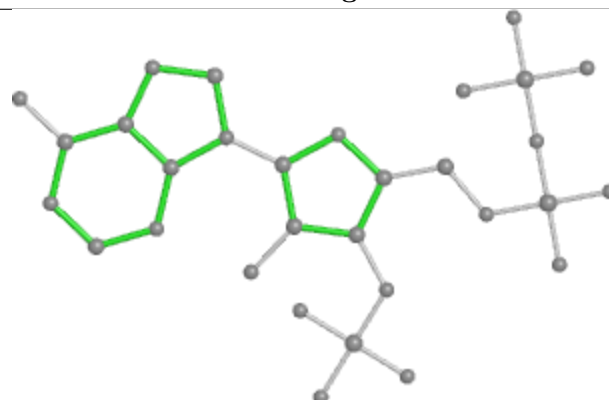
Bond lengths



Bond angles

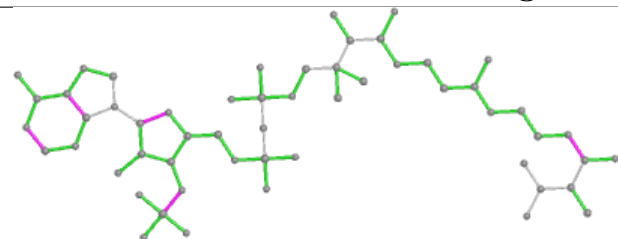


Torsions

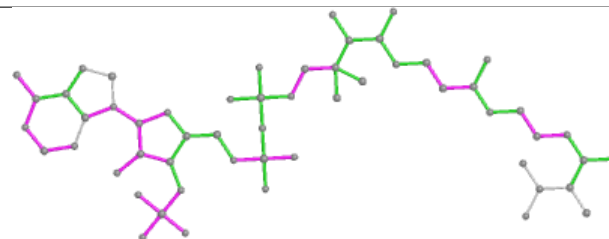


Rings

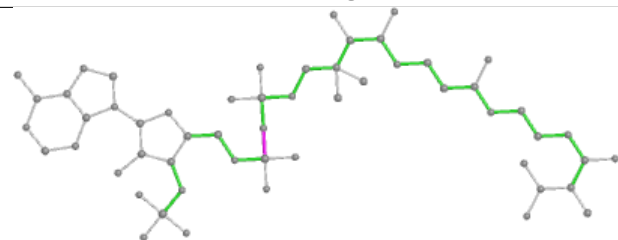
Ligand KGJ A 301



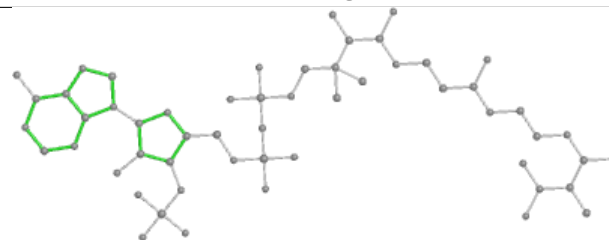
Bond lengths



Bond angles

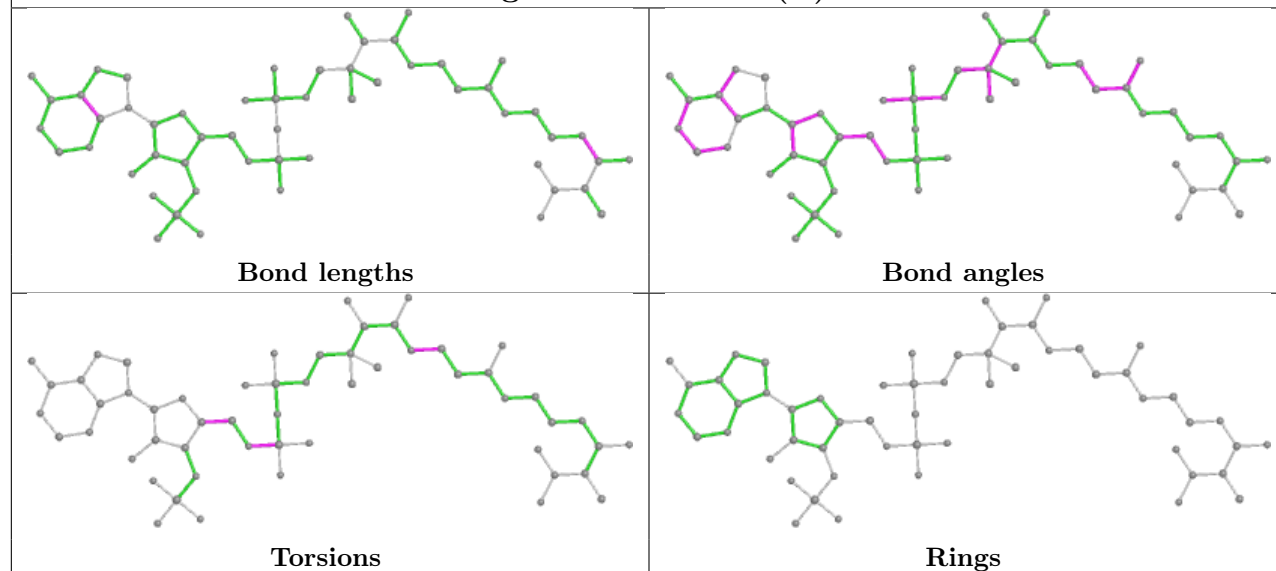


Torsions

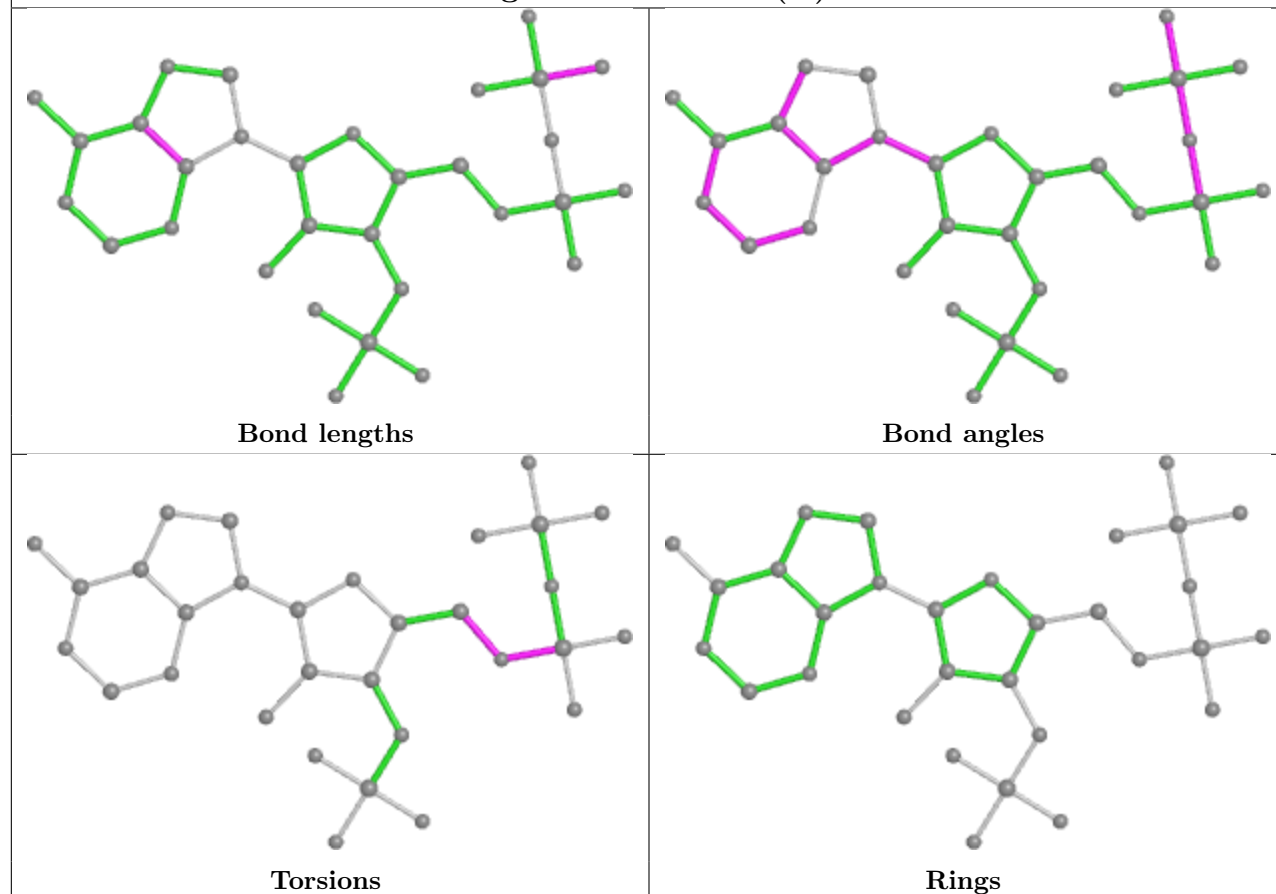


Rings

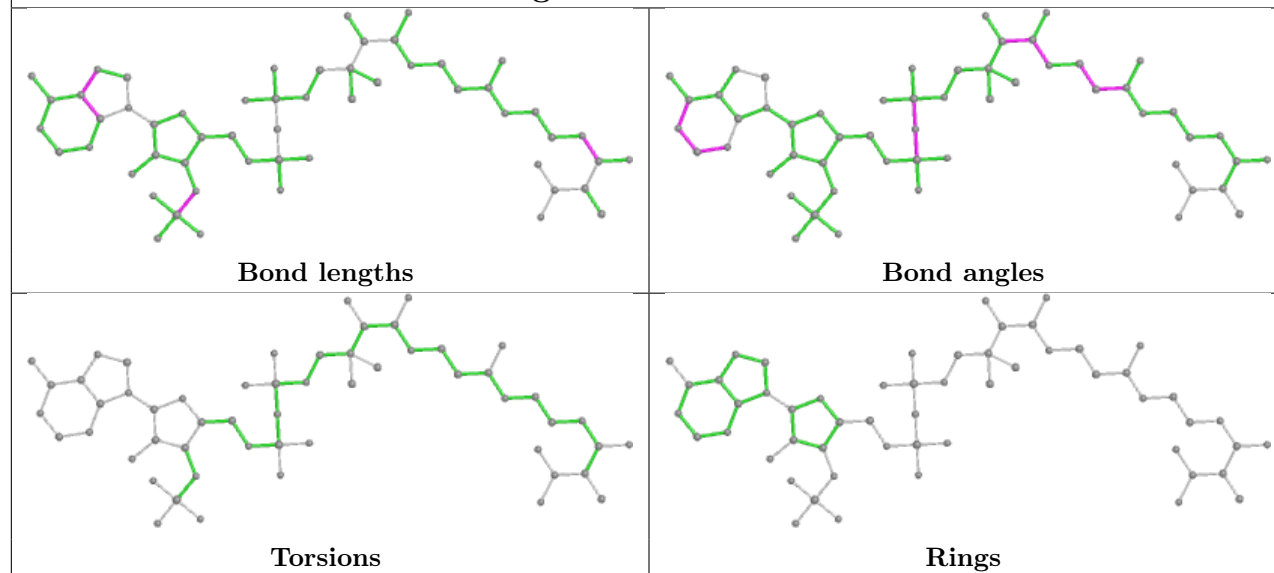
Ligand KGJ F 301 (B)



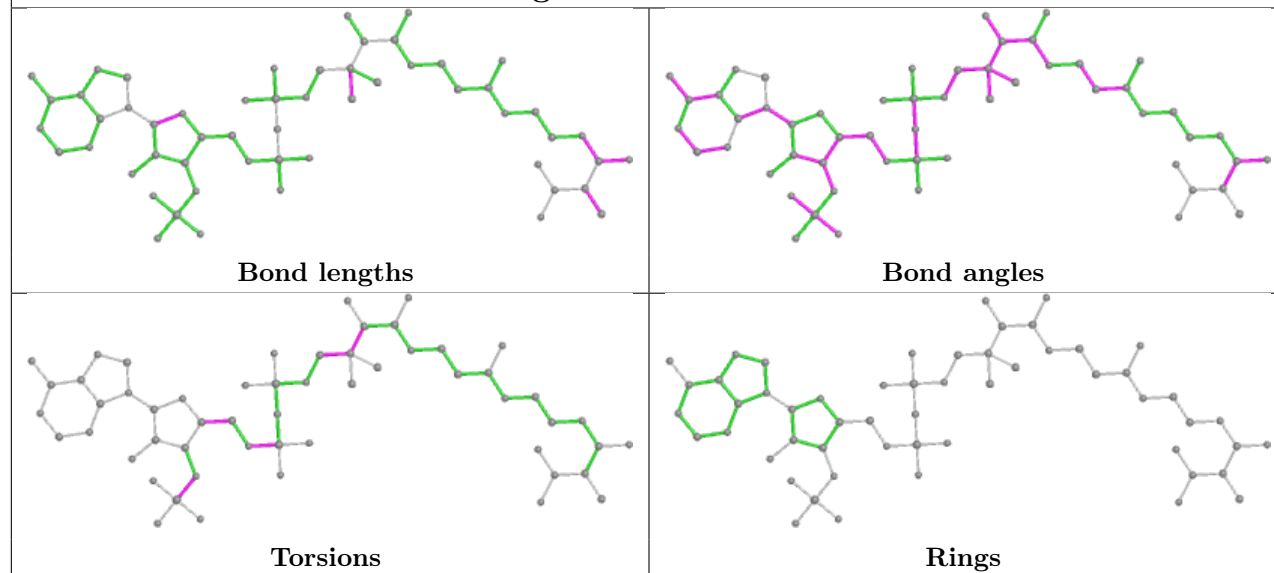
Ligand KGJ F 302 (A)

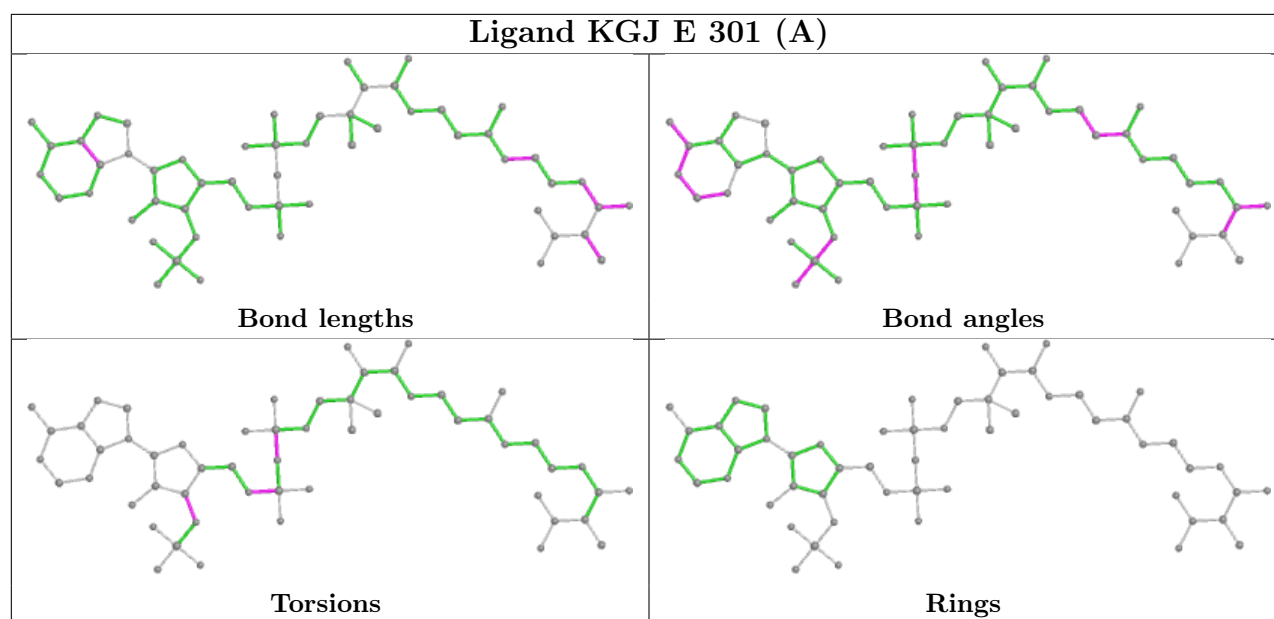


Ligand KGJ C 301



Ligand KGJ B 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	260/261 (99%)	-0.44	2 (0%) 86 90	13, 18, 32, 51	0
1	B	260/261 (99%)	-0.21	6 (2%) 60 67	14, 20, 42, 87	0
1	C	260/261 (99%)	-0.28	6 (2%) 60 67	13, 18, 39, 112	0
1	D	260/261 (99%)	-0.36	4 (1%) 73 80	14, 19, 39, 81	0
1	E	260/261 (99%)	-0.27	7 (2%) 54 60	13, 19, 42, 97	0
1	F	260/261 (99%)	-0.32	6 (2%) 60 67	13, 20, 41, 71	0
All	All	1560/1566 (99%)	-0.31	31 (1%) 65 72	13, 19, 39, 112	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	GLY	8.9
1	E	73	SER	7.8
1	E	74	GLY	7.7
1	B	73	SER	6.4
1	C	75	GLY	6.1
1	C	73	SER	5.6
1	F	74	GLY	5.4
1	B	74	GLY	5.0
1	E	75	GLY	4.3
1	D	73	SER	4.1
1	F	251	LEU	3.8
1	D	251	LEU	3.8
1	B	71	LEU	3.8
1	D	2	ALA	3.5
1	C	72	PRO	3.3
1	F	253	LYS	2.9
1	E	71	LEU	2.8
1	D	74	GLY	2.8
1	E	251	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	250	PHE	2.5
1	A	2	ALA	2.5
1	C	251	LEU	2.5
1	B	2	ALA	2.4
1	E	2	ALA	2.4
1	A	23	ARG	2.4
1	B	72	PRO	2.3
1	F	23	ARG	2.2
1	C	23	ARG	2.2
1	B	251	LEU	2.1
1	F	72	PRO	2.0
1	E	248	ASN	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, 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	KGJ	C	302[A]	31/55	0.68	0.37	35,46,55,57	31
4	PEG	C	304	7/7	0.71	0.23	64,68,79,82	0
4	PEG	B	302	7/7	0.75	0.18	52,62,65,66	0
8	PGE	F	304	10/10	0.78	0.15	52,58,61,62	0
2	KGJ	F	302[A]	31/55	0.80	0.36	32,41,51,52	31
2	KGJ	E	302[A]	31/55	0.82	0.30	36,47,51,53	31
6	PG4	C	305	13/13	0.87	0.13	40,44,50,51	0
2	KGJ	F	301[B]	55/55	0.90	0.15	25,35,46,61	27
2	KGJ	B	301	55/55	0.90	0.12	27,43,64,72	0
2	KGJ	F	301[A]	55/55	0.90	0.15	23,39,48,61	27
2	KGJ	C	301	55/55	0.92	0.11	22,36,50,53	0

Continued on next page...

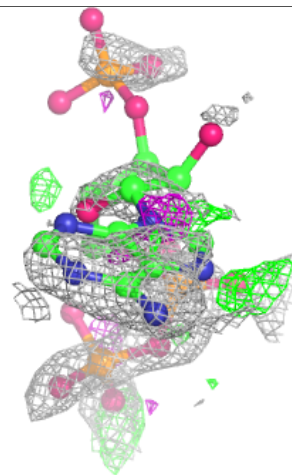
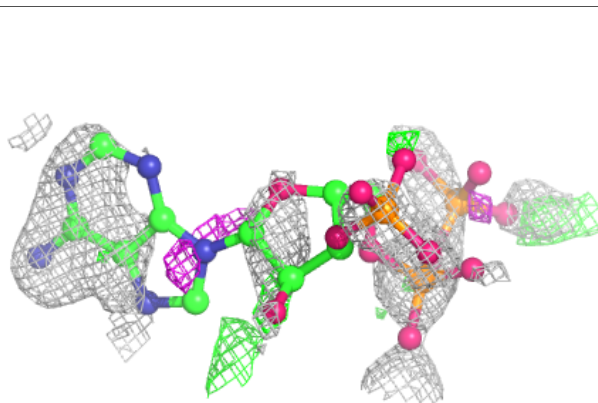
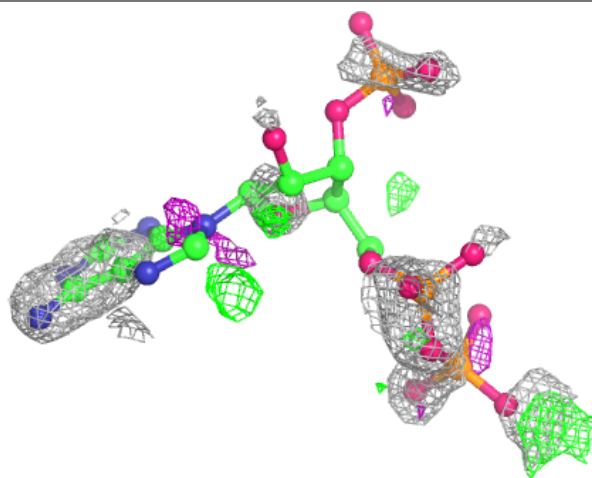
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	KGJ	E	301[B]	55/55	0.93	0.12	26,34,56,69	27
2	KGJ	A	301	55/55	0.93	0.09	19,32,51,61	0
2	KGJ	E	301[A]	55/55	0.93	0.12	22,36,56,69	27
2	KGJ	D	302[A]	55/55	0.94	0.12	19,30,45,57	27
2	KGJ	D	302[B]	55/55	0.94	0.12	25,34,45,57	27
3	NI	D	301	1/1	0.97	0.05	30,30,30,30	0
3	NI	A	302	1/1	0.98	0.06	31,31,31,31	0
7	IMD	D	303	5/5	0.98	0.07	24,26,28,28	0
5	K	F	303	1/1	0.98	0.11	44,44,44,44	0
5	K	C	303	1/1	0.99	0.11	40,40,40,40	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.

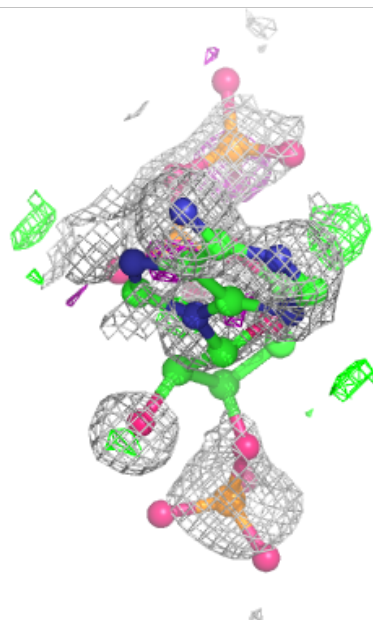
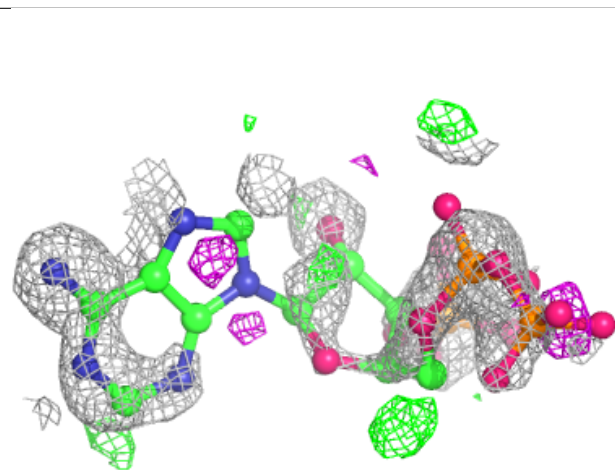
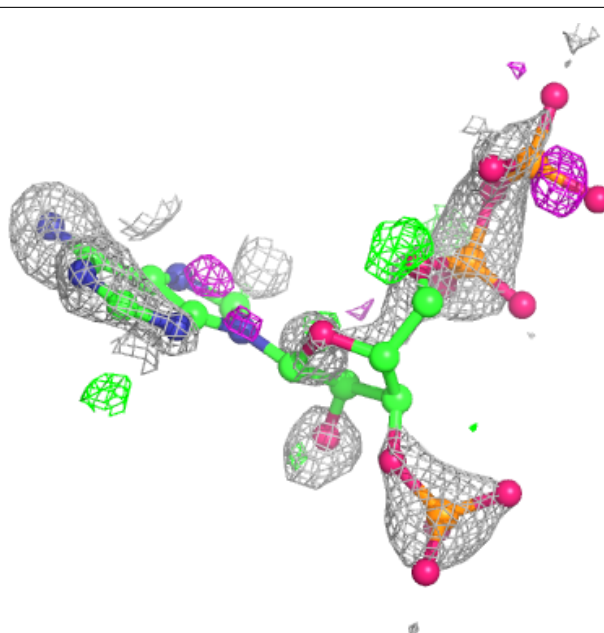
Electron density around KGJ C 302 (A):

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



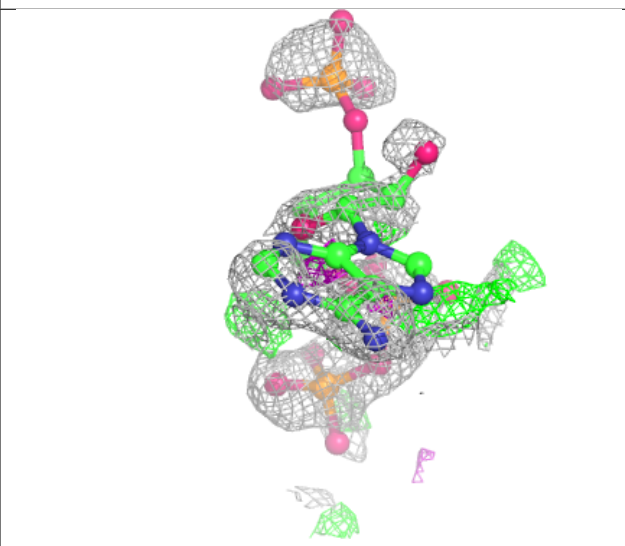
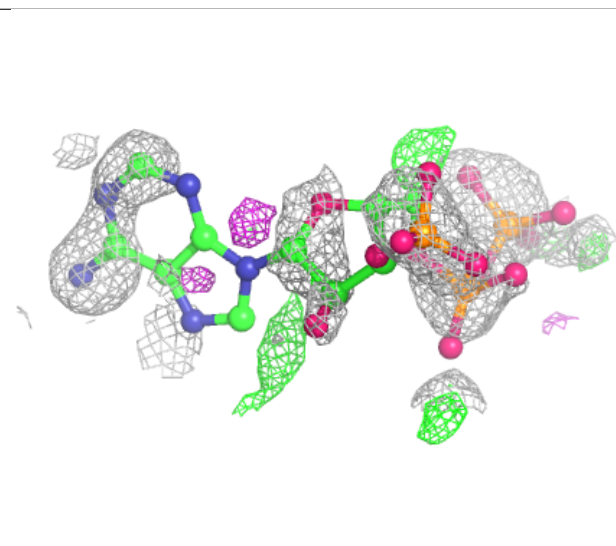
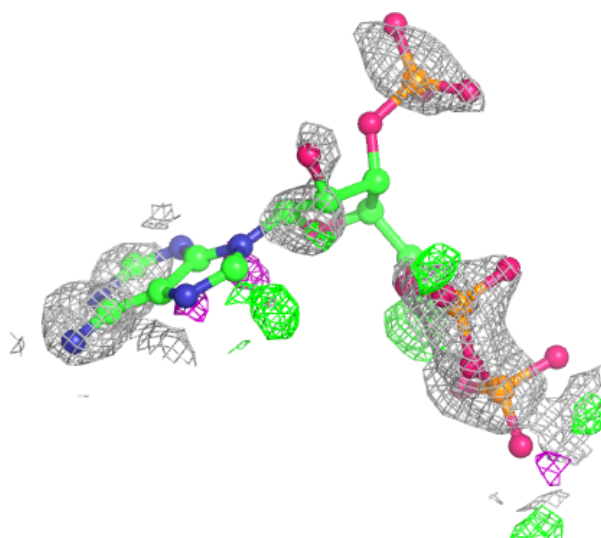
Electron density around KGJ F 302 (A):

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



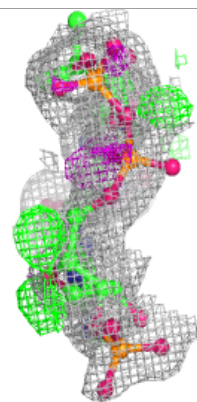
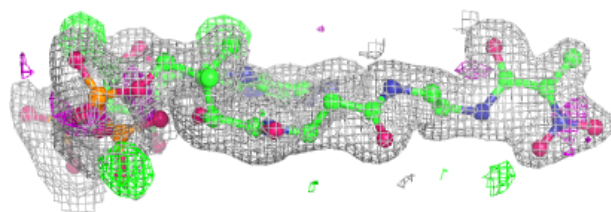
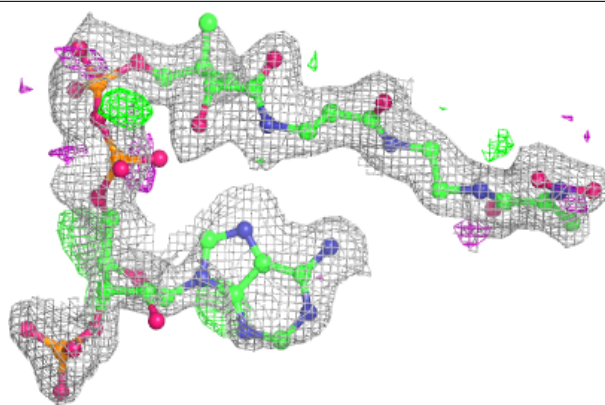
Electron density around KGJ E 302 (A):

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

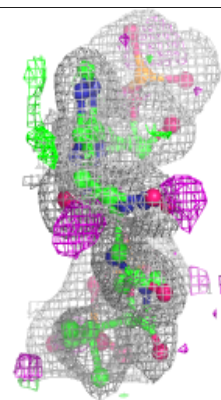
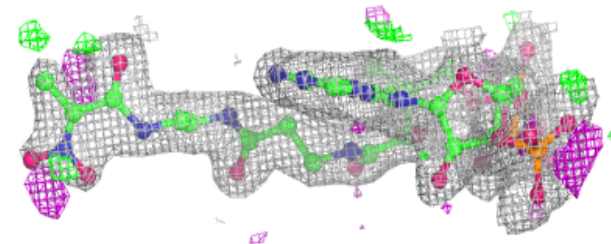
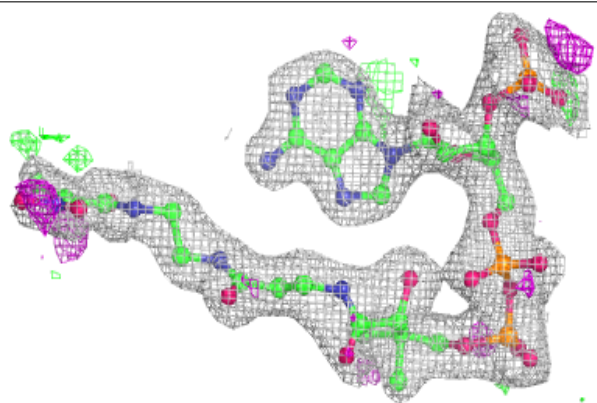


Electron density around KGJ F 301 (B):

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

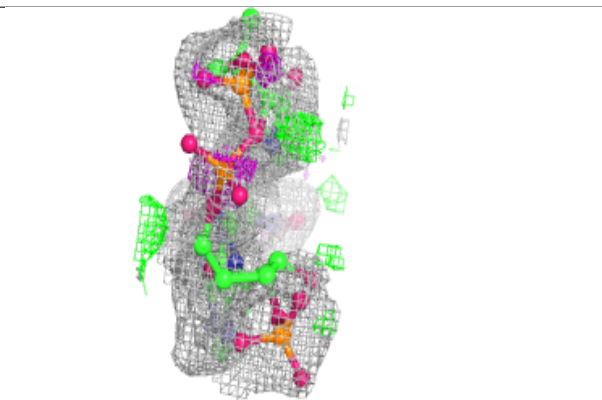
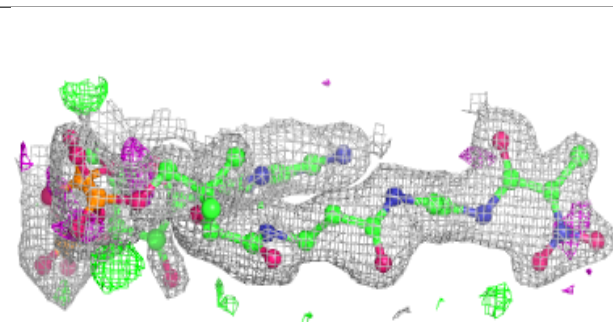
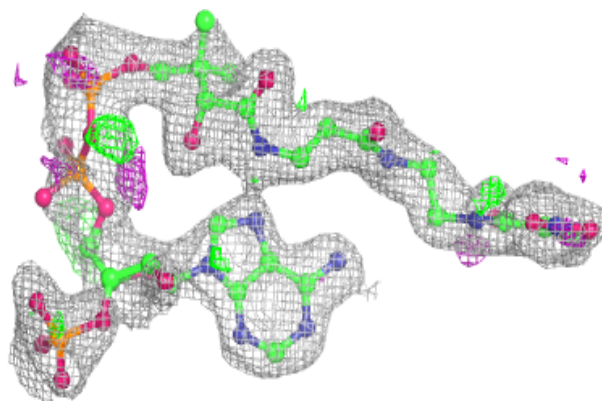
**Electron density around KGJ B 301:**

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

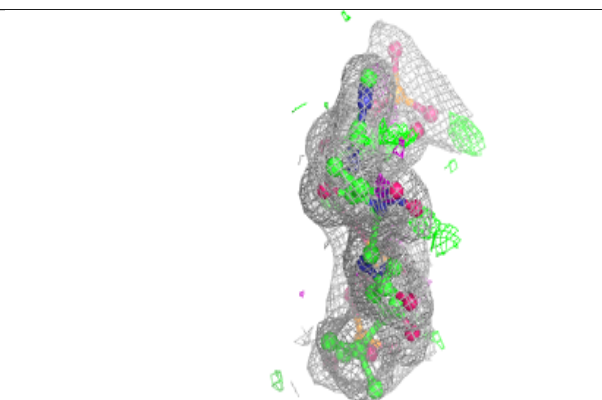
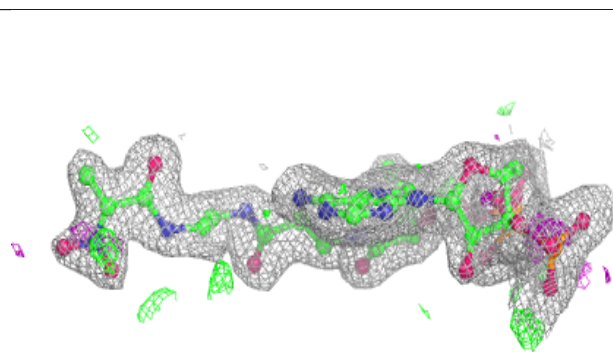
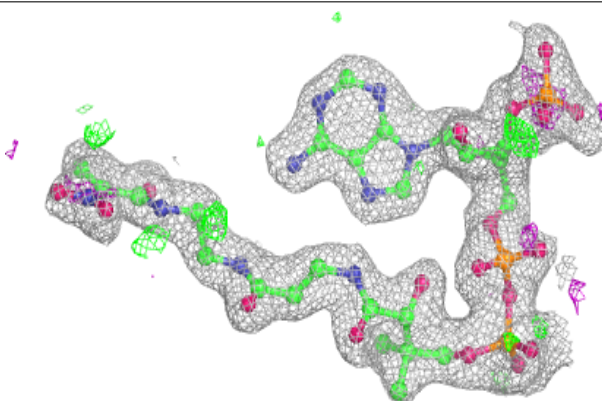


Electron density around KGJ F 301 (A):

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

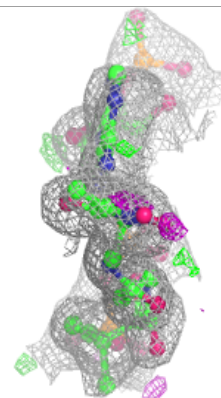
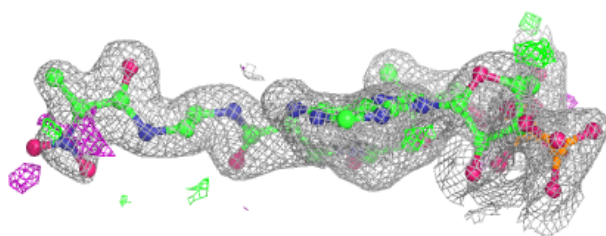
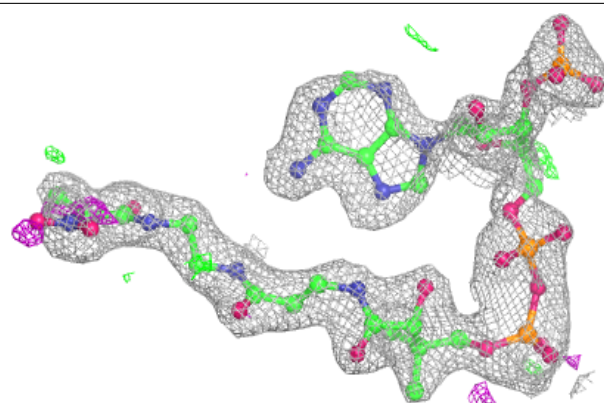
**Electron density around KGJ C 301:**

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

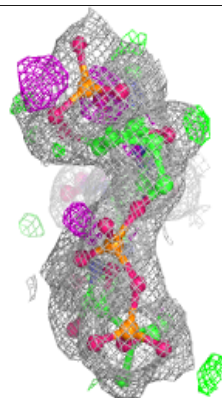
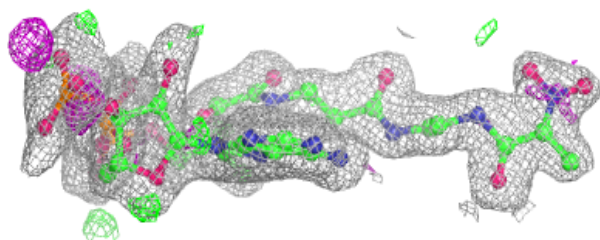
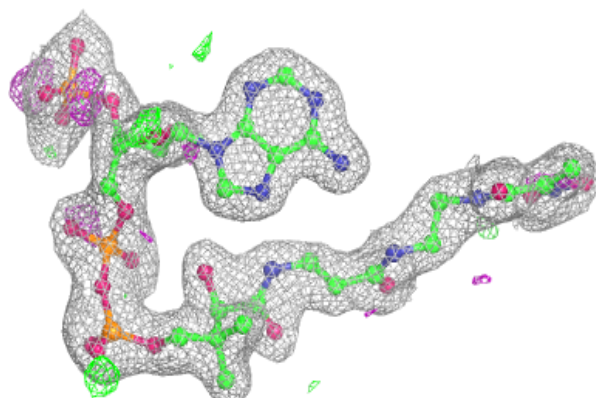


Electron density around KGJ E 301 (B):

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

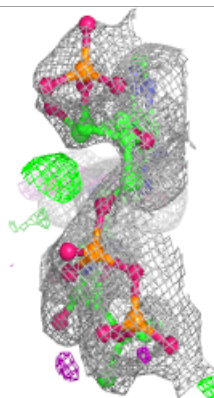
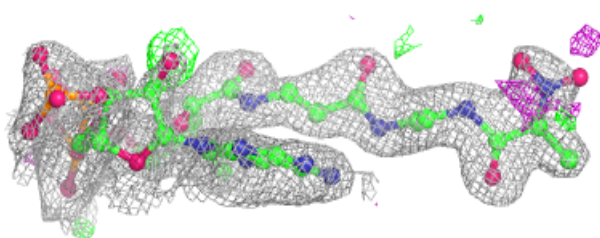
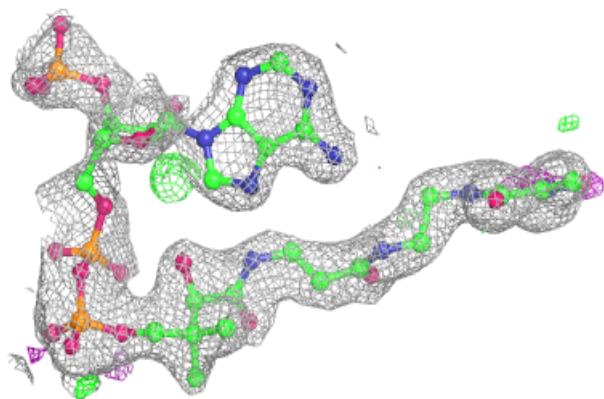
**Electron density around KGJ A 301:**

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

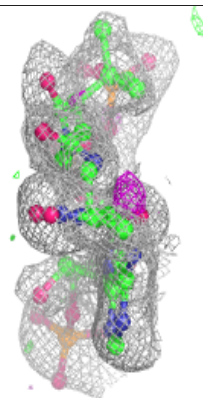
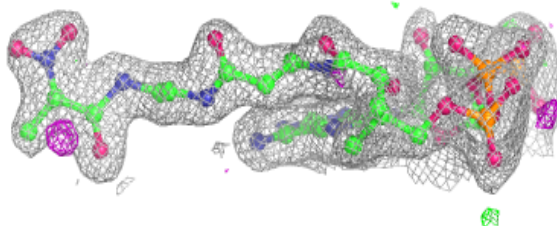
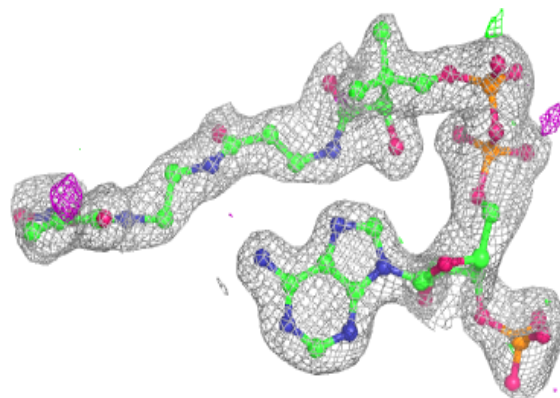


Electron density around KGJ E 301 (A):

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

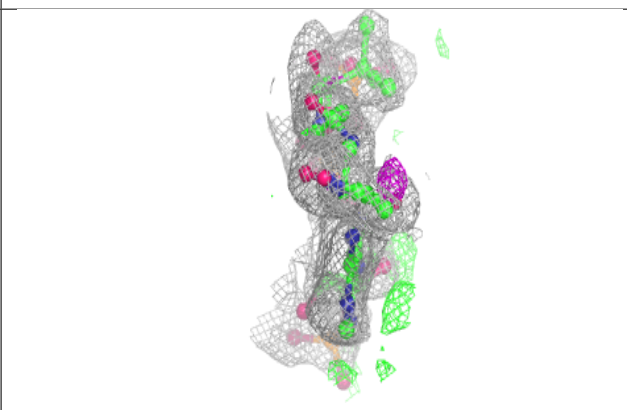
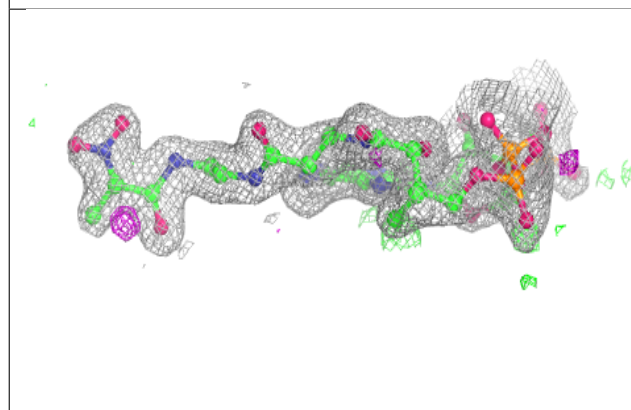
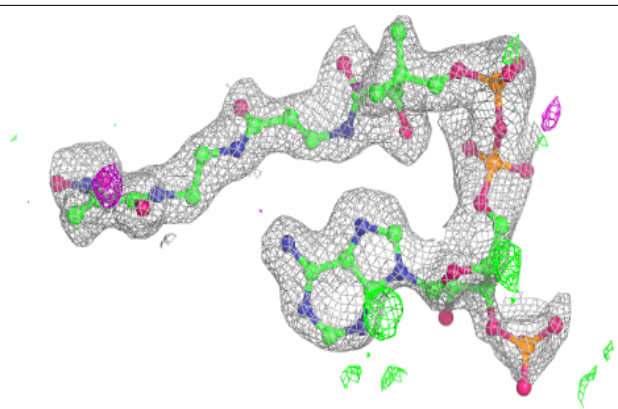
**Electron density around KGJ D 302 (A):**

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



Electron density around KGJ D 302 (B):

$2mF_o-DF_c$ (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.