



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:40 am BST

PDB ID : 6N93
Title : Methylmalonyl-CoA decarboxylase in complex with 2-nitronate-propionyl-ox
a(dethia)-CoA
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on : 2018-11-30
Resolution : 1.70 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 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 : 2.11
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) : 2.11

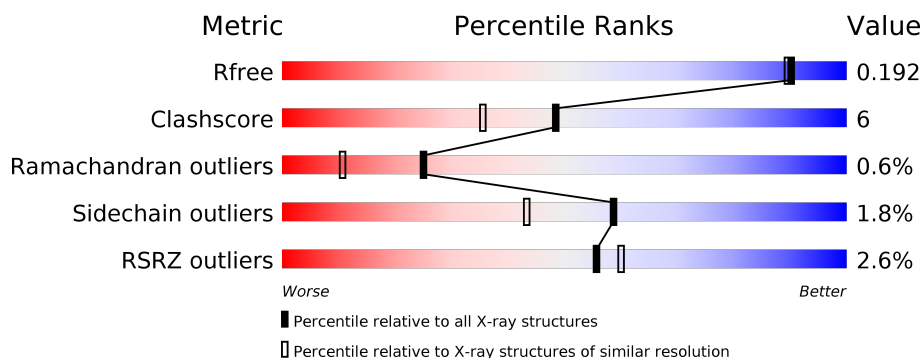
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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>90%</div> <div>9%</div> <div>•</div> </div>
1	B	261	<div> <div>4%</div> <div>92%</div> <div>8%</div> </div>
1	C	261	<div> <div>3%</div> <div>90%</div> <div>9%</div> <div>•</div> </div>
1	D	261	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>
1	E	261	<div> <div>3%</div> <div>87%</div> <div>13%</div> </div>
1	F	261	<div> <div>%</div> <div>90%</div> <div>9%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15344 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.

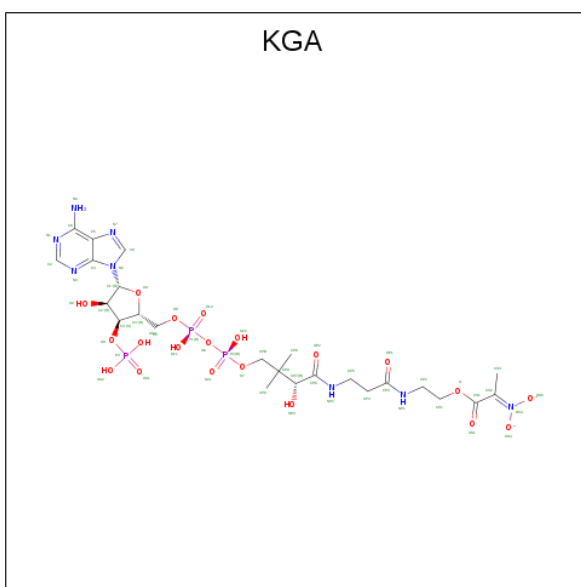
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	24	0
			2172	1397	365	397	13			
1	B	260	Total	C	N	O	S	0	13	0
			2129	1366	360	391	12			
1	C	260	Total	C	N	O	S	0	17	0
			2143	1373	366	392	12			
1	D	260	Total	C	N	O	S	0	16	0
			2123	1365	357	389	12			
1	E	260	Total	C	N	O	S	0	19	0
			2134	1372	357	393	12			
1	F	260	Total	C	N	O	S	0	21	0
			2153	1388	363	390	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-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethoxy]-1-oxidanylidene-propan-2-ylidene]-bis(oxidanidyl)azanium (three-letter code: KGA) (formula: C₂₄H₃₈N₈O₂₀P₃).

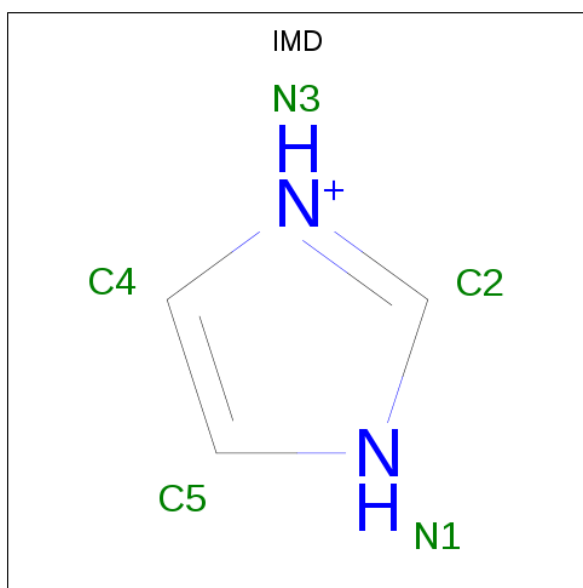


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	1
			86	37	12	31	6		
2	E	1	Total	C	N	O	P	0	0
			55	24	8	20	3		
2	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			55	24	8	20	3		
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		
3	F	1	Total	Ni	0	0
			1	1		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	D	1	Total	C	N	0	0
			5	3	2		
4	F	1	Total	C	N	0	0
			5	3	2		

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

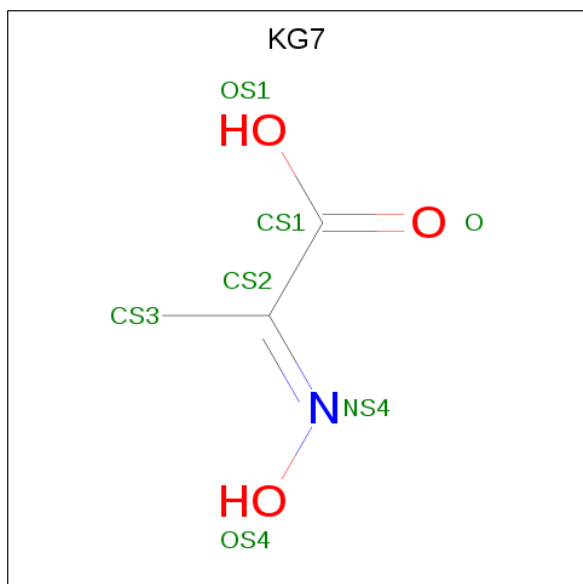
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 7 is (2E)-2-(hydroxyimino)propanoic acid (three-letter code: KG7) (formula: $C_3H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	0
			7	3	1	3		


- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	346	Total 357	O 357	0	13
8	B	323	Total 332	O 332	0	11
8	C	316	Total 326	O 326	0	16
8	D	320	Total 328	O 328	0	9
8	E	328	Total 337	O 337	0	11
8	F	332	Total 338	O 338	0	11

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

Chain A: 



- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain B: 




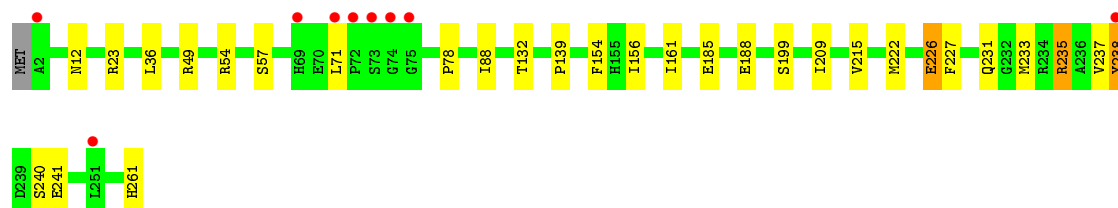
- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain C: 




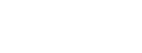
- Molecule 1: Methylmalonyl-CoA decarboxylase

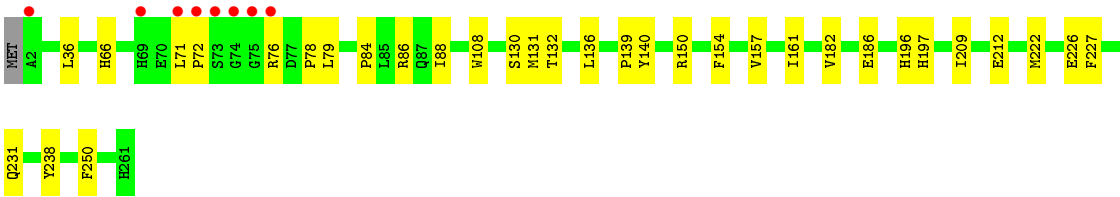
Chain D: 



- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain E: 





• 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	87.18Å 114.65Å 194.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.68 – 1.70 28.66 – 1.69	Depositor EDS
% Data completeness (in resolution range)	86.2 (28.68-1.70) 86.3 (28.66-1.69)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.153 , 0.184 0.165 , 0.192	Depositor DCC
R_{free} test set	9300 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15344	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, IMD, KG7, K, KGA, PG4

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	0.75	0/2281	0.88	2/3085 (0.1%)
1	B	0.83	3/2213 (0.1%)	0.86	1/2994 (0.0%)
1	C	0.82	1/2236 (0.0%)	0.86	1/3025 (0.0%)
1	D	0.83	3/2216 (0.1%)	0.89	3/2998 (0.1%)
1	E	0.80	2/2233 (0.1%)	0.86	2/3022 (0.1%)
1	F	0.78	2/2256 (0.1%)	0.85	2/3052 (0.1%)
All	All	0.80	11/13435 (0.1%)	0.87	11/18176 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	226	GLU	CD-OE2	-10.00	1.14	1.25
1	E	226	GLU	CD-OE2	7.96	1.34	1.25
1	D	185	GLU	CD-OE1	7.85	1.34	1.25
1	E	212	GLU	CD-OE2	-7.69	1.17	1.25
1	F	226[A]	GLU	CD-OE1	-6.27	1.18	1.25
1	B	226[A]	GLU	CD-OE2	-5.94	1.19	1.25
1	B	226[B]	GLU	CD-OE2	-5.94	1.19	1.25
1	D	185	GLU	CD-OE2	5.89	1.32	1.25
1	B	212	GLU	CD-OE2	-5.69	1.19	1.25
1	D	226	GLU	CD-OE2	5.35	1.31	1.25
1	F	212	GLU	CD-OE2	-5.17	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	238[A]	TYR	CB-CA-C	6.05	122.51	110.40
1	D	238[B]	TYR	CB-CA-C	6.05	122.51	110.40
1	B	86	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	D	23	ARG	NE-CZ-NH1	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	86	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	F	235	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	A	76	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	86	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	86	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	F	45	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	E	150	ARG	NE-CZ-NH1	5.00	122.80	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	2172	0	2237	22	0
1	B	2129	0	2159	21	0
1	C	2143	0	2182	32	0
1	D	2123	0	2168	35	0
1	E	2134	0	2177	42	0
1	F	2153	0	2213	24	0
2	A	48	0	0	1	0
2	B	48	0	0	3	0
2	C	79	0	0	13	0
2	D	86	0	0	2	0
2	E	86	0	0	3	0
2	F	86	0	0	8	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	5	0	0
4	D	5	0	5	0	0
4	F	5	0	4	0	0
5	C	1	0	0	0	0
6	C	13	0	18	0	0
7	F	7	0	0	0	0
8	A	357	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	332	0	0	3	0
8	C	326	0	0	5	0
8	D	328	0	0	4	0
8	E	337	0	0	6	0
8	F	338	0	0	5	0
All	All	15344	0	13168	157	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 (157) 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:215[A]:VAL:CG1	1:B:222[A]:MET:SD	2.20	1.29
1:E:78:PRO:HD2	1:E:238[A]:TYR:CZ	1.68	1.27
1:D:215[A]:VAL:CG1	1:E:222[A]:MET:SD	2.36	1.13
1:D:78:PRO:HD2	1:D:238[B]:TYR:CZ	1.84	1.10
1:A:215[A]:VAL:HG12	1:B:222[A]:MET:SD	1.90	1.09
1:B:71:LEU:CD1	1:B:72:PRO:HD2	1.86	1.06
1:A:226[B]:GLU:OE2	8:A:401:HOH:O	1.76	1.04
1:D:215[A]:VAL:HG12	1:E:222[A]:MET:SD	2.06	0.94
1:E:78:PRO:CD	1:E:238[A]:TYR:CZ	2.53	0.92
1:E:222[B]:MET:CG	1:E:227[B]:PHE:CE2	2.53	0.92
1:E:222[B]:MET:HG3	1:E:227[B]:PHE:CE2	2.05	0.92
1:E:78:PRO:HD2	1:E:238[A]:TYR:OH	1.68	0.92
1:B:71:LEU:HD13	1:B:72:PRO:HD2	1.52	0.92
1:A:215[A]:VAL:HG11	1:B:222[A]:MET:SD	2.10	0.90
1:E:222[B]:MET:HG2	1:E:227[B]:PHE:CZ	2.08	0.88
1:B:71:LEU:HD12	1:B:72:PRO:HD2	1.58	0.82
1:F:130[A]:SER:OG	2:F:303[A]:KGA:N7	2.15	0.80
1:E:222[B]:MET:CG	1:E:227[B]:PHE:CZ	2.65	0.79
1:B:78:PRO:HD2	1:B:238[A]:TYR:CZ	2.19	0.78
1:F:108:TRP:CZ3	2:F:303[A]:KGA:C8	2.67	0.78
1:C:108:TRP:CZ3	2:C:303[A]:KGA:C8	2.67	0.77
1:C:108:TRP:CH2	2:C:303[A]:KGA:C4	2.68	0.77
1:B:71:LEU:HD13	1:B:72:PRO:CD	2.17	0.74
1:D:78:PRO:CD	1:D:238[B]:TYR:CZ	2.68	0.73
1:E:222[B]:MET:HG2	1:E:227[B]:PHE:CE2	2.22	0.72
1:D:78:PRO:CD	1:D:238[B]:TYR:CE1	2.73	0.72
1:B:71:LEU:HD12	8:B:492:HOH:O	1.91	0.71
1:A:222[A]:MET:HE2	1:A:226[A]:GLU:HG2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215[A]:VAL:HG11	1:E:222[A]:MET:SD	2.30	0.70
1:E:222[B]:MET:HG3	1:E:227[B]:PHE:CD2	2.27	0.70
1:B:78:PRO:HD2	1:B:238[A]:TYR:OH	1.91	0.69
1:D:78:PRO:HD2	1:D:238[B]:TYR:CE1	2.28	0.69
1:C:68:ILE:HG23	2:C:301:KGA:CP1	2.23	0.69
1:A:200[B]:GLU:CD	8:A:408:HOH:O	2.31	0.68
1:A:215[A]:VAL:HG13	1:B:222[A]:MET:SD	2.27	0.68
1:C:108:TRP:CH2	2:C:303[A]:KGA:C5	2.76	0.68
1:C:227[B]:PHE:HE2	1:D:231[B]:GLN:HG2	1.60	0.67
2:B:301:KGA:O12	2:B:301:KGA:OP3	2.11	0.67
1:F:108:TRP:CH2	2:F:303[A]:KGA:C4	2.77	0.67
1:C:108:TRP:CZ3	2:C:303[A]:KGA:N7	2.63	0.67
1:F:196[B]:HIS:HD2	8:F:598:HOH:O	1.78	0.66
1:D:215[A]:VAL:HG13	1:E:222[A]:MET:SD	2.33	0.66
1:A:23:ARG:H	1:A:23:ARG:HD2	1.62	0.65
1:E:78:PRO:CD	1:E:238[A]:TYR:CE1	2.80	0.65
1:A:68[B]:ILE:HD11	2:A:301:KGA:CP1	2.28	0.63
1:E:222[B]:MET:SD	1:E:227[B]:PHE:CE1	2.92	0.63
1:A:196[B]:HIS:HE1	8:A:629:HOH:O	1.83	0.61
8:C:610:HOH:O	1:D:231[A]:GLN:HG2	2.01	0.60
1:F:130[A]:SER:OG	2:F:303[A]:KGA:C5	2.50	0.59
1:C:166:PRO:HB3	2:C:303[A]:KGA:C5	2.33	0.59
1:D:78:PRO:HD2	1:D:238[B]:TYR:OH	2.03	0.59
1:E:182[B]:VAL:HG12	1:E:186:GLU:HB2	1.83	0.58
1:B:71:LEU:CD1	8:B:492:HOH:O	2.50	0.58
1:A:218[A]:GLU:CD	8:A:417:HOH:O	2.42	0.58
1:E:131:MET:HG2	1:E:161[B]:ILE:HD12	1.85	0.58
1:E:66:HIS:ND1	2:E:301:KGA:CS3	2.65	0.58
1:F:222[A]:MET:HE2	1:F:227[A]:PHE:CE1	2.38	0.58
1:E:78:PRO:CD	1:E:238[A]:TYR:OH	2.46	0.58
1:C:45[B]:ARG:NH1	1:C:47:GLU:OE1	2.30	0.57
1:C:68:ILE:HG12	1:C:250:PHE:CD1	2.39	0.57
1:B:71:LEU:CD1	1:B:72:PRO:CD	2.72	0.57
1:D:241:GLU:OE1	1:D:261:HIS:ND1	2.38	0.56
1:C:78:PRO:HD2	1:C:238:TYR:CZ	2.41	0.55
1:D:156[B]:ILE:CD1	8:D:670:HOH:O	2.54	0.55
1:F:108:TRP:CZ3	2:F:303[A]:KGA:N7	2.74	0.55
1:C:68:ILE:HG12	1:C:250:PHE:CE1	2.41	0.55
1:D:139:PRO:HD2	1:D:238[B]:TYR:CE1	2.41	0.55
1:F:28:LEU:HB3	1:F:33:ILE:HD11	1.89	0.55
1:C:77:ASP:H	1:D:235:ARG:HH22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:VAL:O	1:E:161[B]:ILE:HG12	2.08	0.54
1:E:197[B]:HIS:HD2	8:E:492:HOH:O	1.89	0.54
1:D:49:ARG:NH1	8:D:402:HOH:O	2.24	0.54
1:B:253:LYS:NZ	2:B:301:KGA:O31	2.38	0.53
1:C:128:THR:OG1	2:C:303[A]:KGA:N1	2.41	0.53
1:A:235[A]:ARG:HG3	1:A:238:TYR:CE1	2.45	0.52
1:C:78:PRO:HD2	1:C:238:TYR:OH	2.09	0.52
1:F:188[B]:GLU:HG3	8:F:419:HOH:O	2.09	0.51
1:A:218[A]:GLU:CG	8:A:417:HOH:O	2.59	0.51
2:B:301:KGA:NP2	2:B:301:KGA:CP8	2.71	0.51
1:D:139:PRO:HG2	1:D:238[B]:TYR:CZ	2.46	0.51
1:F:146[A]:HIS:HD2	8:F:631:HOH:O	1.93	0.51
1:C:83[B]:ASP:CG	8:C:402:HOH:O	2.49	0.50
1:D:36:LEU:HD23	1:D:88[B]:ILE:CD1	2.42	0.50
1:F:108:TRP:CH2	2:F:303[A]:KGA:N9	2.80	0.50
1:C:108:TRP:HZ3	2:C:303[A]:KGA:C8	2.22	0.50
1:E:209:ILE:HG21	1:F:161:ILE:HG21	1.92	0.50
1:A:23:ARG:H	1:A:23:ARG:CD	2.23	0.49
1:C:18[B]:GLU:CD	8:C:444:HOH:O	2.50	0.49
1:C:227[B]:PHE:CE2	1:D:231[B]:GLN:HG2	2.45	0.49
1:D:222[A]:MET:HE2	1:F:215[A]:VAL:HG12	1.95	0.48
1:D:161:ILE:HG21	1:F:209:ILE:HG21	1.93	0.48
1:D:222[A]:MET:CE	1:F:215[A]:VAL:HG12	2.44	0.48
1:E:131:MET:HG2	1:E:161[B]:ILE:CD1	2.43	0.48
1:D:54:ARG:HH12	1:D:188[B]:GLU:CD	2.16	0.48
1:C:2:ALA:HB1	8:C:551[A]:HOH:O	2.13	0.47
1:E:136:LEU:HD21	1:E:250:PHE:HB2	1.96	0.47
1:B:49:ARG:HB2	1:B:199[B]:SER:HB2	1.95	0.47
1:B:71:LEU:HA	1:B:71:LEU:HD13	1.54	0.47
1:C:108:TRP:CH2	2:C:303[A]:KGA:N9	2.83	0.47
1:D:209:ILE:HG21	1:E:161[A]:ILE:HG21	1.97	0.47
1:E:197[B]:HIS:CD2	8:E:492:HOH:O	2.66	0.46
1:A:73[A]:SER:O	1:A:244:GLN:OE1	2.34	0.46
1:A:209:ILE:HG21	1:B:161:ILE:HG21	1.97	0.46
1:E:36[A]:LEU:HD23	1:E:88:ILE:CD1	2.45	0.46
1:A:33:ILE:HD13	1:A:36[B]:LEU:HD12	1.97	0.46
1:D:71:LEU:CD2	1:D:78:PRO:HB2	2.46	0.46
1:F:146[B]:HIS:CE1	1:F:220:HIS:HD1	2.34	0.46
1:F:54:ARG:HH12	1:F:188[B]:GLU:CD	2.20	0.46
1:D:156[B]:ILE:HD11	8:D:670:HOH:O	2.15	0.45
1:B:28:LEU:HB3	1:B:33:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:ARG:HD2	8:F:584[A]:HOH:O	2.16	0.45
1:A:161:ILE:HG21	1:C:209:ILE:HG21	1.99	0.45
1:C:227[B]:PHE:HE2	1:D:231[B]:GLN:CG	2.28	0.45
1:C:108:TRP:CH2	2:C:303[A]:KGA:C8	2.99	0.45
1:C:67:ASP:HA	2:C:301:KGA:N1	2.32	0.45
1:E:130[A]:SER:OG	2:E:302[A]:KGA:N7	2.50	0.45
1:E:222[B]:MET:SD	1:E:227[B]:PHE:CD1	3.11	0.45
1:A:166:PRO:HD3	8:A:468:HOH:O	2.17	0.44
1:F:49[B]:ARG:NH1	8:F:554[B]:HOH:O	2.25	0.44
1:D:222[A]:MET:HE2	1:F:215[A]:VAL:CG1	2.47	0.44
1:C:68:ILE:CD1	1:C:69[B]:HIS:CD2	3.01	0.44
1:A:45[A]:ARG:NH1	1:A:47:GLU:OE2	2.43	0.43
1:E:222[B]:MET:SD	1:E:227[B]:PHE:CZ	3.11	0.43
1:E:72:PRO:HD2	1:E:78:PRO:HB3	2.00	0.43
1:F:128:THR:OG1	2:F:303[A]:KGA:N1	2.52	0.43
1:B:78:PRO:HD2	1:B:238[A]:TYR:CE2	2.52	0.43
1:A:226[A]:GLU:OE1	8:A:403[A]:HOH:O	2.22	0.43
1:E:196[B]:HIS:HE1	8:E:562:HOH:O	2.02	0.43
1:C:222[A]:MET:HE3	1:C:226:GLU:HB3	2.00	0.43
1:B:224:SER:HA	1:E:227[B]:PHE:CE1	2.54	0.43
1:D:199[B]:SER:OG	8:D:401:HOH:O	2.21	0.42
1:C:222[A]:MET:HB2	1:C:222[A]:MET:HE2	1.77	0.42
1:B:182:VAL:CG1	1:B:186:GLU:HB2	2.49	0.42
8:B:466[B]:HOH:O	1:C:255:LYS:HG2	2.19	0.42
1:D:241:GLU:OE1	1:D:261:HIS:CE1	2.72	0.42
1:F:108:TRP:CH2	2:F:303[A]:KGA:C5	3.03	0.42
1:D:237:VAL:O	1:D:240[B]:SER:HB2	2.20	0.42
1:E:139:PRO:HD2	1:E:238[A]:TYR:CE1	2.54	0.42
1:C:108:TRP:HH2	2:C:303[A]:KGA:C4	2.30	0.41
1:A:222[A]:MET:HB3	1:A:222[A]:MET:HE3	1.90	0.41
1:E:182[B]:VAL:CG1	1:E:186:GLU:HB2	2.48	0.41
1:C:68:ILE:HG23	2:C:301:KGA:CP2	2.50	0.41
1:C:7:ASN:ND2	8:C:551[B]:HOH:O	2.53	0.41
1:C:227[B]:PHE:CD2	1:D:227[B]:PHE:HB3	2.56	0.41
1:D:233:MET:HE2	1:F:208:VAL:HG23	2.03	0.41
1:E:231[B]:GLN:NE2	8:E:421:HOH:O	2.52	0.41
1:F:40[A]:LEU:HA	1:F:40[A]:LEU:HD12	1.88	0.41
1:E:227[A]:PHE:CE2	1:E:231[A]:GLN:HG2	2.56	0.41
1:E:108:TRP:CZ3	2:E:302[A]:KGA:C8	3.04	0.41
1:D:71:LEU:HD22	1:D:78:PRO:HB2	2.02	0.41
1:D:237:VAL:O	1:D:240[B]:SER:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:HIS:CE1	1:E:79:LEU:HD21	2.57	0.40
1:E:84:PRO:HB2	8:E:474:HOH:O	2.21	0.40
1:E:76:ARG:NH2	8:E:431:HOH:O	2.54	0.40
1:E:78:PRO:HD2	1:E:238[A]:TYR:HH	1.76	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	282/261 (108%)	270 (96%)	9 (3%)	3 (1%)	14	3
1	B	272/261 (104%)	262 (96%)	8 (3%)	2 (1%)	22	8
1	C	275/261 (105%)	264 (96%)	9 (3%)	2 (1%)	22	8
1	D	274/261 (105%)	266 (97%)	7 (3%)	1 (0%)	34	18
1	E	276/261 (106%)	266 (96%)	9 (3%)	1 (0%)	34	18
1	F	278/261 (106%)	270 (97%)	7 (2%)	1 (0%)	34	18
All	All	1657/1566 (106%)	1598 (96%)	49 (3%)	10 (1%)	25	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74[A]	GLY
1	A	74[B]	GLY
1	B	74	GLY
1	C	76	ARG
1	A	132	THR
1	C	132	THR
1	D	132	THR
1	E	132	THR

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Mol	Chain	Res	Type
1	F	132	THR
1	B	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	246/224 (110%)	240 (98%)	6 (2%)	49	31
1	B	237/224 (106%)	234 (99%)	3 (1%)	69	56
1	C	240/224 (107%)	237 (99%)	3 (1%)	69	56
1	D	239/224 (107%)	233 (98%)	6 (2%)	47	29
1	E	241/224 (108%)	238 (99%)	3 (1%)	71	59
1	F	243/224 (108%)	237 (98%)	6 (2%)	47	29
All	All	1446/1344 (108%)	1419 (98%)	27 (2%)	59	41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	24	LYS
1	A	140	TYR
1	A	154	PHE
1	A	222[A]	MET
1	A	222[B]	MET
1	B	71	LEU
1	B	154	PHE
1	B	251	LEU
1	C	68	ILE
1	C	136	LEU
1	C	154	PHE
1	D	12	ASN
1	D	57[A]	SER
1	D	57[B]	SER
1	D	154	PHE

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Mol	Chain	Res	Type
1	D	226	GLU
1	D	235	ARG
1	E	71	LEU
1	E	140	TYR
1	E	154	PHE
1	F	140	TYR
1	F	146[A]	HIS
1	F	146[B]	HIS
1	F	154	PHE
1	F	235	ARG
1	F	251	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	193	GLN
1	C	4	GLN
1	C	7	ASN
1	D	7	ASN
1	D	12	ASN
1	E	244	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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$
4	IMD	D	303	-	3,5,5	0.22	0	4,5,5	0.71	0
7	KG7	F	304	3	4,6,6	1.98	1 (25%)	3,7,7	4.86	2 (66%)
4	IMD	A	303	3	3,5,5	0.21	0	4,5,5	0.65	0
2	KGA	A	301	-	42,50,57	1.12	3 (7%)	53,75,85	1.62	12 (22%)
2	KGA	C	301	-	42,50,57	1.02	2 (4%)	53,75,85	1.47	8 (15%)
2	KGA	E	301	-	45,57,57	1.51	3 (6%)	56,85,85	1.11	4 (7%)
4	IMD	F	305	3	3,5,5	0.23	0	4,5,5	0.48	0
2	KGA	D	302[B]	-	42,50,57	0.88	2 (4%)	53,75,85	1.63	10 (18%)
2	KGA	C	303[A]	-	28,33,57	1.17	3 (10%)	35,52,85	1.30	4 (11%)
2	KGA	E	302[A]	-	28,33,57	1.42	6 (21%)	35,52,85	1.51	6 (17%)
2	KGA	D	302[A]	-	42,50,57	0.85	2 (4%)	53,75,85	1.69	10 (18%)
6	PG4	C	304	5	12,12,12	0.26	0	11,11,11	0.22	0
2	KGA	B	301	-	42,50,57	0.82	1 (2%)	53,75,85	1.69	11 (20%)
2	KGA	F	303[A]	-	28,33,57	1.39	5 (17%)	35,52,85	1.43	6 (17%)
2	KGA	F	301	-	45,57,57	1.75	3 (6%)	56,85,85	1.67	11 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMD	D	303	-	-	-	0/1/1/1
7	KG7	F	304	3	-	0/1/6/6	-
4	IMD	A	303	3	-	-	0/1/1/1
2	KGA	A	301	-	-	4/44/64/75	0/3/3/3
2	KGA	C	301	-	-	5/44/64/75	0/3/3/3
2	KGA	E	301	-	-	0/49/75/75	0/3/3/3
4	IMD	F	305	3	-	-	0/1/1/1
2	KGA	D	302[B]	-	-	10/44/64/75	0/3/3/3
2	KGA	C	303[A]	-	-	5/17/37/75	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KGA	E	302[A]	-	-	2/17/37/75	0/3/3/3
2	KGA	D	302[A]	-	-	12/44/64/75	0/3/3/3
6	PG4	C	304	5	-	1/10/10/10	-
2	KGA	B	301	-	-	25/44/64/75	0/3/3/3
2	KGA	F	303[A]	-	-	1/17/37/75	0/3/3/3
2	KGA	F	301	-	-	4/49/75/75	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	KGA	O-CS1	9.65	1.51	1.33
2	E	301	KGA	O-CS1	7.62	1.47	1.33
2	A	301	KGA	O4'-C1'	4.24	1.47	1.41
7	F	304	KG7	CS3-CS2	3.78	1.57	1.50
2	E	301	KGA	O4'-C1'	3.35	1.45	1.41
2	F	303[A]	KGA	C5-C4	3.25	1.49	1.40
2	E	301	KGA	P3-O3'	3.25	1.65	1.59
2	F	301	KGA	O4'-C1'	3.03	1.45	1.41
2	F	303[A]	KGA	O4'-C1'	3.00	1.45	1.41
2	E	302[A]	KGA	O4'-C1'	2.92	1.45	1.41
2	C	303[A]	KGA	C5-C4	2.88	1.48	1.40
2	E	302[A]	KGA	P3-O3'	2.82	1.64	1.59
2	E	302[A]	KGA	C2-N3	2.80	1.36	1.32
2	A	301	KGA	P3-O3'	2.74	1.64	1.59
2	A	301	KGA	C5-C4	2.74	1.48	1.40
2	D	302[A]	KGA	O4'-C1'	2.73	1.44	1.41
2	E	302[A]	KGA	C4-N3	2.71	1.39	1.35
2	E	302[A]	KGA	C5-C4	2.61	1.47	1.40
2	F	303[A]	KGA	C2'-C1'	-2.60	1.49	1.53
2	F	303[A]	KGA	C2-N3	2.59	1.36	1.32
2	C	301	KGA	C5-C4	2.59	1.47	1.40
2	B	301	KGA	O4'-C1'	2.55	1.44	1.41
2	D	302[B]	KGA	O4'-C1'	2.49	1.44	1.41
2	F	301	KGA	C5-C4	2.48	1.47	1.40
2	D	302[B]	KGA	C5-C4	2.26	1.46	1.40
2	C	303[A]	KGA	C2-N3	2.24	1.35	1.32
2	F	303[A]	KGA	P2-O7	2.24	1.63	1.54
2	C	303[A]	KGA	C2'-C1'	-2.17	1.50	1.53
2	C	301	KGA	O4'-C1'	2.17	1.44	1.41
2	E	302[A]	KGA	P2-O7	2.16	1.63	1.54
2	D	302[A]	KGA	C5-C4	2.11	1.46	1.40

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	KGA	CP1-O-CS1	6.83	129.66	116.58
7	F	304	KG7	OS4-NS4-CS2	6.17	121.52	112.68
7	F	304	KG7	CS3-CS2-CS1	5.49	124.00	117.92
2	E	302[A]	KGA	N3-C2-N1	-4.99	120.88	128.68
2	A	301	KGA	CP7-CP6-NP2	-4.34	107.94	116.58
2	D	302[B]	KGA	CP4-CP3-NP1	4.22	123.52	116.42
2	D	302[A]	KGA	CP4-CP3-NP1	4.22	123.52	116.42
2	C	303[A]	KGA	N3-C2-N1	-4.03	122.38	128.68
2	D	302[A]	KGA	CP5-NP2-CP6	3.90	129.55	122.59
2	F	303[A]	KGA	N3-C2-N1	-3.80	122.74	128.68
2	D	302[B]	KGA	CP5-NP2-CP6	3.76	129.30	122.59
2	D	302[A]	KGA	CP9-CPA-CP7	3.76	115.34	108.82
2	B	301	KGA	N3-C2-N1	-3.70	122.89	128.68
2	D	302[A]	KGA	N3-C2-N1	-3.64	122.99	128.68
2	E	301	KGA	CP1-O-CS1	3.63	123.54	116.58
2	E	301	KGA	CP9-CPA-CP7	3.59	115.04	108.82
2	B	301	KGA	P2-O6-P1	-3.56	120.62	132.83
2	B	301	KGA	CP5-NP2-CP6	-3.55	116.26	122.59
2	E	302[A]	KGA	C1'-N9-C4	-3.49	120.51	126.64
2	F	303[A]	KGA	C4-C5-N7	-3.48	105.77	109.40
2	F	301	KGA	CP5-CP4-CP3	-3.44	106.63	112.36
2	C	301	KGA	CP9-CPA-CP7	3.42	114.74	108.82
2	B	301	KGA	C1'-N9-C4	-3.40	120.67	126.64
2	B	301	KGA	CP8-CPA-CPB	-3.34	102.78	108.23
2	A	301	KGA	C1'-N9-C4	-3.33	120.79	126.64
2	C	301	KGA	CP9-CPA-CPB	-3.29	102.86	108.23
2	C	303[A]	KGA	P1-O6-P2	-3.27	121.59	132.83
2	D	302[B]	KGA	N3-C2-N1	-3.24	123.62	128.68
2	D	302[B]	KGA	CP9-CPA-CP7	3.22	114.40	108.82
2	D	302[B]	KGA	OP1-CP3-CP4	-3.20	116.17	122.02
2	D	302[A]	KGA	OP1-CP3-CP4	-3.20	116.17	122.02
2	E	301	KGA	C4-C5-N7	-3.19	106.07	109.40
2	D	302[B]	KGA	P2-O6-P1	-3.16	121.97	132.83
2	A	301	KGA	OP2-CP6-NP2	3.11	129.67	122.99
2	F	301	KGA	C2'-C3'-C4'	3.09	108.69	103.22
2	A	301	KGA	O4'-C1'-C2'	3.07	111.42	106.93
2	B	301	KGA	CP8-CPA-CP7	3.07	114.14	108.82
2	D	302[B]	KGA	CP7-CP6-NP2	3.03	122.61	116.58
2	C	301	KGA	C4-C5-N7	-3.02	106.25	109.40
2	B	301	KGA	CP7-CP6-NP2	-3.01	110.58	116.58
2	F	301	KGA	N3-C2-N1	-3.00	123.99	128.68
2	D	302[A]	KGA	CP7-CP6-NP2	3.00	122.54	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	303[A]	KGA	C1'-N9-C4	-2.96	121.44	126.64
2	F	301	KGA	O7-CPB-CPA	-2.94	105.81	110.55
2	F	303[A]	KGA	C2-N1-C6	2.90	123.71	118.75
2	C	301	KGA	CP2-NP1-CP3	2.89	128.20	122.84
2	C	303[A]	KGA	C2-N1-C6	2.87	123.66	118.75
2	A	301	KGA	N3-C2-N1	-2.80	124.30	128.68
2	F	301	KGA	CS3-CS2-CS1	2.74	125.80	119.89
2	B	301	KGA	CP4-CP3-NP1	-2.71	111.86	116.42
2	A	301	KGA	N6-C6-N1	2.67	124.12	118.57
2	E	301	KGA	N3-C2-N1	-2.63	124.56	128.68
2	F	303[A]	KGA	O7-P2-O6	2.57	113.25	104.64
2	C	301	KGA	N3-C2-N1	-2.56	124.68	128.68
2	F	301	KGA	C4-C5-N7	-2.54	106.76	109.40
2	E	302[A]	KGA	C2-N1-C6	2.53	123.08	118.75
2	D	302[B]	KGA	CP1-CP2-NP1	-2.51	106.00	111.64
2	D	302[A]	KGA	CP1-CP2-NP1	-2.51	106.00	111.64
2	D	302[A]	KGA	C4-C5-N7	-2.48	106.81	109.40
2	C	301	KGA	O4'-C1'-C2'	-2.42	103.39	106.93
2	B	301	KGA	OP1-CP3-NP1	2.39	127.52	123.01
2	E	302[A]	KGA	O32-P3-O33	2.38	116.72	107.64
2	C	301	KGA	O4'-C4'-C5'	2.37	117.18	109.37
2	F	301	KGA	O5'-C5'-C4'	-2.35	100.92	108.99
2	D	302[B]	KGA	C1'-N9-C4	-2.32	122.56	126.64
2	A	301	KGA	CP4-CP5-NP2	2.32	116.57	111.90
2	D	302[A]	KGA	C2-N1-C6	2.27	122.63	118.75
2	F	301	KGA	P2-O6-P1	-2.26	125.06	132.83
2	B	301	KGA	N6-C6-N1	2.24	123.22	118.57
2	D	302[B]	KGA	CP4-CP5-NP2	-2.23	107.39	111.90
2	D	302[A]	KGA	CP4-CP5-NP2	-2.23	107.39	111.90
2	A	301	KGA	C2-N1-C6	2.23	122.57	118.75
2	E	302[A]	KGA	N6-C6-N1	2.22	123.19	118.57
2	B	301	KGA	O4'-C1'-C2'	2.22	110.17	106.93
2	A	301	KGA	CP5-CP4-CP3	-2.17	108.74	112.36
2	C	301	KGA	CP7-CP6-NP2	2.16	120.88	116.58
2	F	301	KGA	OP1-CP3-CP4	-2.11	118.16	122.02
2	E	302[A]	KGA	O4'-C1'-C2'	2.07	109.95	106.93
2	F	301	KGA	O2'-C2'-C3'	2.06	117.03	111.17
2	A	301	KGA	O5'-P1-O12	2.03	117.02	109.07
2	A	301	KGA	O32-P3-O31	2.02	118.60	110.68
2	A	301	KGA	CP1-CP2-NP1	2.02	116.19	111.64
2	C	303[A]	KGA	N6-C6-N1	2.02	122.76	118.57
2	F	303[A]	KGA	O4'-C1'-C2'	-2.02	103.98	106.93

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	KGA	CP6-CP7-CPA-CPB
2	D	302[B]	KGA	C5'-O5'-P1-O11
2	D	302[B]	KGA	C5'-O5'-P1-O12
2	D	302[B]	KGA	C5'-O5'-P1-O6
2	D	302[B]	KGA	P1-O6-P2-O7
2	D	302[B]	KGA	CP7-CP6-NP2-CP5
2	D	302[B]	KGA	CP3-CP4-CP5-NP2
2	D	302[B]	KGA	CP4-CP3-NP1-CP2
2	D	302[B]	KGA	OP1-CP3-NP1-CP2
2	C	303[A]	KGA	P1-O6-P2-O22
2	C	303[A]	KGA	P1-O6-P2-O7
2	D	302[A]	KGA	C4'-C3'-O3'-P3
2	D	302[A]	KGA	C3'-O3'-P3-O31
2	D	302[A]	KGA	CP7-CP6-NP2-CP5
2	D	302[A]	KGA	CP3-CP4-CP5-NP2
2	D	302[A]	KGA	CP4-CP3-NP1-CP2
2	D	302[A]	KGA	OP1-CP3-NP1-CP2
2	B	301	KGA	OP3-CP7-CPA-CPB
2	B	301	KGA	CP6-CP7-CPA-CPB
2	B	301	KGA	OP3-CP7-CPA-CP9
2	B	301	KGA	CP6-CP7-CPA-CP9
2	B	301	KGA	OP3-CP7-CPA-CP8
2	B	301	KGA	CP6-CP7-CPA-CP8
2	B	301	KGA	OP2-CP6-CP7-OP3
2	B	301	KGA	NP2-CP6-CP7-OP3
2	B	301	KGA	CP7-CP6-NP2-CP5
2	B	301	KGA	CP3-CP4-CP5-NP2
2	F	303[A]	KGA	P2-O6-P1-O5'
2	F	301	KGA	O-CS1-CS2-CS3
2	A	301	KGA	CP4-CP5-NP2-CP6
2	D	302[B]	KGA	OP2-CP6-NP2-CP5
2	D	302[A]	KGA	OP2-CP6-NP2-CP5
2	B	301	KGA	C3'-C4'-C5'-O5'
2	B	301	KGA	O4'-C4'-C5'-O5'
2	C	303[A]	KGA	C4'-C3'-O3'-P3
2	B	301	KGA	CP8-CPA-CPB-O7
2	D	302[B]	KGA	O-CP1-CP2-NP1
2	D	302[A]	KGA	O-CP1-CP2-NP1
2	A	301	KGA	CP4-CP3-NP1-CP2
2	C	301	KGA	O-CP1-CP2-NP1

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Mol	Chain	Res	Type	Atoms
2	C	303[A]	KGA	P2-O6-P1-O5'
2	D	302[A]	KGA	P1-O6-P2-O7
2	F	301	KGA	P1-O6-P2-O7
2	B	301	KGA	CP4-CP3-NP1-CP2
2	F	301	KGA	OS1-CS1-CS2-CS3
2	C	301	KGA	CP6-CP7-CPA-CP8
2	C	301	KGA	C5'-O5'-P1-O6
2	E	302[A]	KGA	C3'-O3'-P3-O33
2	D	302[A]	KGA	C3'-O3'-P3-O33
2	B	301	KGA	C5'-O5'-P1-O6
2	B	301	KGA	CPB-O7-P2-O6
2	D	302[A]	KGA	P2-O6-P1-O12
2	B	301	KGA	P1-O6-P2-O22
2	B	301	KGA	C5'-O5'-P1-O12
2	B	301	KGA	CP7-CPA-CPB-O7
2	B	301	KGA	CP9-CPA-CPB-O7
2	C	303[A]	KGA	C2'-C3'-O3'-P3
2	A	301	KGA	O-CP1-CP2-NP1
2	F	301	KGA	CP4-CP5-NP2-CP6
2	B	301	KGA	NP2-CP6-CP7-CPA
6	C	304	PG4	C3-C4-O3-C5
2	C	301	KGA	CP6-CP7-CPA-CP9
2	A	301	KGA	P2-O6-P1-O11
2	D	302[A]	KGA	P1-O6-P2-O22
2	B	301	KGA	P1-O6-P2-O21
2	B	301	KGA	CPA-CPB-O7-P2
2	E	302[A]	KGA	C5'-O5'-P1-O12
2	B	301	KGA	C5'-O5'-P1-O11
2	B	301	KGA	CPB-O7-P2-O22

There are no ring outliers.

9 monomers are involved in 30 short contacts:

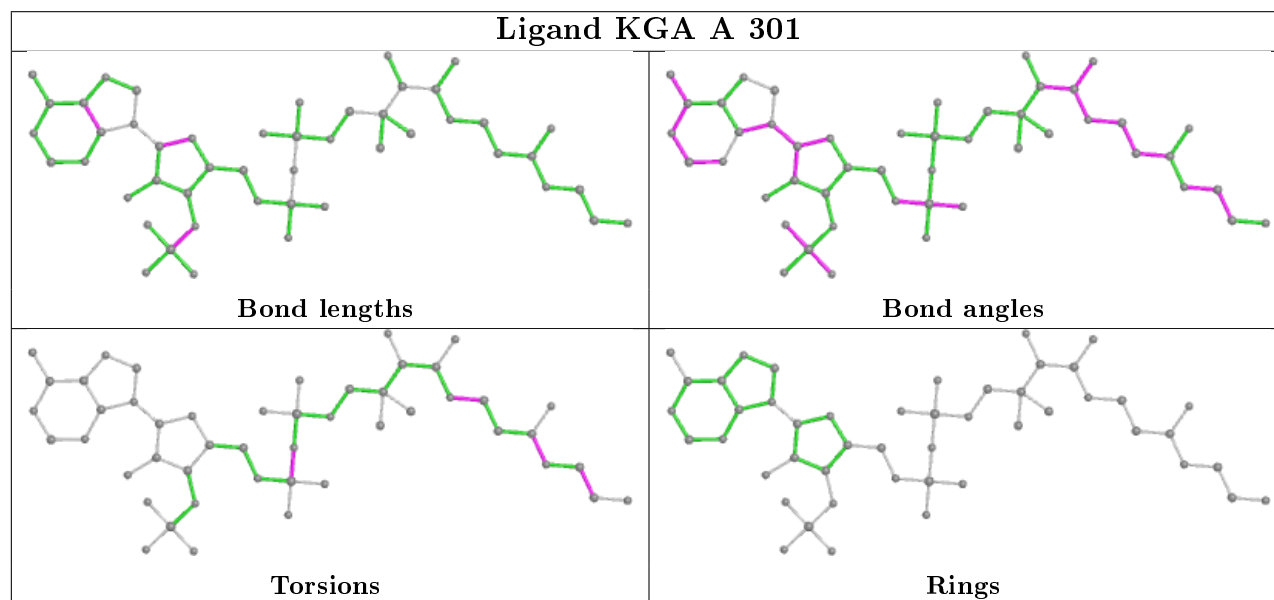
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	KGA	1	0
2	C	301	KGA	3	0
2	E	301	KGA	1	0
2	D	302[B]	KGA	1	0
2	C	303[A]	KGA	10	0
2	E	302[A]	KGA	2	0
2	D	302[A]	KGA	1	0
2	B	301	KGA	3	0

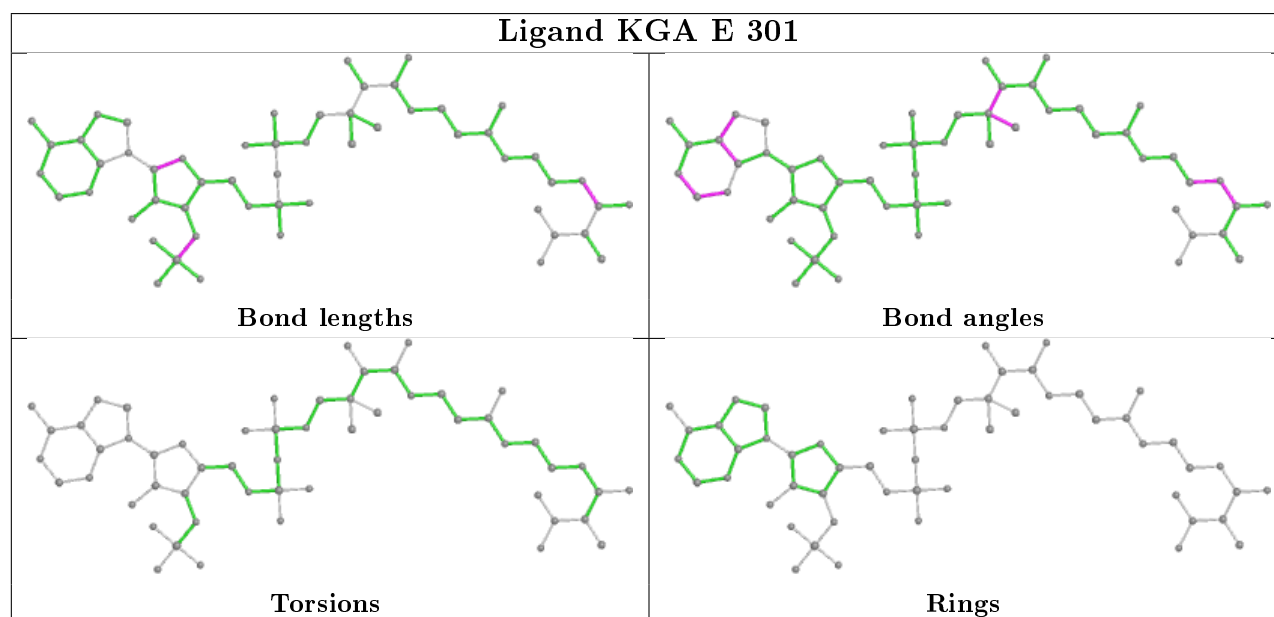
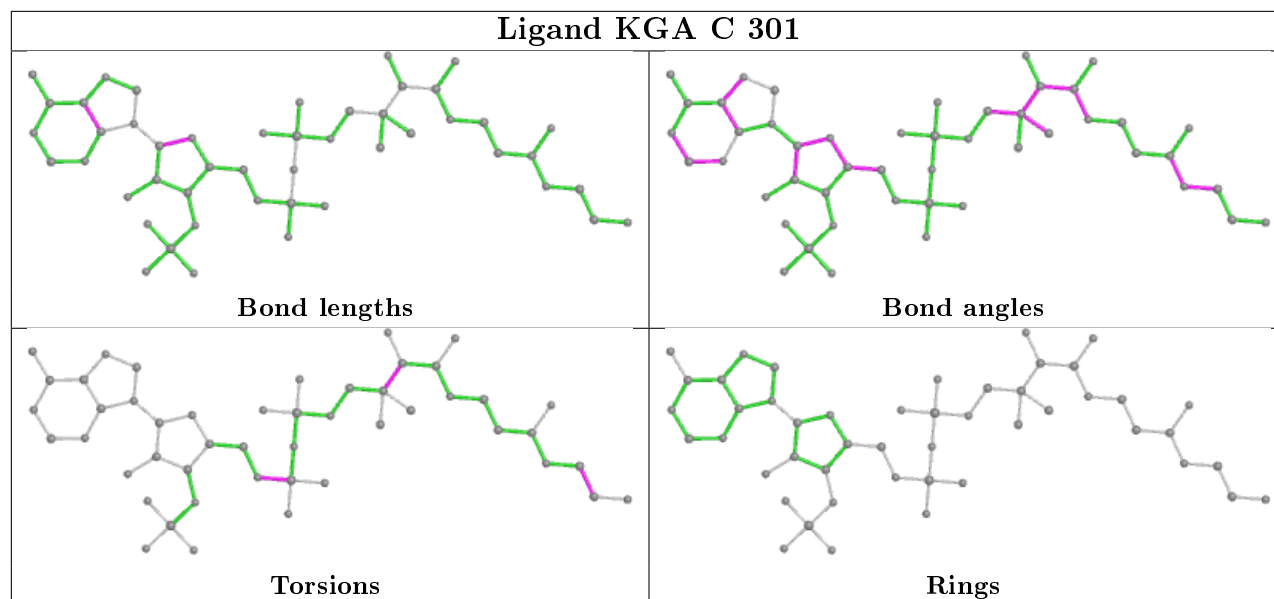
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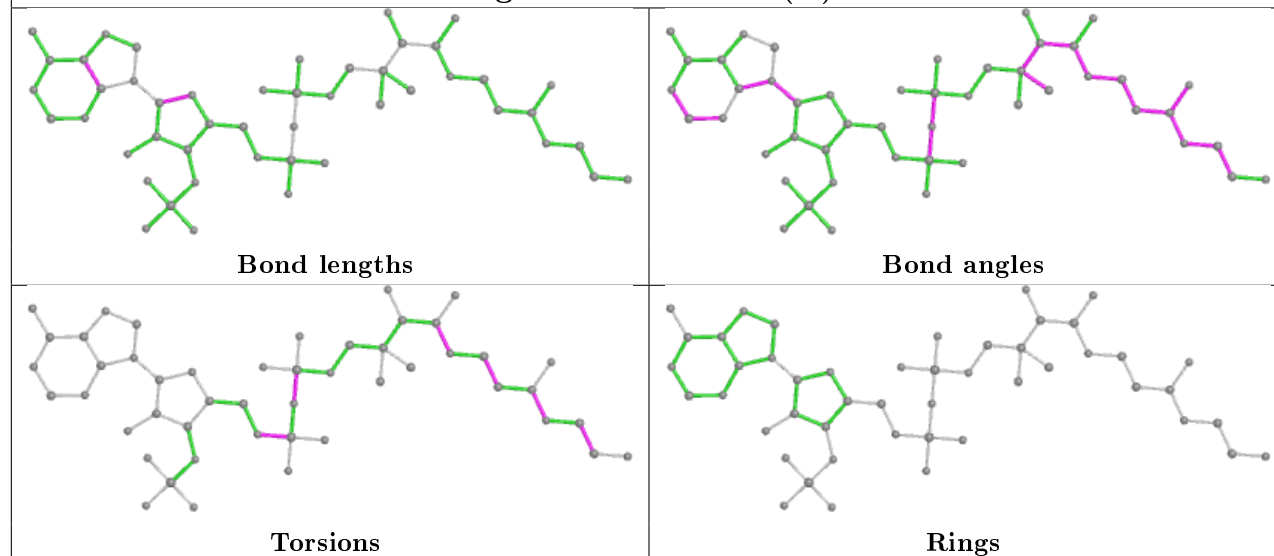
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	303[A]	KGA	8	0

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.

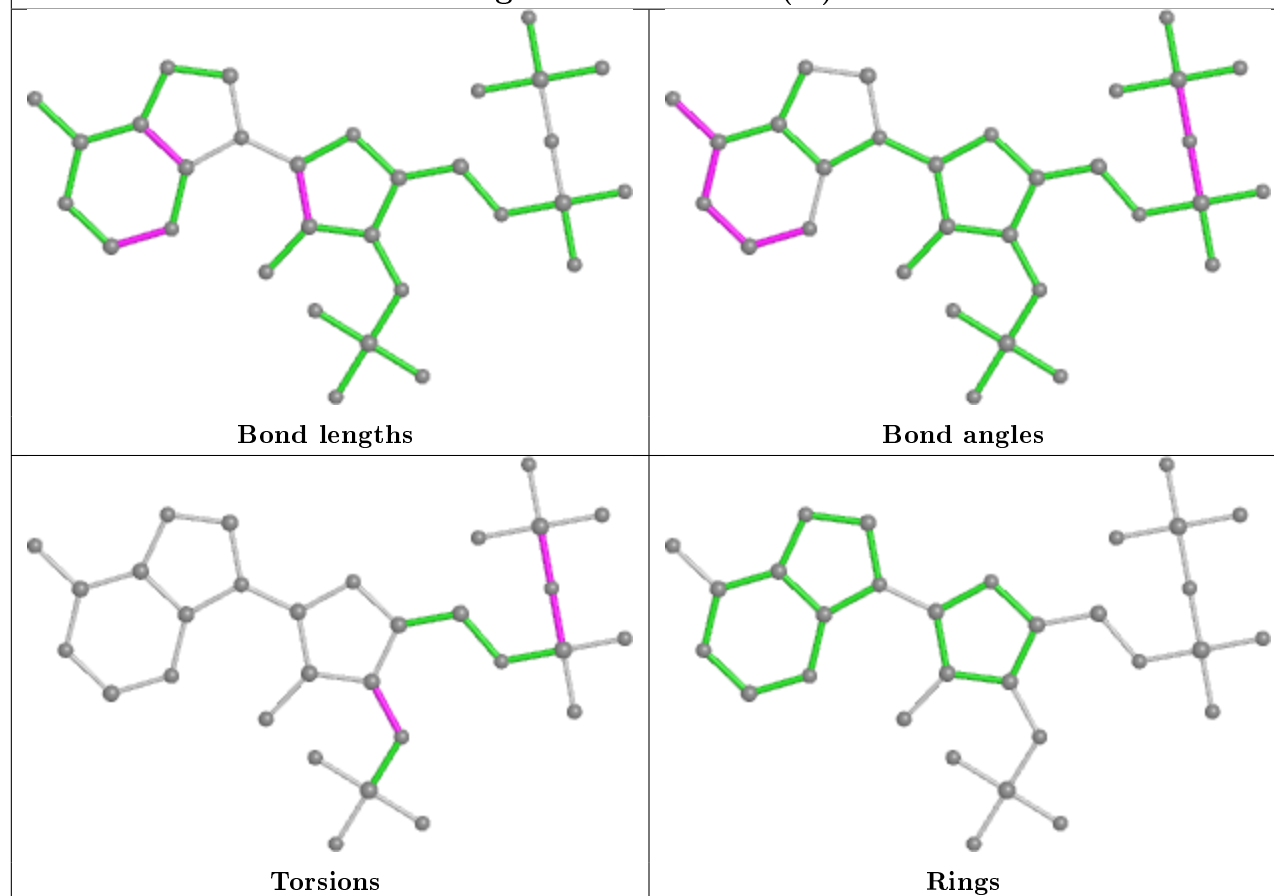




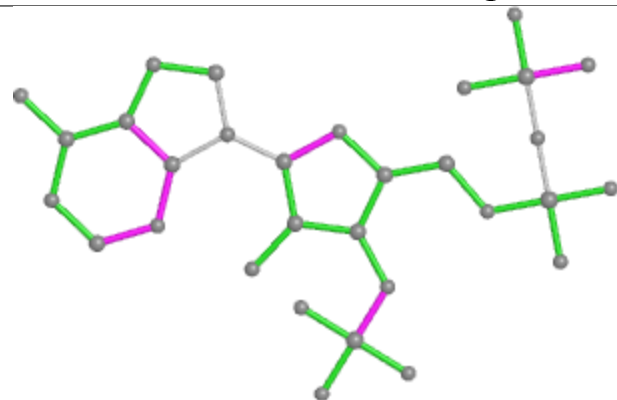
Ligand KGA D 302 (B)



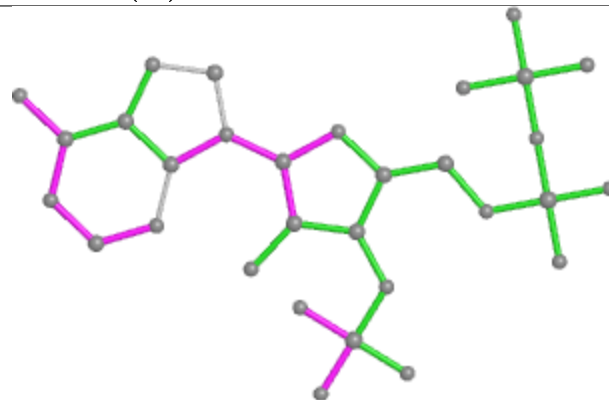
Ligand KGA C 303 (A)



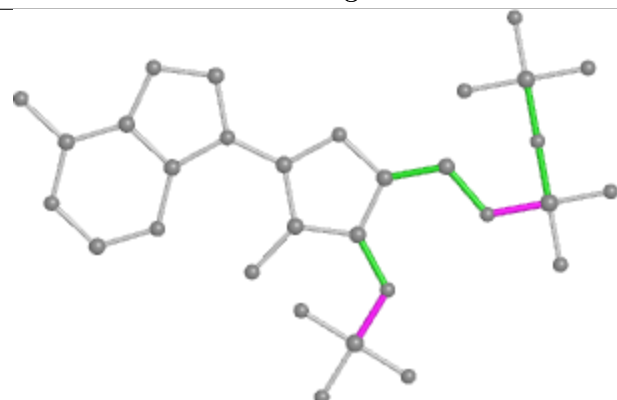
Ligand KGA E 302 (A)



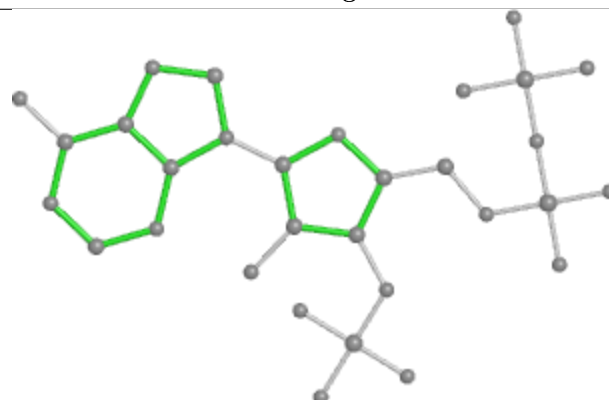
Bond lengths



Bond angles

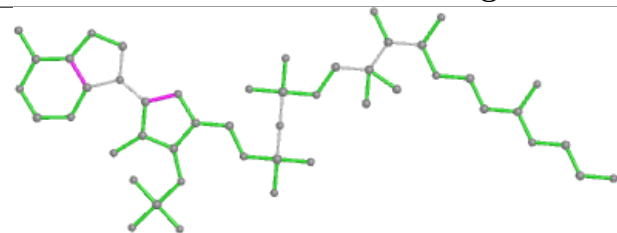


Torsions

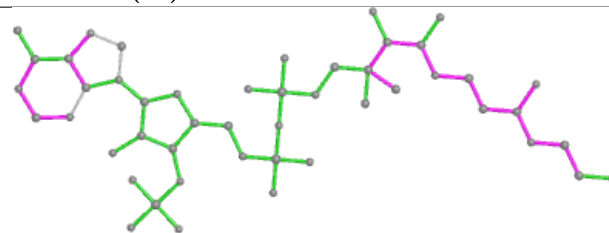


Rings

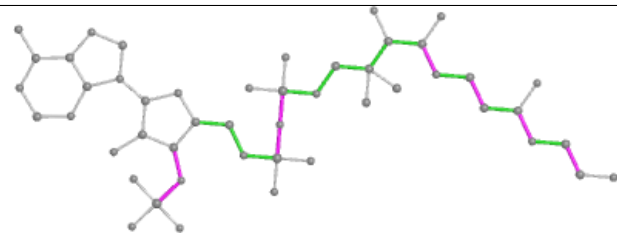
Ligand KGA D 302 (A)



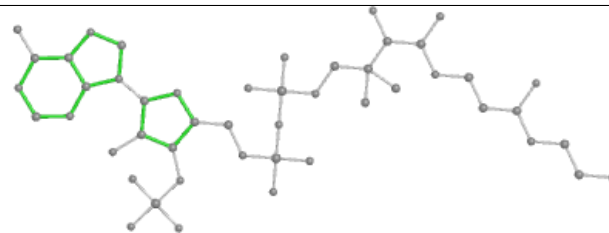
Bond lengths



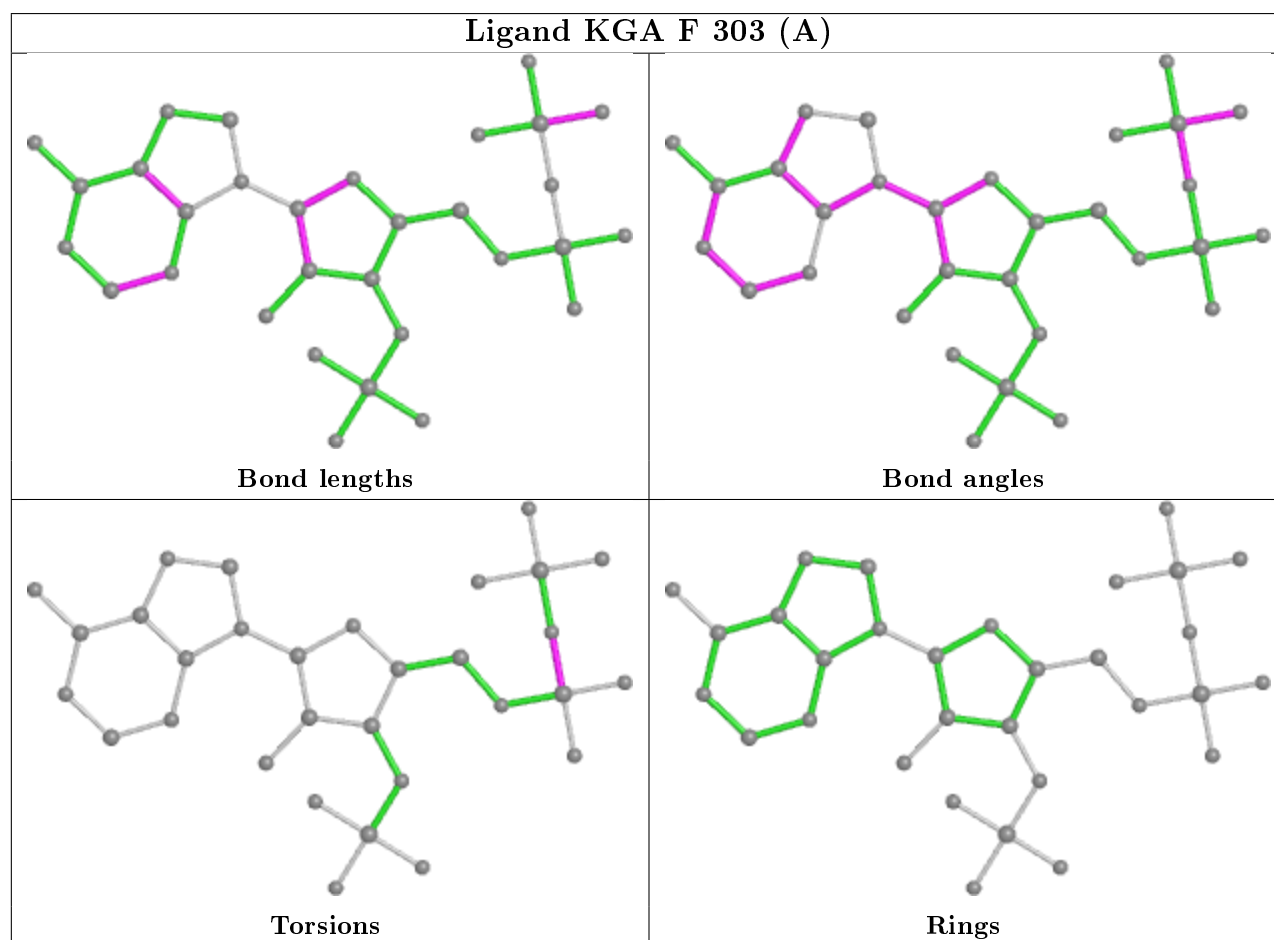
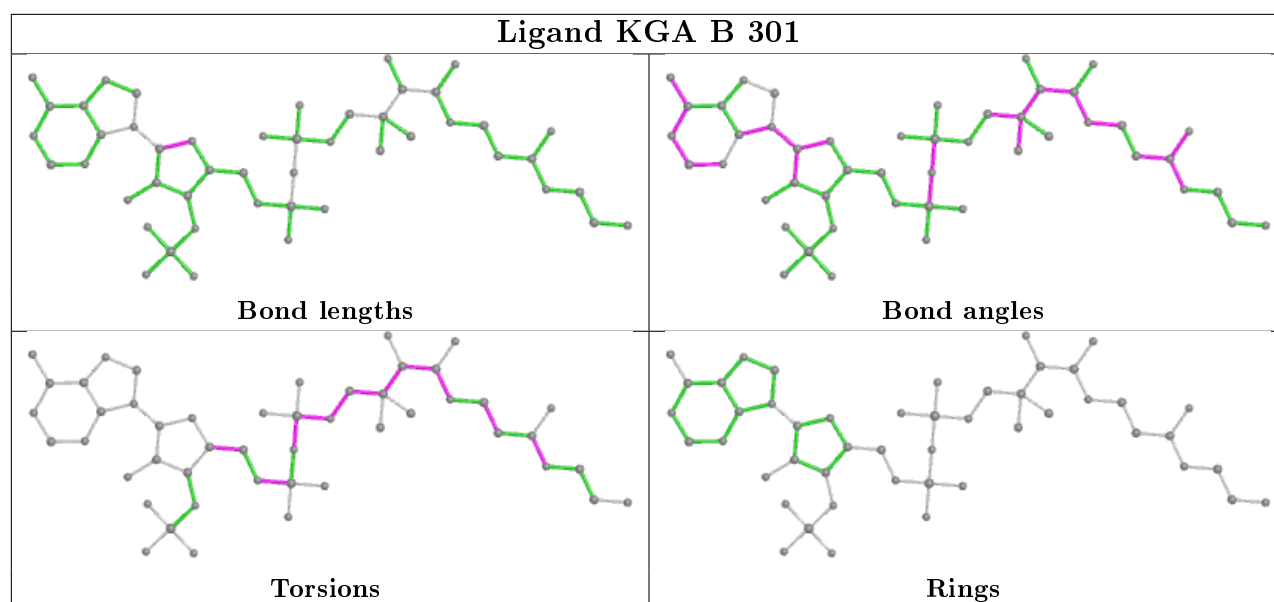
Bond angles

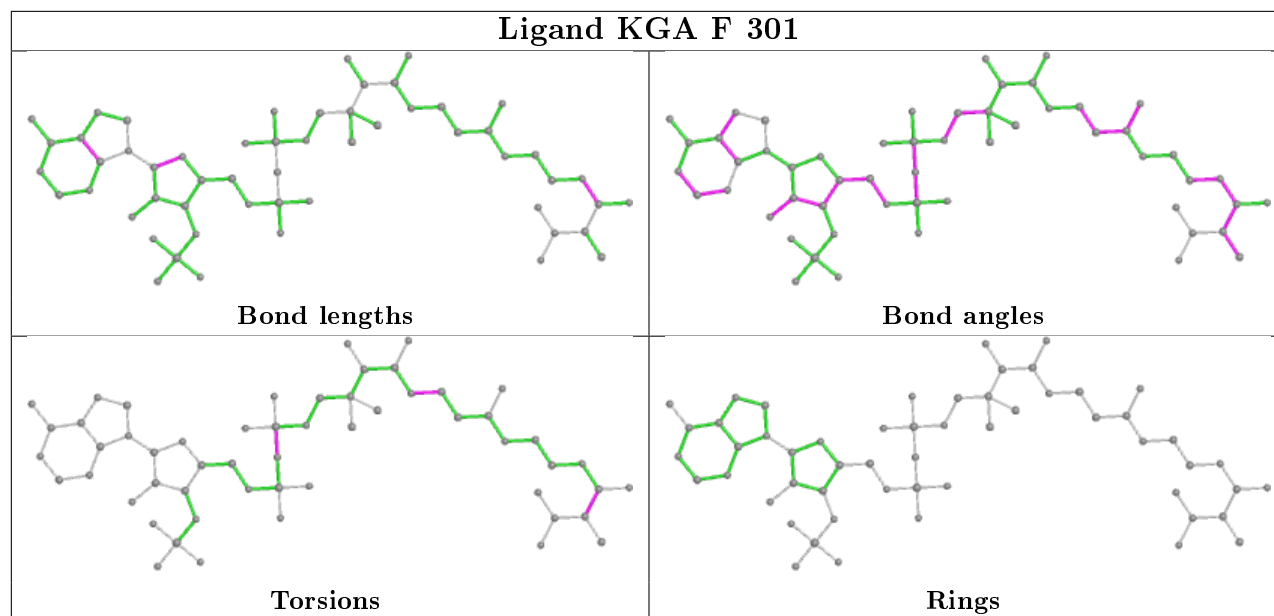


Torsions



Rings





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%)	-0.41	1 (0%) 92 93	8, 12, 27, 47	0
1	B	260/261 (99%)	-0.13	10 (3%) 40 45	8, 14, 36, 62	5 (1%)
1	C	260/261 (99%)	-0.19	9 (3%) 44 49	8, 13, 34, 124	0
1	D	260/261 (99%)	-0.24	9 (3%) 44 49	8, 13, 34, 87	0
1	E	260/261 (99%)	-0.16	8 (3%) 49 53	8, 14, 35, 93	0
1	F	260/261 (99%)	-0.30	3 (1%) 79 82	8, 14, 33, 63	0
All	All	1560/1566 (99%)	-0.24	40 (2%) 56 60	8, 14, 34, 124	5 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	74	GLY	8.9
1	C	72	PRO	8.7
1	C	73	SER	8.6
1	C	71	LEU	6.6
1	E	75	GLY	6.3
1	E	73	SER	6.0
1	F	73	SER	5.8
1	C	74	GLY	5.3
1	D	71	LEU	5.2
1	B	75	GLY	4.8
1	D	75	GLY	4.7
1	C	75	GLY	4.7
1	B	73	SER	3.7
1	D	2	ALA	3.6
1	B	251	LEU	3.6
1	D	74	GLY	3.5
1	E	71	LEU	3.4
1	E	2	ALA	3.4
1	B	71	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	3.3
1	E	72	PRO	3.2
1	D	72	PRO	3.1
1	D	73	SER	2.9
1	F	23	ARG	2.9
1	E	76	ARG	2.9
1	C	69[A]	HIS	2.9
1	C	68	ILE	2.8
1	B	68	ILE	2.7
1	D	69	HIS	2.7
1	F	72	PRO	2.7
1	C	76	ARG	2.5
1	A	23	ARG	2.5
1	D	238[A]	TYR	2.4
1	C	238	TYR	2.3
1	B	238[A]	TYR	2.2
1	B	72	PRO	2.2
1	D	251	LEU	2.2
1	B	69	HIS	2.1
1	E	69	HIS	2.1
1	B	76	ARG	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 carbohydrates 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(\AA^2)	Q<0.9
2	KGA	B	301	48/55	0.72	0.21	29,60,86,90	0
2	KGA	F	301	55/55	0.77	0.21	26,42,69,76	0

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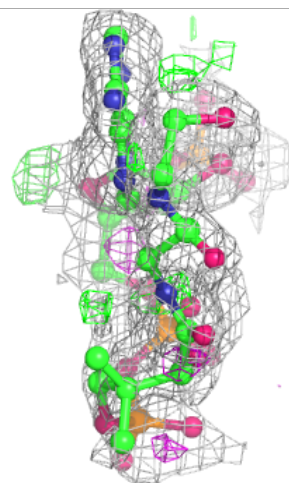
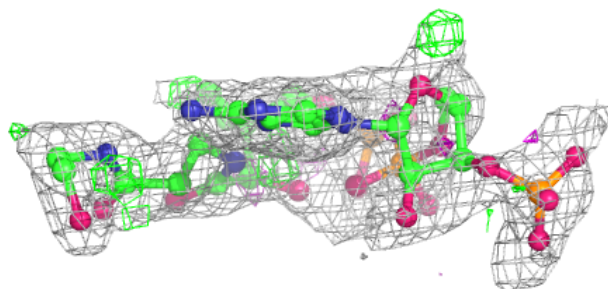
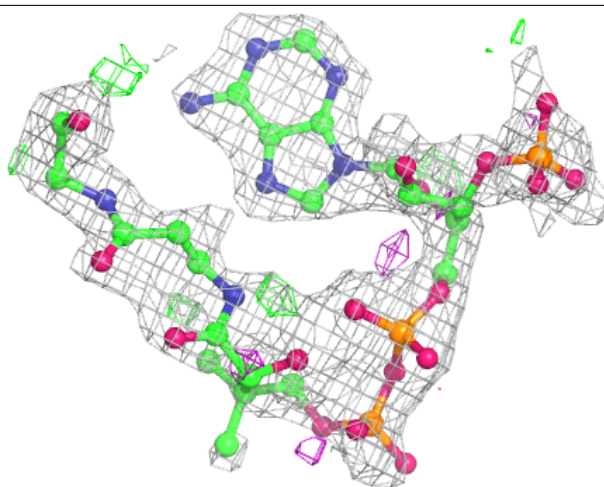
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	KGA	C	303[A]	31/55	0.78	0.26	30,33,41,46	31
2	KGA	D	302[B]	48/55	0.81	0.23	28,37,52,57	38
2	KGA	D	302[A]	48/55	0.81	0.23	30,42,56,62	38
2	KGA	F	303[A]	31/55	0.82	0.26	29,37,52,56	31
2	KGA	C	301	48/55	0.84	0.16	28,41,56,63	0
6	PG4	C	304	13/13	0.85	0.22	40,46,53,57	0
2	KGA	E	302[A]	31/55	0.86	0.27	23,43,52,58	0
4	IMD	A	303	5/5	0.89	0.13	38,41,43,43	0
2	KGA	A	301	48/55	0.90	0.12	18,36,48,53	0
4	IMD	D	303	5/5	0.92	0.14	30,31,33,34	0
2	KGA	E	301	55/55	0.92	0.13	23,30,51,57	0
7	KG7	F	304	7/7	0.93	0.11	19,21,24,25	0
4	IMD	F	305	5/5	0.95	0.10	31,33,33,34	0
5	K	C	302	1/1	0.96	0.14	48,48,48,48	0
3	NI	A	302	1/1	0.98	0.06	23,23,23,23	0
3	NI	D	301	1/1	0.99	0.04	21,21,21,21	0
3	NI	F	302	1/1	0.99	0.03	20,20,20,20	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.

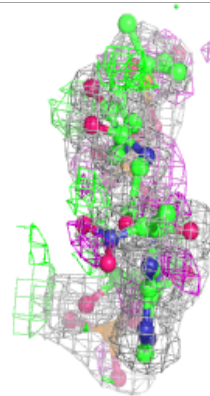
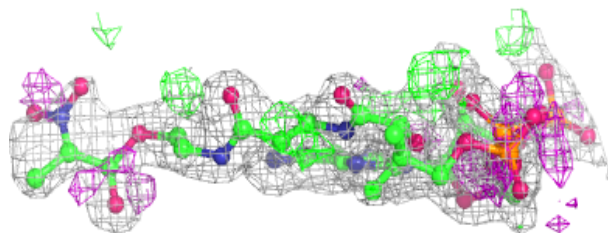
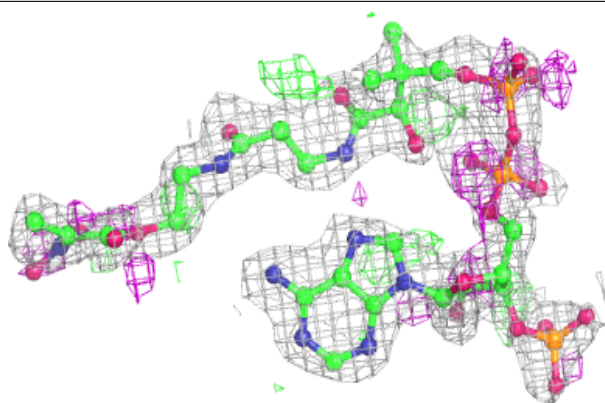
Electron density around KGA B 301:

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



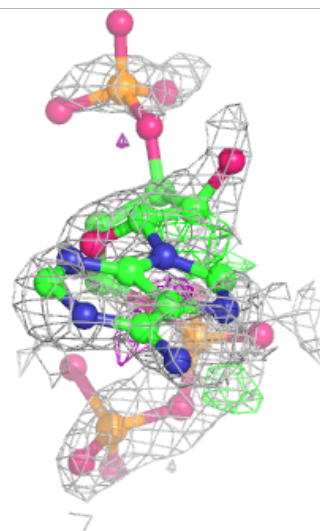
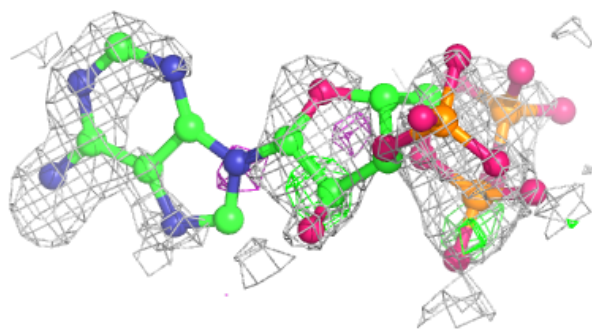
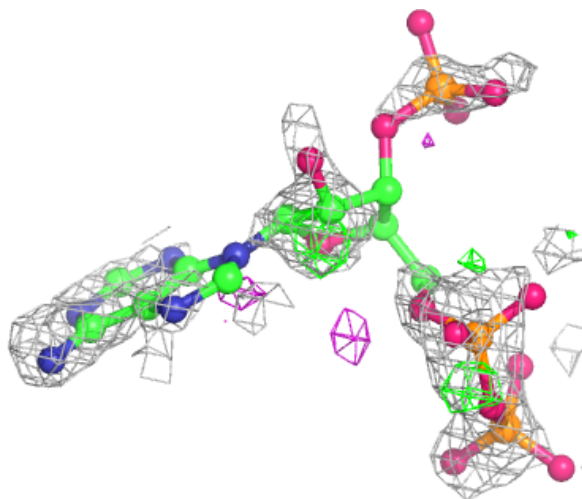
Electron density around KGA F 301:

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



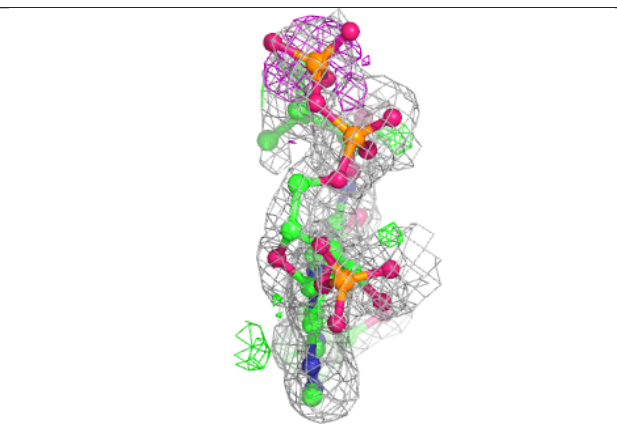
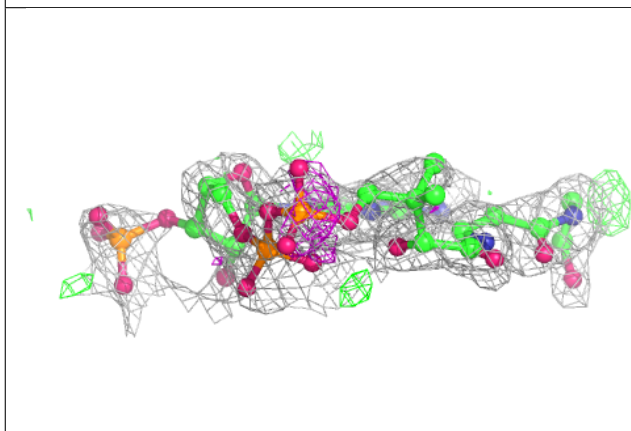
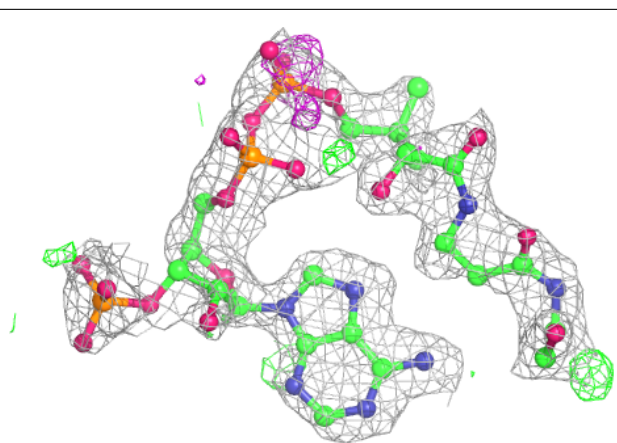
Electron density around KGA C 303 (A):

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

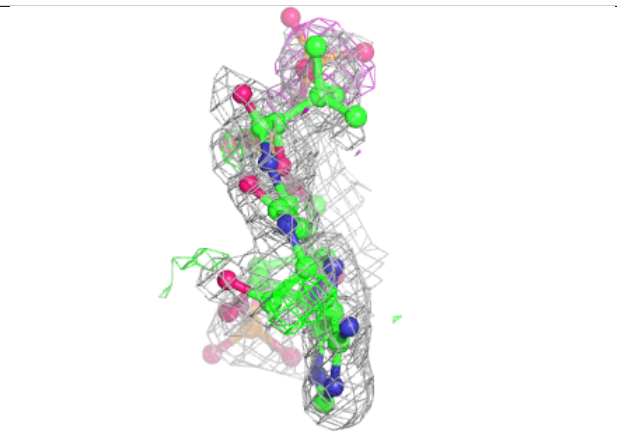
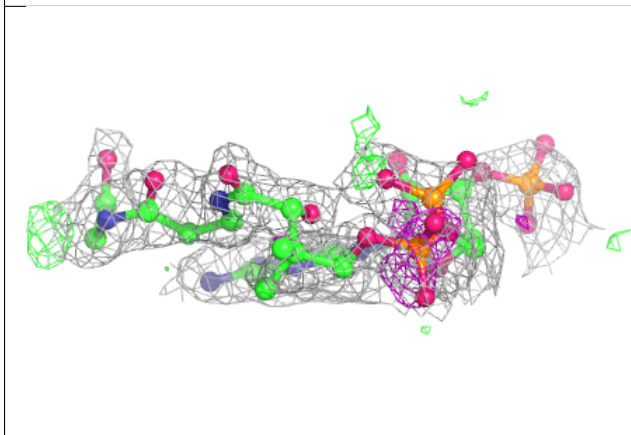
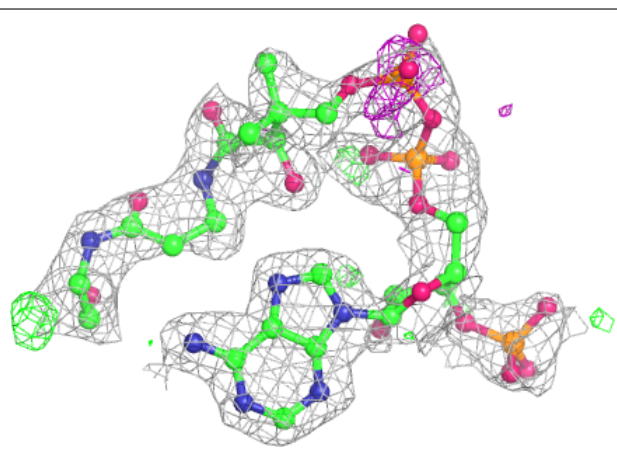
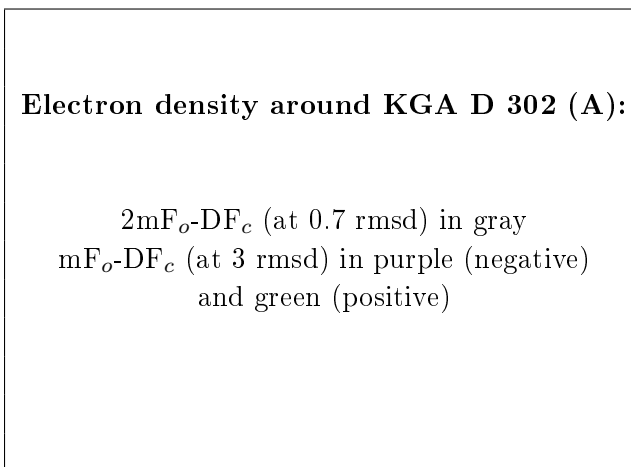


Electron density around KGA D 302 (B):

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

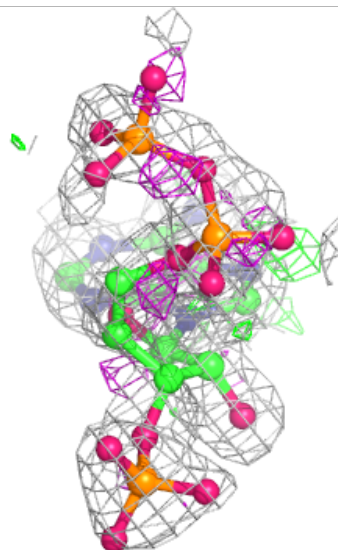
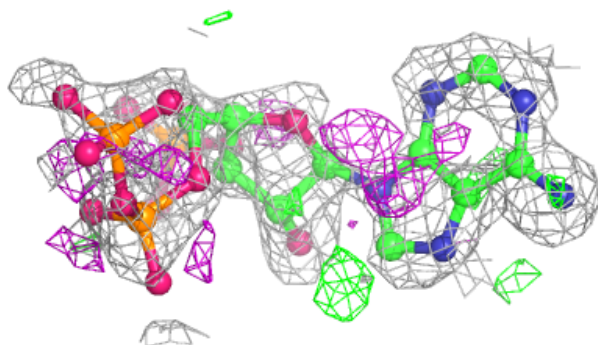
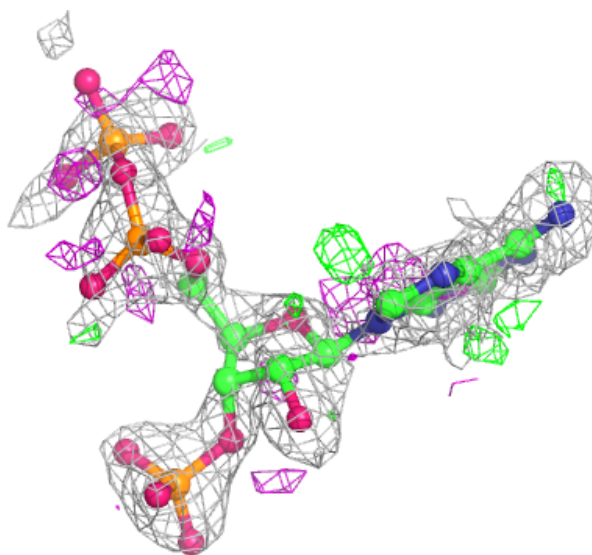
**Electron density around KGA D 302 (A):**

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



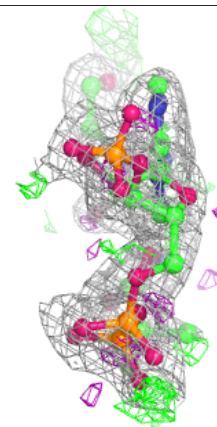
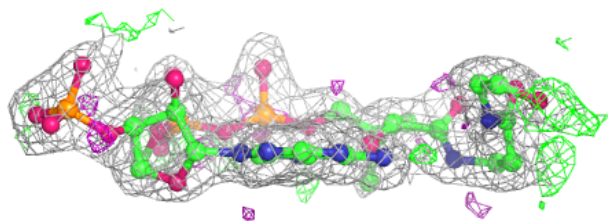
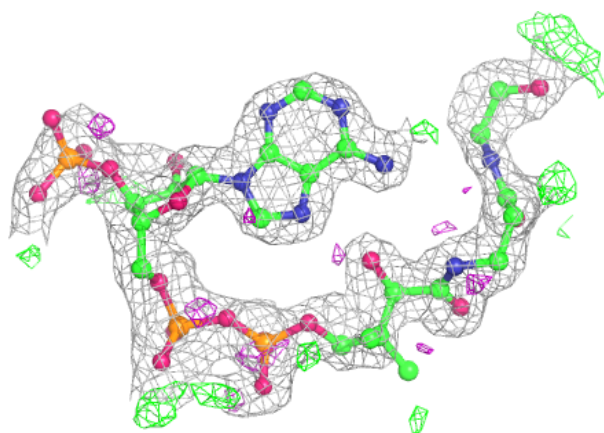
Electron density around KGA F 303 (A):

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



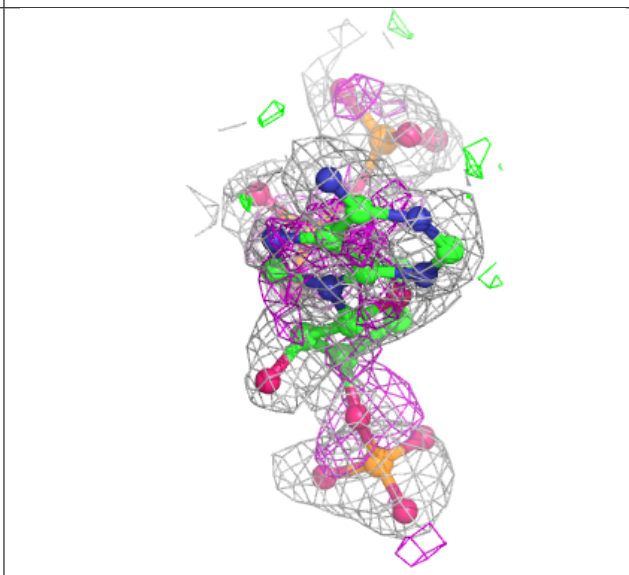
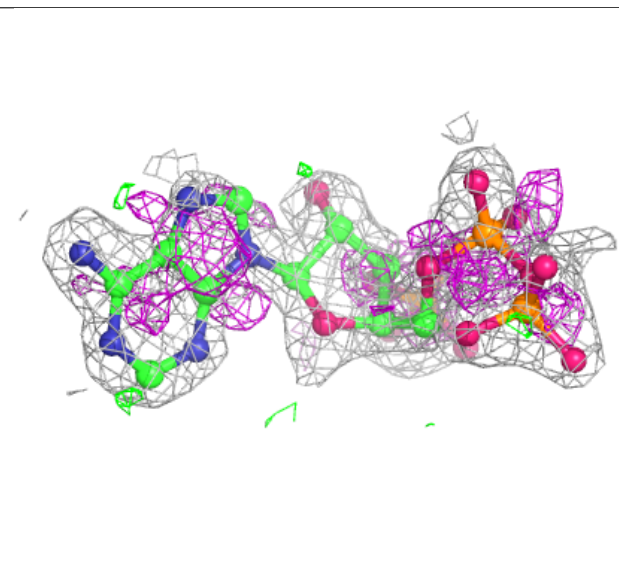
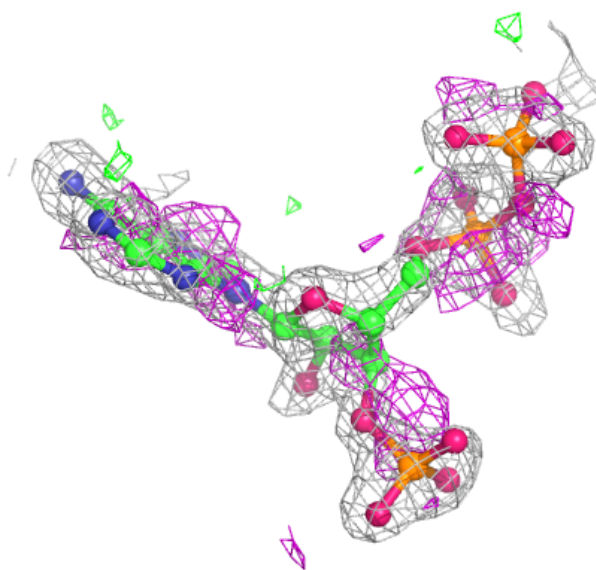
Electron density around KGA C 301:

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



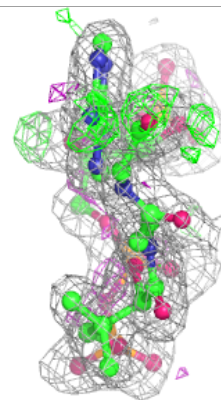
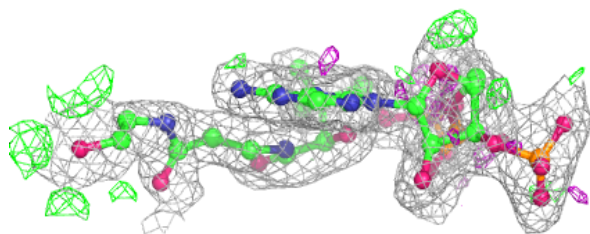
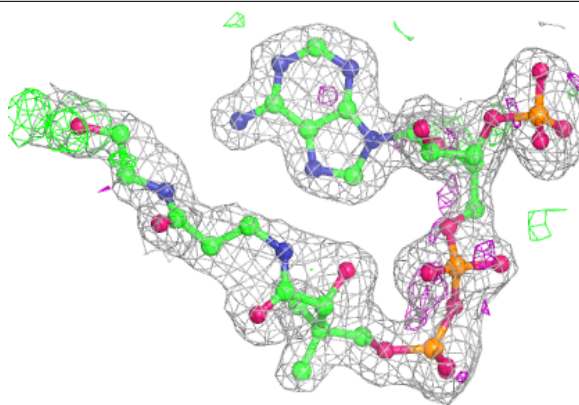
Electron density around KGA E 302 (A):

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

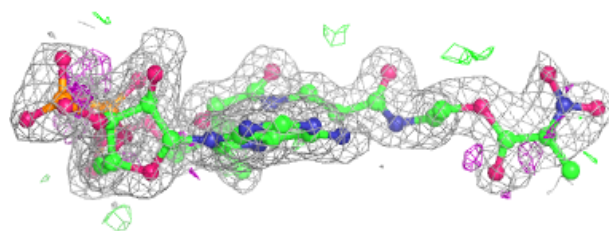
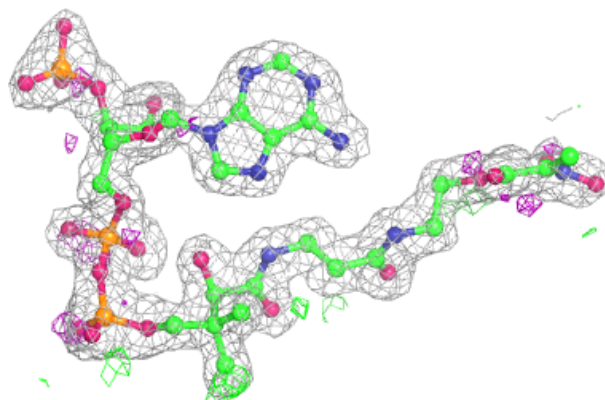


Electron density around KGA A 301:

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

**Electron density around KGA E 301:**

$2mF_o-DF_c$ (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.