



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:10 AM UTC

PDB ID : 6N93 / pdb_00006n93
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 types of validation reports are described at

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

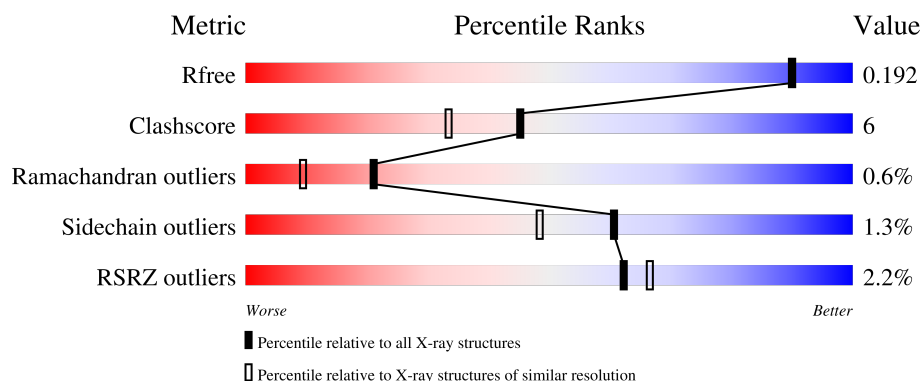
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

i

X-RAY DIFFRACTION

A.

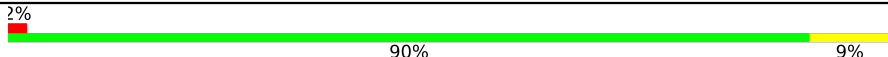


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

Mol	Chain	Length	Quality of chain
1	A	261	91% 8%
1	B	261	2% 92% 7%
1	C	261	3% 90% 10%
1	D	261	3% 90% 10%
1	E	261	2% 87% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	261	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	KG7	F	304	-	X	-	-

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.

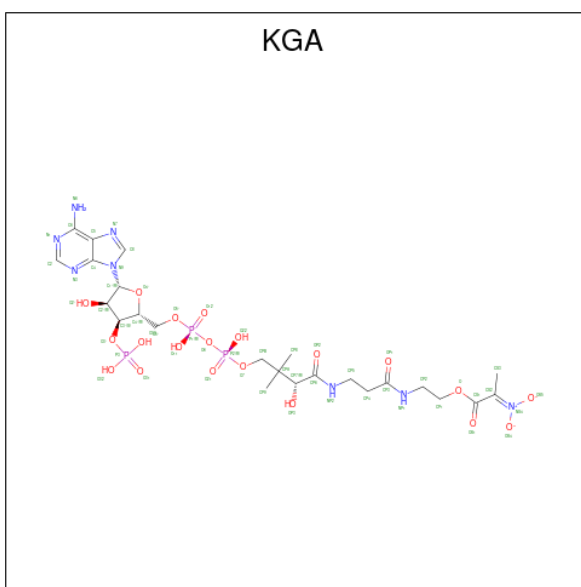
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

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)azanum (CCD ID: KGA) (formula: C₂₄H₃₈N₈O₂₀P₃).

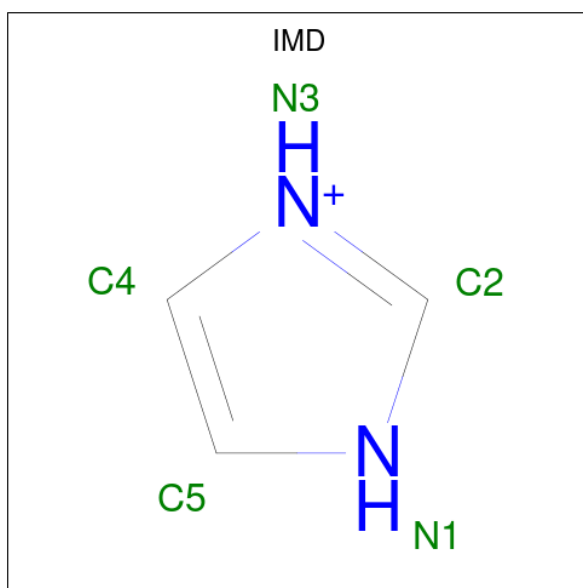


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	1
			86	37	12	31	6		
2	E	1	Total	C	N	O	P	0	0
			55	24	8	20	3		
2	E	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 (CCD ID: 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 (CCD ID: 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 (CCD ID: K) (formula: K).

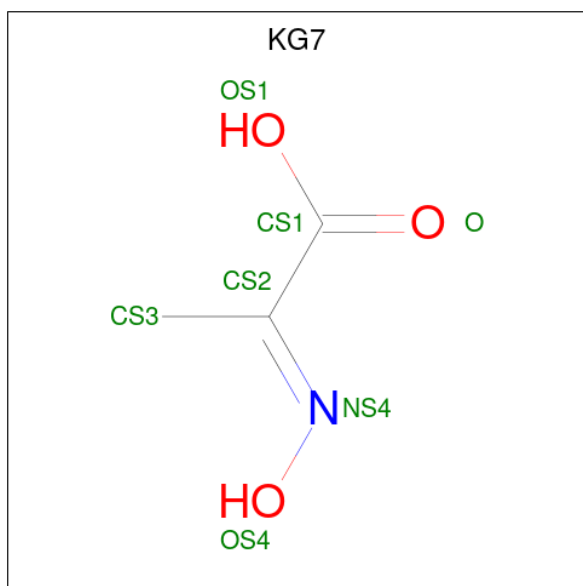
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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 [i](#)

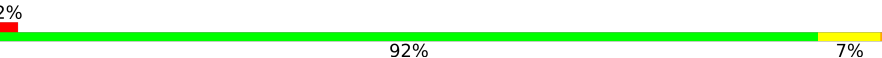
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain A: 



- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain B: 

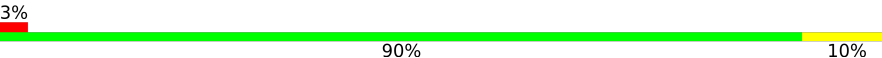


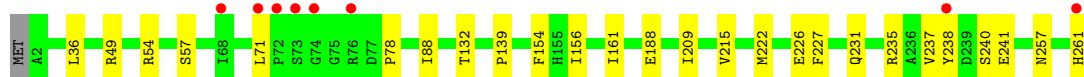
- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain C: 



- Molecule 1: Methylmalonyl-CoA decarboxylase

Chain D: 



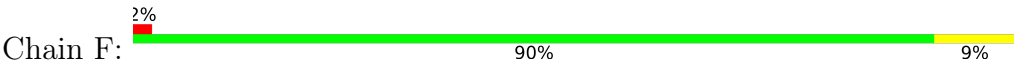
- Molecule 1: Methylmalonyl-CoA decarboxylase

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 28.68 – 1.70	Depositor EDS
% Data completeness (in resolution range)	86.2 (28.68-1.70) 87.2 (28.68-1.70)	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 (4.29%)	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 , 53.5	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, PG4, KGA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	0/2281	1.22	1/3085 (0.0%)
1	B	1.11	0/2213	1.20	1/2994 (0.0%)
1	C	1.10	2/2236 (0.1%)	1.20	2/3025 (0.1%)
1	D	1.10	0/2216	1.23	1/2998 (0.0%)
1	E	1.09	2/2233 (0.1%)	1.21	0/3022
1	F	1.06	0/2256	1.19	0/3052
All	All	1.09	4/13435 (0.0%)	1.21	5/18176 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	167	ILE	C-O	6.21	1.30	1.24
1	E	146	HIS	CE1-NE2	5.80	1.38	1.32
1	C	226	GLU	CD-OE2	-5.63	1.14	1.25
1	E	256	PRO	C-O	-5.31	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	ILE	CB-CA-C	-6.20	103.77	112.14
1	C	68	ILE	N-CA-CB	5.89	118.55	110.54
1	B	132	THR	O-C-N	-5.53	114.96	121.32
1	A	83	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	257	ASN	CA-CB-CG	-5.23	107.37	112.60

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	21	0
1	B	2129	0	2159	19	0
1	C	2143	0	2182	31	0
1	D	2123	0	2168	33	0
1	E	2134	0	2177	44	0
1	F	2153	0	2213	25	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	6	0
8	B	332	0	0	4	0
8	C	326	0	0	5	0
8	D	328	0	0	3	0
8	E	337	0	0	6	0
8	F	338	0	0	5	0
All	All	15344	0	13168	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: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: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: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: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:A:222[A]:MET:HE2	1:A:226[A]:GLU:HG2	1.70	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:A:200[B]:GLU:CD	8:A:408:HOH:O	2.31	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:D:215[A]:VAL:HG11	1:E:222[A]:MET:SD	2.30	0.70
1:F:222[A]:MET:HE2	1:F:227[A]:PHE:CE1	2.27	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: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:OP3	2:B:301:KGA:O12	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:HD2	1:A:23:ARG:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218[A]:GLU:CD	8:A:417:HOH:O	2.42	0.62
1:B:222[A]:MET:HE3	1:B:227[A]:PHE:CE1	2.34	0.62
1:A:196[B]:HIS:HE1	8:A:629:HOH:O	1.83	0.61
1:E:222[B]:MET:HE2	1:E:226:GLU:HB3	1.82	0.60
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:E:66:HIS:ND1	2:E:301:KGA:CS3	2.65	0.58
1:E:131:MET:HG2	1:E:161[B]:ILE:HD12	1.85	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:F:33:ILE:HG22	1:F:37:MET:HE2	1.86	0.57
1:C:68:ILE:HG12	1:C:250:PHE:CD1	2.39	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:83[B]:ASP:CG	8:C:402:HOH:O	2.49	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
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:D:222[B]:MET:HE3	1:D:227[B]:PHE:CE1	2.43	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:C:18[B]:GLU:CD	8:C:444:HOH:O	2.50	0.53
1:D:54:ARG:HH12	1:D:188[B]:GLU:CD	2.16	0.52
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:F:222[A]:MET:HE2	1:F:227[A]:PHE:CD1	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:54:ARG:HH12	1:F:188[B]:GLU:CD	2.20	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:227[B]:PHE:CE2	1:D:231[B]:GLN:HG2	2.45	0.49
1:D:161:ILE:HG21	1:F:209:ILE:HG21	1.93	0.48
1:C:222[A]:MET:HE2	1:C:227[A]:PHE:CE1	2.49	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:222[A]:MET:HE1	1:F:215[A]:VAL:HG12	1.95	0.48
1:F:243:TYR:CE1	1:F:247:MET:HE3	2.49	0.47
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: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: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
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:E:71:LEU:HB3	1:E:247:MET:HE1	1.99	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:222[B]:MET:HE2	1:E:226:GLU:CB	2.48	0.43
1:A:226[A]:GLU:OE1	8:A:403[A]:HOH:O	2.22	0.43
1:B:188[B]:GLU:CD	8:B:438:HOH:O	2.60	0.43
1:E:196[B]:HIS:HE1	8:E:562:HOH:O	2.02	0.43
1:B:224:SER:HA	1:E:227[B]:PHE:CE1	2.54	0.43
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:B:71:LEU:HD21	1:B:247:MET:HE3	2.02	0.42
1:C:108:TRP:HH2	2:C:303[A]:KGA:C4	2.30	0.41
1:E:182[B]:VAL:CG1	1:E:186:GLU:HB2	2.48	0.41
1:C:7:ASN:ND2	8:C:551[B]:HOH:O	2.53	0.41
1:C:68:ILE:HG23	2:C:301:KGA:CP2	2.50	0.41
1:C:227[B]:PHE:CD2	1:D:227[B]:PHE:HB3	2.56	0.41
1:E:231[B]:GLN:NE2	8:E:421:HOH:O	2.52	0.41
1:F:40[A]:LEU:HD12	1:F:40[A]:LEU:HA	1.88	0.41
1:A:222[A]:MET:HE3	1:A:222[A]:MET:HB3	1.85	0.41
1:E:108:TRP:CZ3	2:E:302[A]:KGA:C8	3.04	0.41
1:E:227[A]:PHE:CE2	1:E:231[A]:GLN:HG2	2.56	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
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:B:33:ILE:HG22	1:B:37:MET:HE2	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	282/261 (108%)	270 (96%)	9 (3%)	3 (1%)	11	3
1	B	272/261 (104%)	262 (96%)	8 (3%)	2 (1%)	18	7
1	C	275/261 (105%)	264 (96%)	9 (3%)	2 (1%)	18	7
1	D	274/261 (105%)	266 (97%)	7 (3%)	1 (0%)	30	16
1	E	276/261 (106%)	266 (96%)	9 (3%)	1 (0%)	30	16
1	F	278/261 (106%)	270 (97%)	7 (2%)	1 (0%)	30	16
All	All	1657/1566 (106%)	1598 (96%)	49 (3%)	10 (1%)	21	9

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
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%)	242 (98%)	4 (2%)	55	41
1	B	237/224 (106%)	234 (99%)	3 (1%)	61	48
1	C	240/224 (107%)	237 (99%)	3 (1%)	61	48
1	D	239/224 (107%)	235 (98%)	4 (2%)	53	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	241/224 (108%)	237 (98%)	4 (2%)	53	38
1	F	243/224 (108%)	241 (99%)	2 (1%)	73	65
All	All	1446/1344 (108%)	1426 (99%)	20 (1%)	61	46

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	24	LYS
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	57[A]	SER
1	D	57[B]	SER
1	D	154	PHE
1	D	226	GLU
1	E	66	HIS
1	E	71	LEU
1	E	154	PHE
1	E	235	ARG
1	F	154	PHE
1	F	251	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	26	ASN
1	B	26	ASN
1	B	66	HIS
1	B	193	GLN
1	C	4	GLN
1	C	7	ASN
1	C	26	ASN
1	D	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	12	ASN
1	D	66	HIS
1	F	26	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	KGA	B	301	-	48,50,57	1.16	4 (8%)	70,75,85	1.97	21 (30%)
2	KGA	A	301	-	48,50,57	1.34	7 (14%)	70,75,85	1.90	21 (30%)
2	KGA	D	302[B]	-	48,50,57	1.18	5 (10%)	70,75,85	1.75	17 (24%)
2	KGA	F	303[A]	-	32,33,57	1.62	5 (15%)	50,52,85	1.92	13 (26%)
4	IMD	D	303	-	5,5,5	0.26	0	5,5,5	0.50	0
6	PG4	C	304	5	12,12,12	0.25	0	11,11,11	0.22	0
4	IMD	F	305	3	5,5,5	0.22	0	5,5,5	0.45	0
7	KG7	F	304	3	6,6,6	1.85	2 (33%)	7,7,7	3.56	6 (85%)
2	KGA	E	302[A]	-	32,33,57	1.69	7 (21%)	50,52,85	2.09	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KGA	C	301	-	48,50,57	1.42	7 (14%)	70,75,85	1.66	12 (17%)
2	KGA	F	301	-	51,57,57	1.96	8 (15%)	74,85,85	1.82	17 (22%)
4	IMD	A	303	3	5,5,5	0.42	0	5,5,5	0.51	0
2	KGA	E	301	-	51,57,57	1.65	7 (13%)	74,85,85	1.74	14 (18%)
2	KGA	D	302[A]	-	48,50,57	1.22	6 (12%)	70,75,85	2.05	18 (25%)
2	KGA	C	303[A]	-	32,33,57	1.44	4 (12%)	50,52,85	1.73	10 (20%)

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	KGA	B	301	-	-	22/48/64/75	0/3/3/3
2	KGA	A	301	-	-	4/48/64/75	0/3/3/3
2	KGA	D	302[B]	-	-	10/48/64/75	0/3/3/3
2	KGA	F	303[A]	-	-	3/21/37/75	0/3/3/3
4	IMD	D	303	-	-	-	0/1/1/1
6	PG4	C	304	5	-	1/10/10/10	-
4	IMD	F	305	3	-	-	0/1/1/1
7	KG7	F	304	3	-	0/6/6/6	-
2	KGA	E	302[A]	-	-	4/21/37/75	0/3/3/3
2	KGA	C	301	-	-	4/48/64/75	0/3/3/3
2	KGA	F	301	-	-	4/53/75/75	0/3/3/3
4	IMD	A	303	3	-	-	0/1/1/1
2	KGA	E	301	-	-	1/53/75/75	0/3/3/3
2	KGA	D	302[A]	-	-	13/48/64/75	0/3/3/3
2	KGA	C	303[A]	-	-	7/21/37/75	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	KGA	O-CS1	9.55	1.51	1.33
2	E	301	KGA	O-CS1	7.54	1.47	1.33
2	F	303[A]	KGA	C5-C4	5.86	1.49	1.39
2	C	303[A]	KGA	C5-C4	5.31	1.48	1.39
2	A	301	KGA	C5-C4	5.09	1.48	1.39
2	E	302[A]	KGA	C5-C4	4.90	1.47	1.39
2	C	301	KGA	C5-C4	4.88	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	KGA	C5-C4	4.72	1.47	1.39
2	F	301	KGA	P1-O6	4.65	1.64	1.59
2	D	302[B]	KGA	C5-C4	4.39	1.46	1.39
2	D	302[A]	KGA	C5-C4	4.17	1.46	1.39
7	F	304	KG7	CS3-CS2	3.94	1.57	1.49
2	E	301	KGA	C5-C4	3.90	1.46	1.39
2	E	301	KGA	P1-O6	3.80	1.63	1.59
2	C	301	KGA	P1-O6	3.73	1.63	1.59
2	E	302[A]	KGA	P1-O6	3.67	1.63	1.59
2	B	301	KGA	C5-C4	3.58	1.45	1.39
2	E	301	KGA	P3-O3'	3.37	1.65	1.59
2	F	303[A]	KGA	C5-C6	3.25	1.50	1.41
2	A	301	KGA	P1-O6	3.24	1.63	1.59
2	B	301	KGA	C5-N7	-2.98	1.33	1.39
2	D	302[B]	KGA	C8-N7	2.97	1.37	1.31
2	C	301	KGA	C5-N7	-2.94	1.33	1.39
2	E	302[A]	KGA	P3-O3'	2.91	1.64	1.59
2	C	301	KGA	C5-C6	2.87	1.49	1.41
2	D	302[A]	KGA	P2-O6	2.84	1.62	1.59
2	A	301	KGA	P3-O3'	2.83	1.64	1.59
2	D	302[A]	KGA	P1-O6	2.83	1.62	1.59
2	F	301	KGA	C8-N7	2.80	1.37	1.31
2	B	301	KGA	C4-N9	-2.79	1.31	1.37
2	E	302[A]	KGA	C5-C6	2.77	1.48	1.41
2	C	303[A]	KGA	C8-N7	2.70	1.36	1.31
2	F	301	KGA	P2-O6	2.67	1.62	1.59
2	E	302[A]	KGA	C4-N3	2.66	1.39	1.34
2	C	301	KGA	C4-N9	-2.61	1.32	1.37
2	F	301	KGA	C5-N7	-2.56	1.34	1.39
2	A	301	KGA	C5-N7	-2.55	1.34	1.39
2	D	302[A]	KGA	C5-N7	-2.55	1.34	1.39
2	D	302[B]	KGA	C4-N9	-2.50	1.32	1.37
2	A	301	KGA	C8-N7	2.47	1.36	1.31
2	B	301	KGA	P2-O6	2.45	1.62	1.59
2	E	301	KGA	C5-C6	2.44	1.47	1.41
2	D	302[A]	KGA	C5-C6	2.41	1.47	1.41
2	F	301	KGA	C5-C6	2.40	1.47	1.41
2	D	302[B]	KGA	C5-N7	-2.37	1.34	1.39
2	D	302[B]	KGA	C5-C6	2.36	1.47	1.41
2	A	301	KGA	C4-N9	-2.36	1.32	1.37
2	F	303[A]	KGA	P2-O7	2.34	1.63	1.54
2	E	301	KGA	C8-N7	2.26	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	KGA	C5-N7	-2.25	1.35	1.39
2	E	302[A]	KGA	P2-O7	2.25	1.63	1.54
2	F	301	KGA	C4-N9	-2.19	1.33	1.37
2	E	302[A]	KGA	C8-N7	2.18	1.35	1.31
7	F	304	KG7	O-CS1	2.17	1.27	1.22
2	A	301	KGA	O4'-C1'	2.16	1.47	1.42
2	C	301	KGA	C8-N7	2.15	1.35	1.31
2	C	303[A]	KGA	C5-C6	2.12	1.46	1.41
2	C	301	KGA	P2-O6	2.08	1.61	1.59
2	F	303[A]	KGA	C8-N7	2.08	1.35	1.31
2	C	303[A]	KGA	P2-O7	2.05	1.62	1.54
2	F	303[A]	KGA	C4-N3	2.05	1.38	1.34
2	D	302[A]	KGA	C8-N7	2.01	1.35	1.31

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	KGA	CP1-O-CS1	6.44	129.66	116.55
7	F	304	KG7	CS3-CS2-CS1	6.24	124.00	118.11
2	E	301	KGA	C5-C4-N3	-6.11	118.31	126.72
2	C	301	KGA	C5-C4-N3	-5.65	118.94	126.72
2	E	302[A]	KGA	C4-N9-C8	5.48	111.50	105.74
2	D	302[A]	KGA	C5-C4-N3	-5.41	119.26	126.72
2	F	301	KGA	C5-C4-N3	-5.27	119.46	126.72
2	B	301	KGA	C4-N9-C8	5.25	111.25	105.74
2	E	301	KGA	O-CS1-CS2	5.17	123.14	110.25
2	A	301	KGA	C4-N9-C8	5.12	111.12	105.74
2	E	302[A]	KGA	N3-C2-N1	-5.09	120.88	128.58
2	E	302[A]	KGA	N3-C4-N9	4.94	135.57	127.17
2	D	302[B]	KGA	C5-C4-N3	-4.85	120.03	126.72
2	D	302[A]	KGA	N3-C4-N9	4.81	135.35	127.17
2	E	301	KGA	N3-C4-N9	4.71	135.18	127.17
2	F	303[A]	KGA	C5-C4-N3	-4.62	120.35	126.72
2	C	303[A]	KGA	C5-C4-N3	-4.57	120.43	126.72
2	A	301	KGA	N3-C4-N9	4.55	134.90	127.17
2	E	302[A]	KGA	C5-C4-N3	-4.52	120.49	126.72
2	B	301	KGA	N3-C4-N9	4.50	134.82	127.17
2	A	301	KGA	CP7-CP6-NP2	-4.50	107.94	116.48
2	C	303[A]	KGA	N3-C4-N9	4.44	134.72	127.17
2	B	301	KGA	C5-C4-N3	-4.25	120.87	126.72
2	F	303[A]	KGA	C4-C5-N7	-4.21	105.77	110.58
2	F	301	KGA	N3-C4-N9	4.12	134.18	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303[A]	KGA	N3-C2-N1	-4.10	122.38	128.58
2	E	302[A]	KGA	C2-N3-C4	4.06	121.76	111.83
2	D	302[A]	KGA	O4'-C1'-N9	4.06	115.88	108.09
7	F	304	KG7	O-CS1-CS2	-4.04	116.42	121.35
2	F	303[A]	KGA	N3-C4-N9	3.98	133.94	127.17
2	A	301	KGA	C5-C4-N3	-3.96	121.27	126.72
2	E	301	KGA	C4-C5-N7	-3.94	106.07	110.58
2	C	301	KGA	N3-C4-N9	3.94	133.87	127.17
2	D	302[A]	KGA	CP4-CP3-NP1	3.94	123.52	116.34
2	D	302[B]	KGA	CP4-CP3-NP1	3.94	123.52	116.34
2	D	302[A]	KGA	C4-N9-C8	3.92	109.85	105.74
2	D	302[A]	KGA	CP5-NP2-CP6	3.90	129.55	122.55
2	C	303[A]	KGA	O4'-C1'-N9	3.88	115.54	108.09
2	F	303[A]	KGA	N3-C2-N1	-3.86	122.74	128.58
2	D	302[A]	KGA	CP9-CPA-CP7	3.85	115.34	108.77
2	A	301	KGA	O22-P2-O6	-3.85	96.87	107.27
2	F	303[A]	KGA	C5-N7-C8	3.85	109.50	103.45
2	C	301	KGA	C4-C5-N7	-3.79	106.25	110.58
2	B	301	KGA	N3-C2-N1	-3.76	122.89	128.58
2	D	302[B]	KGA	CP5-NP2-CP6	3.76	129.30	122.55
2	F	303[A]	KGA	O11-P1-O6	3.71	117.30	107.27
2	D	302[B]	KGA	N3-C4-N9	3.70	133.46	127.17
2	D	302[A]	KGA	N3-C2-N1	-3.70	122.99	128.58
2	E	301	KGA	CP9-CPA-CP7	3.68	115.04	108.77
2	E	301	KGA	C2-N3-C4	3.67	120.80	111.83
2	B	301	KGA	N9-C8-N7	-3.59	108.84	113.94
2	D	302[A]	KGA	C2-N3-C4	3.59	120.60	111.83
2	E	302[A]	KGA	N9-C8-N7	-3.55	108.90	113.94
2	F	303[A]	KGA	C4-N9-C8	3.52	109.43	105.74
2	C	301	KGA	CP9-CPA-CP7	3.51	114.74	108.77
2	B	301	KGA	CP5-NP2-CP6	-3.50	116.26	122.55
2	B	301	KGA	C2-N3-C4	3.47	120.31	111.83
2	F	301	KGA	CP5-CP4-CP3	-3.46	106.63	112.39
2	E	301	KGA	CP1-O-CS1	3.43	123.54	116.55
2	C	303[A]	KGA	C4-N9-C8	3.41	109.31	105.74
2	F	303[A]	KGA	C2-N3-C4	3.40	120.13	111.83
2	F	301	KGA	C4-C5-N7	-3.35	106.76	110.58
2	E	301	KGA	C5-N7-C8	3.34	108.70	103.45
2	D	302[B]	KGA	CP9-CPA-CP7	3.30	114.40	108.77
2	B	301	KGA	CP8-CPA-CPB	-3.30	102.78	108.22
2	D	302[A]	KGA	C4-C5-N7	-3.30	106.81	110.58
2	D	302[B]	KGA	C2-N3-C4	3.29	119.86	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302[B]	KGA	N3-C2-N1	-3.28	123.62	128.58
2	F	301	KGA	C2-N3-C4	3.26	119.78	111.83
2	C	301	KGA	C2-N3-C4	3.25	119.76	111.83
2	C	301	KGA	CP9-CPA-CPB	-3.25	102.86	108.22
2	D	302[A]	KGA	C2'-C1'-N9	-3.24	105.24	113.30
2	D	302[B]	KGA	CP7-CP6-NP2	3.23	122.61	116.48
2	D	302[A]	KGA	OP1-CP3-CP4	-3.23	116.17	122.02
2	D	302[B]	KGA	OP1-CP3-CP4	-3.23	116.17	122.02
2	D	302[A]	KGA	CP7-CP6-NP2	3.19	122.54	116.48
2	E	301	KGA	C4-N9-C8	3.16	109.06	105.74
2	A	301	KGA	OP2-CP6-NP2	3.16	129.67	122.98
2	B	301	KGA	CP8-CPA-CP7	3.15	114.14	108.77
2	D	302[A]	KGA	C5-N7-C8	3.15	108.40	103.45
2	D	302[A]	KGA	N9-C8-N7	-3.12	109.51	113.94
2	F	301	KGA	C2'-C3'-C4'	3.12	108.69	103.24
2	B	301	KGA	CP7-CP6-NP2	-3.11	110.58	116.48
2	C	303[A]	KGA	C2-N3-C4	3.11	119.42	111.83
2	A	301	KGA	N9-C8-N7	-3.08	109.56	113.94
2	F	303[A]	KGA	N9-C8-N7	-3.08	109.57	113.94
2	F	301	KGA	CS3-CS2-CS1	3.07	125.80	119.29
2	E	301	KGA	N9-C8-N7	-3.05	109.61	113.94
2	F	301	KGA	N3-C2-N1	-3.04	123.99	128.58
2	E	302[A]	KGA	C5-N7-C8	3.03	108.22	103.45
2	F	303[A]	KGA	C2-N1-C6	3.03	123.71	118.73
2	C	303[A]	KGA	C2-N1-C6	3.00	123.66	118.73
7	F	304	KG7	OS4-NS4-CS2	2.99	121.52	112.25
2	D	302[B]	KGA	P3-O3'-C3'	-2.96	115.53	123.43
2	F	301	KGA	O7-CPB-CPA	-2.94	105.81	110.55
7	F	304	KG7	CS3-CS2-NS4	-2.92	118.84	124.83
7	F	304	KG7	OS1-CS1-CS2	2.91	122.70	116.50
2	C	301	KGA	CP2-NP1-CP3	2.89	128.20	122.82
2	F	301	KGA	C4-N9-C8	2.84	108.72	105.74
2	F	303[A]	KGA	C6-C5-N7	2.83	137.55	132.09
2	A	301	KGA	N3-C2-N1	-2.83	124.30	128.58
2	E	302[A]	KGA	C6-C5-N7	2.79	137.47	132.09
2	D	302[B]	KGA	C4-N9-C8	2.75	108.62	105.74
2	E	302[A]	KGA	C4-C5-N7	-2.71	107.49	110.58
2	F	301	KGA	O-CS1-CS2	2.70	116.98	110.25
2	B	301	KGA	C5-N7-C8	2.69	107.68	103.45
2	E	301	KGA	O11-P1-O6	-2.67	100.05	107.27
2	E	301	KGA	N3-C2-N1	-2.65	124.56	128.58
2	E	302[A]	KGA	C2-N1-C6	2.65	123.08	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302[B]	KGA	C4-C5-N7	-2.63	107.57	110.58
2	B	301	KGA	O4'-C1'-N9	2.62	113.12	108.09
2	E	302[A]	KGA	C4-N9-C1'	-2.62	120.51	126.63
2	C	301	KGA	N3-C2-N1	-2.58	124.68	128.58
2	C	301	KGA	C5-N7-C8	2.58	107.50	103.45
2	A	301	KGA	N6-C6-N1	2.58	124.12	118.38
2	F	303[A]	KGA	O7-P2-O6	2.57	113.25	104.64
2	E	302[A]	KGA	C4'-O4'-C1'	-2.56	103.82	109.47
2	B	301	KGA	C4-N9-C1'	-2.55	120.67	126.63
2	B	301	KGA	C6-C5-N7	2.53	136.97	132.09
2	A	301	KGA	C4-N9-C1'	-2.50	120.79	126.63
7	F	304	KG7	CS1-CS2-NS4	2.47	117.15	114.72
2	B	301	KGA	CP4-CP3-NP1	-2.46	111.86	116.34
2	C	301	KGA	O4'-C4'-C5'	2.45	117.18	109.33
2	A	301	KGA	O4'-C1'-N9	2.43	112.75	108.09
2	B	301	KGA	C5-C6-N6	-2.38	117.39	123.29
2	A	301	KGA	O11-P1-O6	-2.38	100.84	107.27
2	E	302[A]	KGA	O32-P3-O33	2.38	116.72	107.80
2	D	302[A]	KGA	CP1-CP2-NP1	-2.37	106.00	111.60
2	D	302[B]	KGA	CP1-CP2-NP1	-2.37	106.00	111.60
2	D	302[A]	KGA	C2-N1-C6	2.37	122.63	118.73
2	F	301	KGA	O5'-C5'-C4'	-2.37	100.92	108.99
2	A	301	KGA	C2-N1-C6	2.34	122.57	118.73
2	B	301	KGA	C4-C5-N7	-2.33	107.92	110.58
2	C	301	KGA	CP7-CP6-NP2	2.32	120.88	116.48
2	A	301	KGA	C5-N7-C8	2.29	107.05	103.45
2	B	301	KGA	OP1-CP3-NP1	2.29	127.52	123.03
2	F	301	KGA	C5-N7-C8	2.29	107.05	103.45
2	D	302[B]	KGA	N9-C8-N7	-2.26	110.73	113.94
2	A	301	KGA	O4'-C1'-C2'	2.24	111.42	106.62
2	F	303[A]	KGA	C4-N9-C1'	-2.22	121.44	126.63
2	B	301	KGA	O22-P2-O6	2.22	113.26	107.27
2	A	301	KGA	CP5-CP4-CP3	-2.19	108.74	112.39
2	C	303[A]	KGA	O11-P1-O6	2.19	113.18	107.27
2	F	301	KGA	C6-C5-N7	2.18	136.28	132.09
2	B	301	KGA	N6-C6-N1	2.17	123.22	118.38
2	E	301	KGA	C6-C5-N7	2.17	136.27	132.09
2	D	302[A]	KGA	CP4-CP5-NP2	-2.17	107.39	112.00
2	D	302[B]	KGA	CP4-CP5-NP2	-2.17	107.39	112.00
2	E	302[A]	KGA	N6-C6-N1	2.16	123.19	118.38
2	A	301	KGA	CP4-CP5-NP2	2.15	116.57	112.00
2	F	301	KGA	OP1-CP3-CP4	-2.13	118.16	122.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302[B]	KGA	C6-C5-N7	2.13	136.19	132.09
2	E	302[A]	KGA	C5-C6-N6	-2.11	118.06	123.29
2	A	301	KGA	C2-N3-C4	2.10	116.95	111.83
2	F	301	KGA	O2'-C2'-C3'	2.09	117.03	111.19
2	A	301	KGA	C5-C6-N6	-2.09	118.12	123.29
2	C	301	KGA	C2-N1-C6	2.08	122.15	118.73
2	C	303[A]	KGA	N9-C8-N7	-2.07	110.99	113.94
2	E	301	KGA	O6-P2-O21	-2.07	104.48	110.70
2	A	301	KGA	C4'-O4'-C1'	-2.07	104.90	109.47
2	B	301	KGA	O6-P1-O12	2.06	116.90	110.70
2	A	301	KGA	O5'-P1-O12	2.04	117.02	108.94
2	D	302[B]	KGA	C2-N1-C6	2.02	122.05	118.73
2	C	303[A]	KGA	C4-C5-N7	-2.01	108.29	110.58

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	KGA	CP8-CPA-CPB-O7
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	NP2-CP6-CP7-OP3
2	B	301	KGA	CP7-CP6-NP2-CP5
2	B	301	KGA	CP3-CP4-CP5-NP2
2	C	301	KGA	CP6-CP7-CPA-CPB
2	C	303[A]	KGA	C2'-C1'-N9-C8
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	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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	E	302[A]	KGA	C2'-C1'-N9-C4
2	E	302[A]	KGA	C2'-C1'-N9-C8
2	F	301	KGA	O-CS1-CS2-CS3
2	F	303[A]	KGA	C2'-C1'-N9-C8
2	F	303[A]	KGA	P2-O6-P1-O5'
2	A	301	KGA	CP4-CP5-NP2-CP6
2	D	302[A]	KGA	OP2-CP6-NP2-CP5
2	D	302[B]	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	C2'-C1'-N9-C4
2	F	303[A]	KGA	C2'-C1'-N9-C4
2	C	303[A]	KGA	C4'-C3'-O3'-P3
2	D	302[A]	KGA	O-CP1-CP2-NP1
2	D	302[B]	KGA	O-CP1-CP2-NP1
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	F	301	KGA	OS1-CS1-CS2-CS3
2	A	301	KGA	CP4-CP3-NP1-CP2
2	C	301	KGA	O-CP1-CP2-NP1
2	C	301	KGA	CP6-CP7-CPA-CP8
2	B	301	KGA	P1-O6-P2-O22
2	D	302[A]	KGA	P2-O6-P1-O12
2	B	301	KGA	CP4-CP3-NP1-CP2
2	B	301	KGA	OP2-CP6-CP7-OP3
2	B	301	KGA	CP9-CPA-CPB-O7
2	B	301	KGA	CP7-CPA-CPB-O7
2	B	301	KGA	C5'-O5'-P1-O12
2	B	301	KGA	C5'-O5'-P1-O6
2	E	302[A]	KGA	C5'-O5'-P1-O12
2	A	301	KGA	O-CP1-CP2-NP1
2	C	303[A]	KGA	C2'-C3'-O3'-P3
2	B	301	KGA	NP2-CP6-CP7-CPA
2	F	301	KGA	CP4-CP5-NP2-CP6
6	C	304	PG4	C3-C4-O3-C5
2	D	302[A]	KGA	C3'-O3'-P3-O31
2	C	301	KGA	CP6-CP7-CPA-CP9
2	A	301	KGA	P2-O6-P1-O11

Continued on next page...

Continued from previous page...

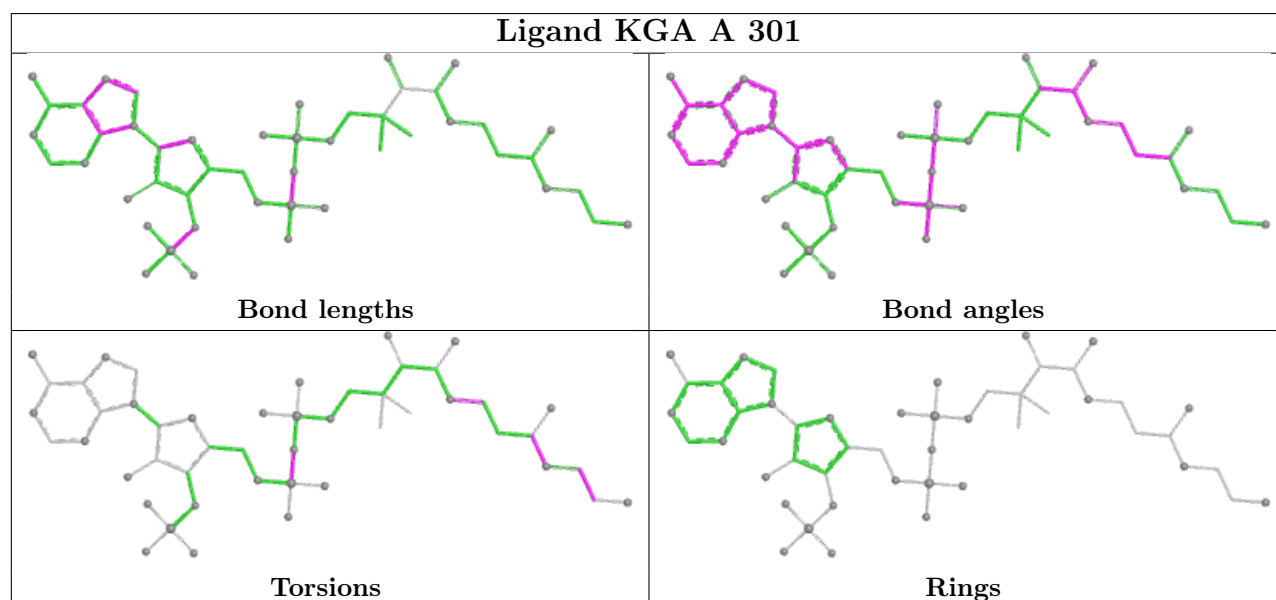
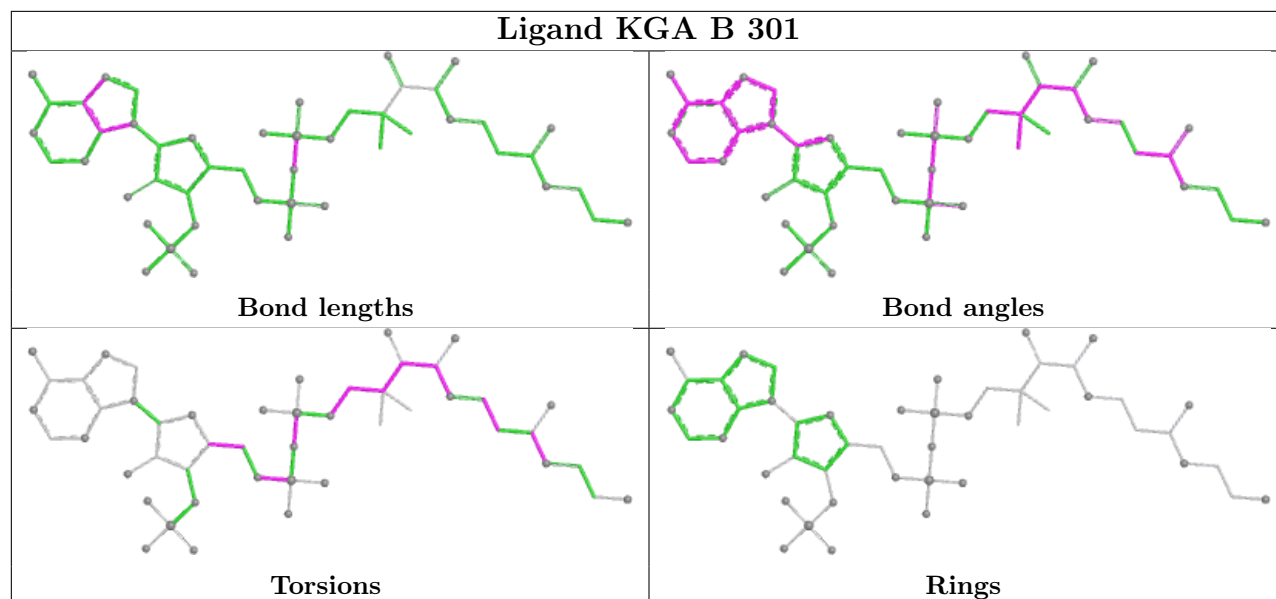
Mol	Chain	Res	Type	Atoms
2	B	301	KGA	P1-O6-P2-O21
2	D	302[A]	KGA	P1-O6-P2-O22
2	D	302[A]	KGA	C3'-O3'-P3-O32
2	E	302[A]	KGA	C3'-O3'-P3-O33
2	B	301	KGA	CPA-CPB-O7-P2
2	E	301	KGA	CP9-CPA-CPB-O7
2	D	302[A]	KGA	P2-O6-P1-O11

There are no ring outliers.

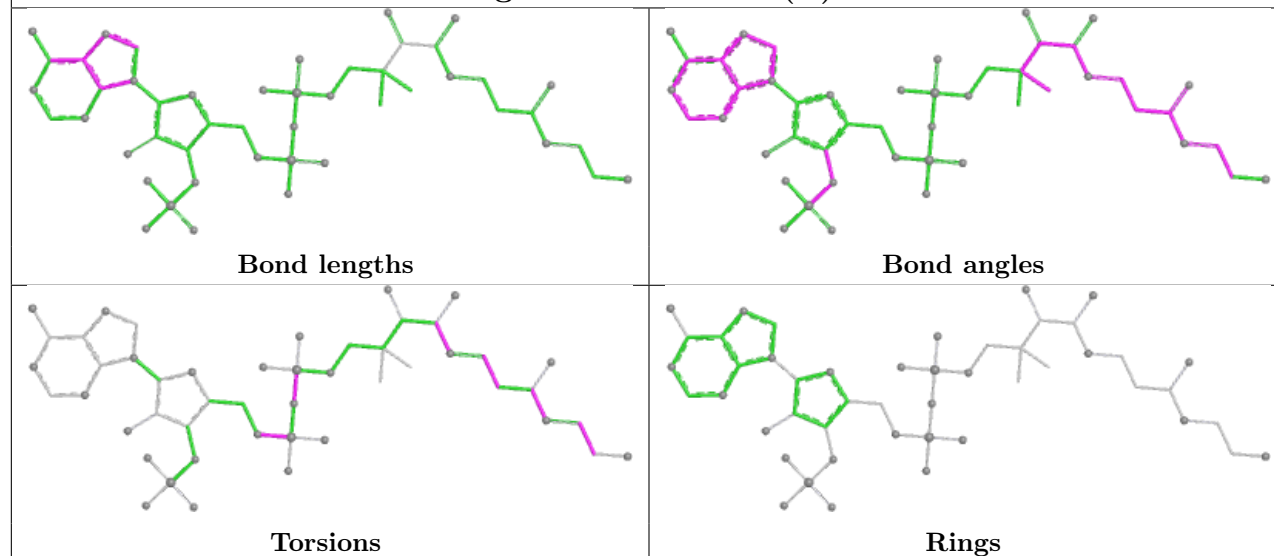
9 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	KGA	3	0
2	A	301	KGA	1	0
2	D	302[B]	KGA	1	0
2	F	303[A]	KGA	8	0
2	E	302[A]	KGA	2	0
2	C	301	KGA	3	0
2	E	301	KGA	1	0
2	D	302[A]	KGA	1	0
2	C	303[A]	KGA	10	0

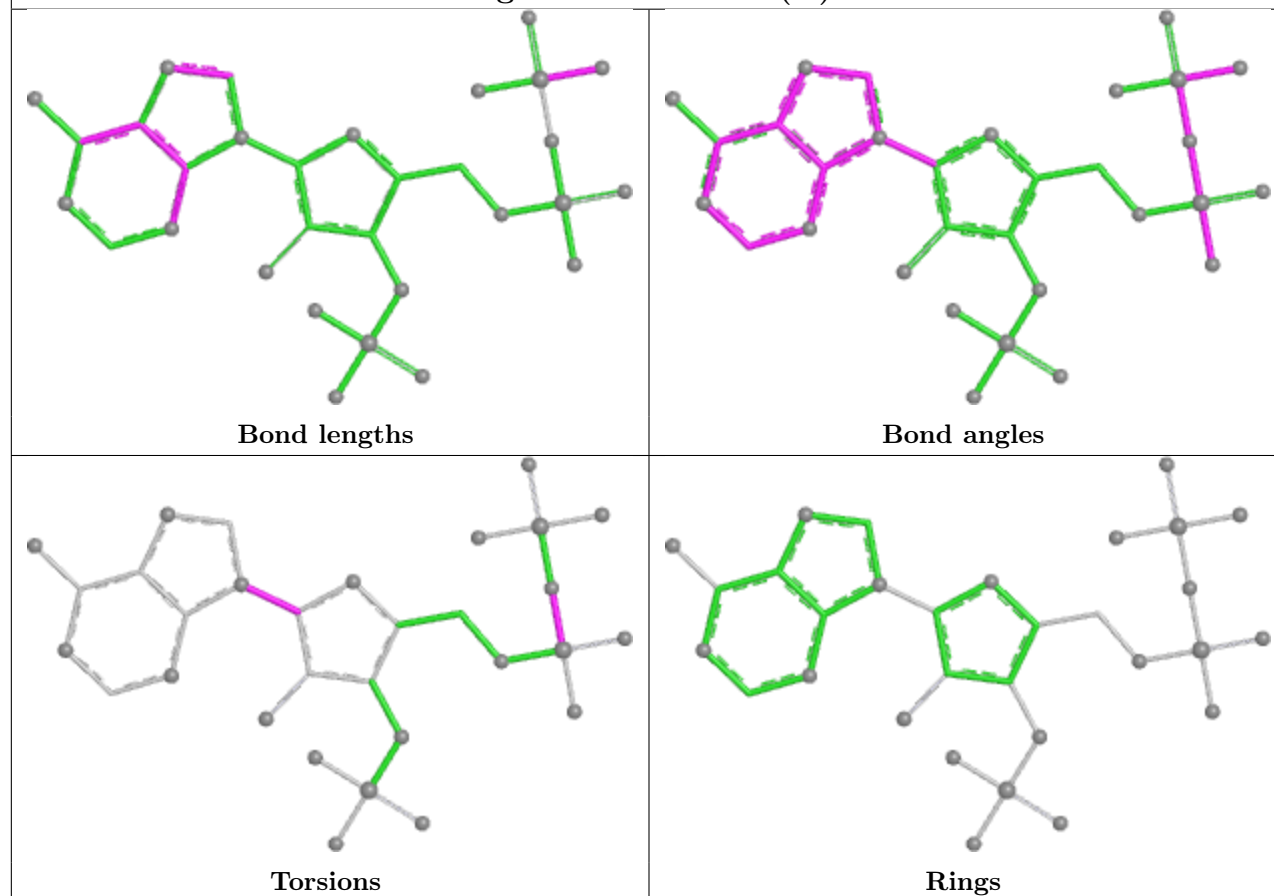
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



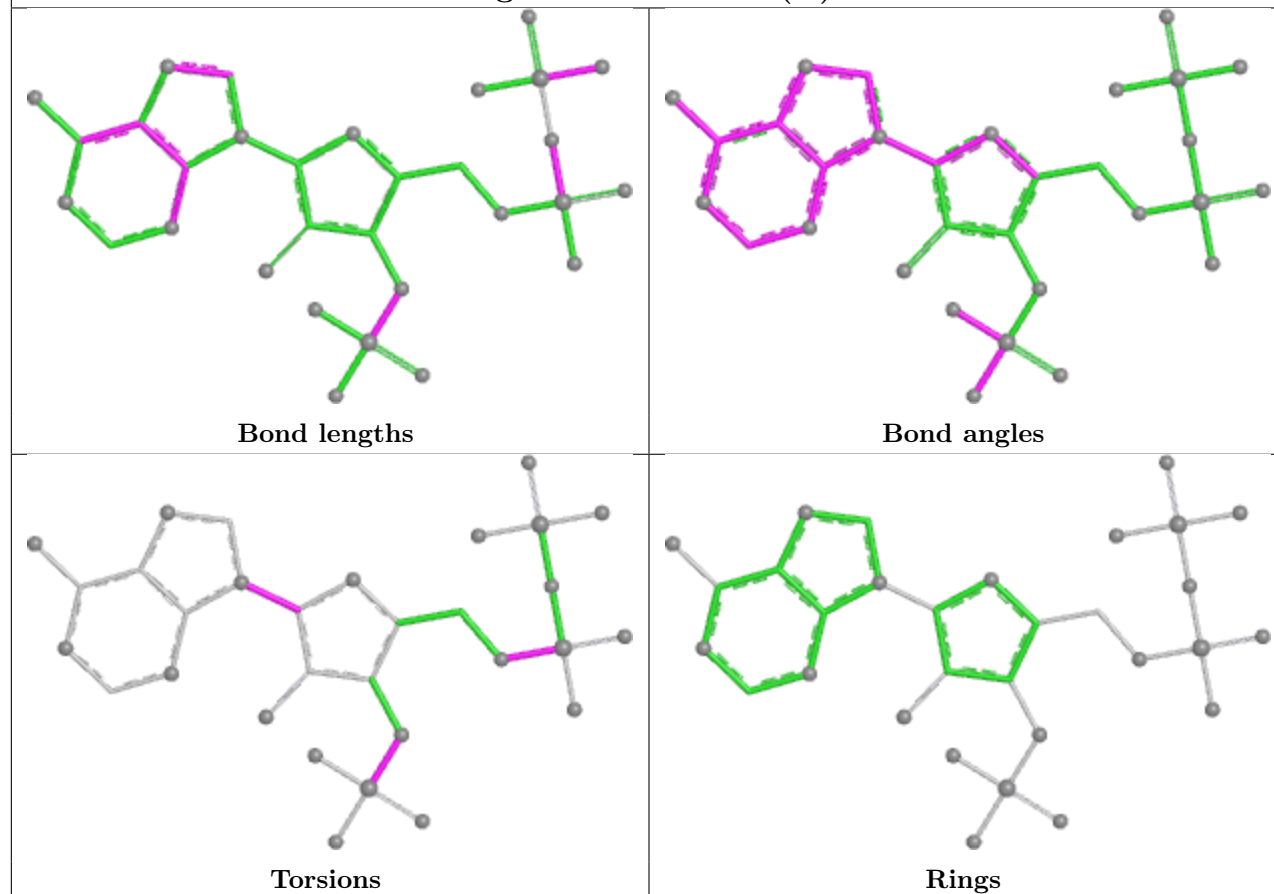
Ligand KGA D 302 (B)



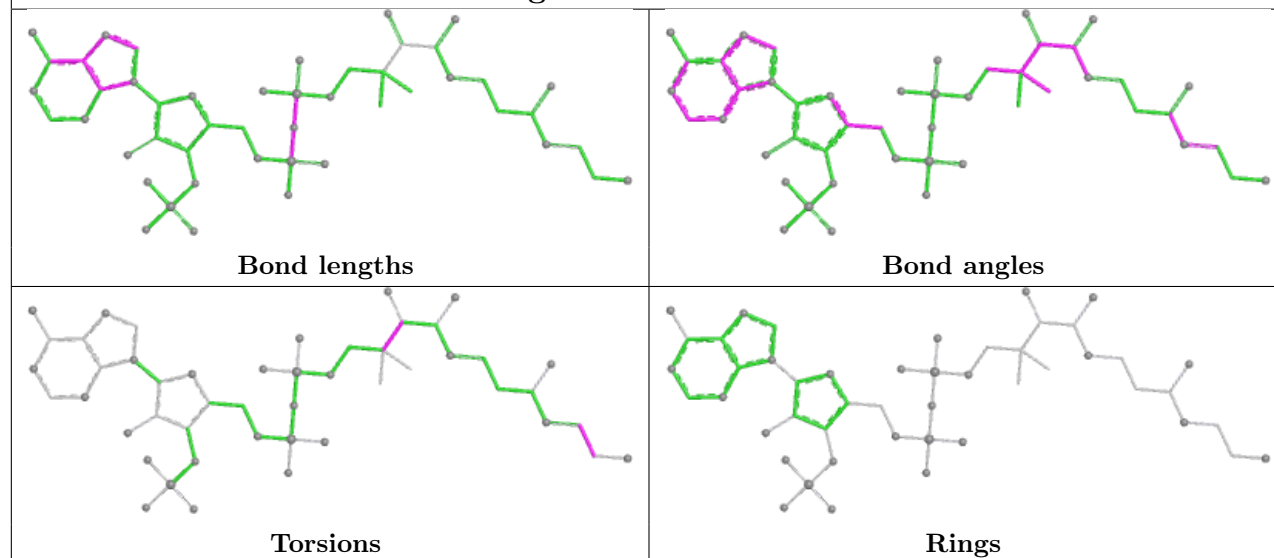
Ligand KGA F 303 (A)

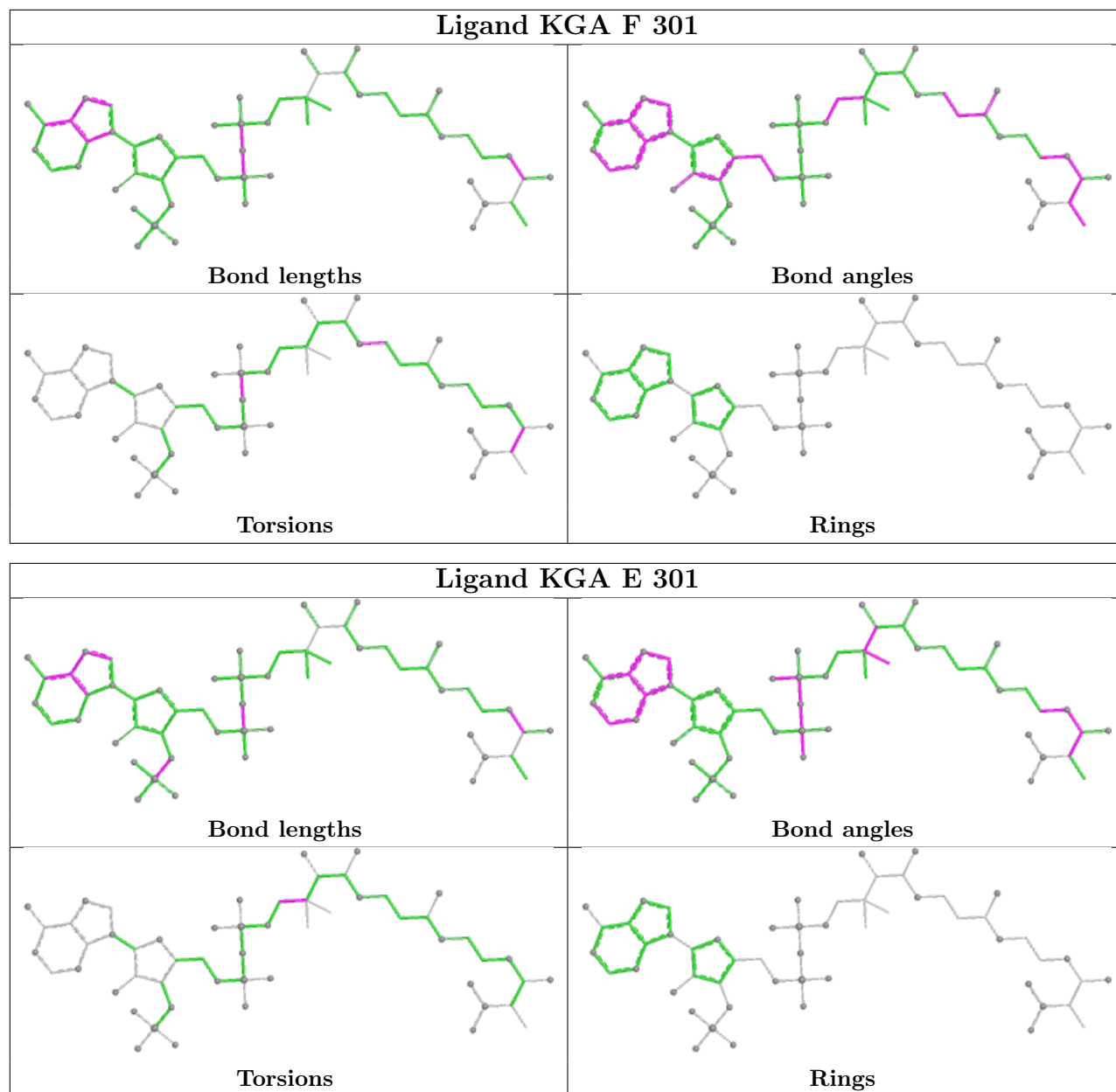


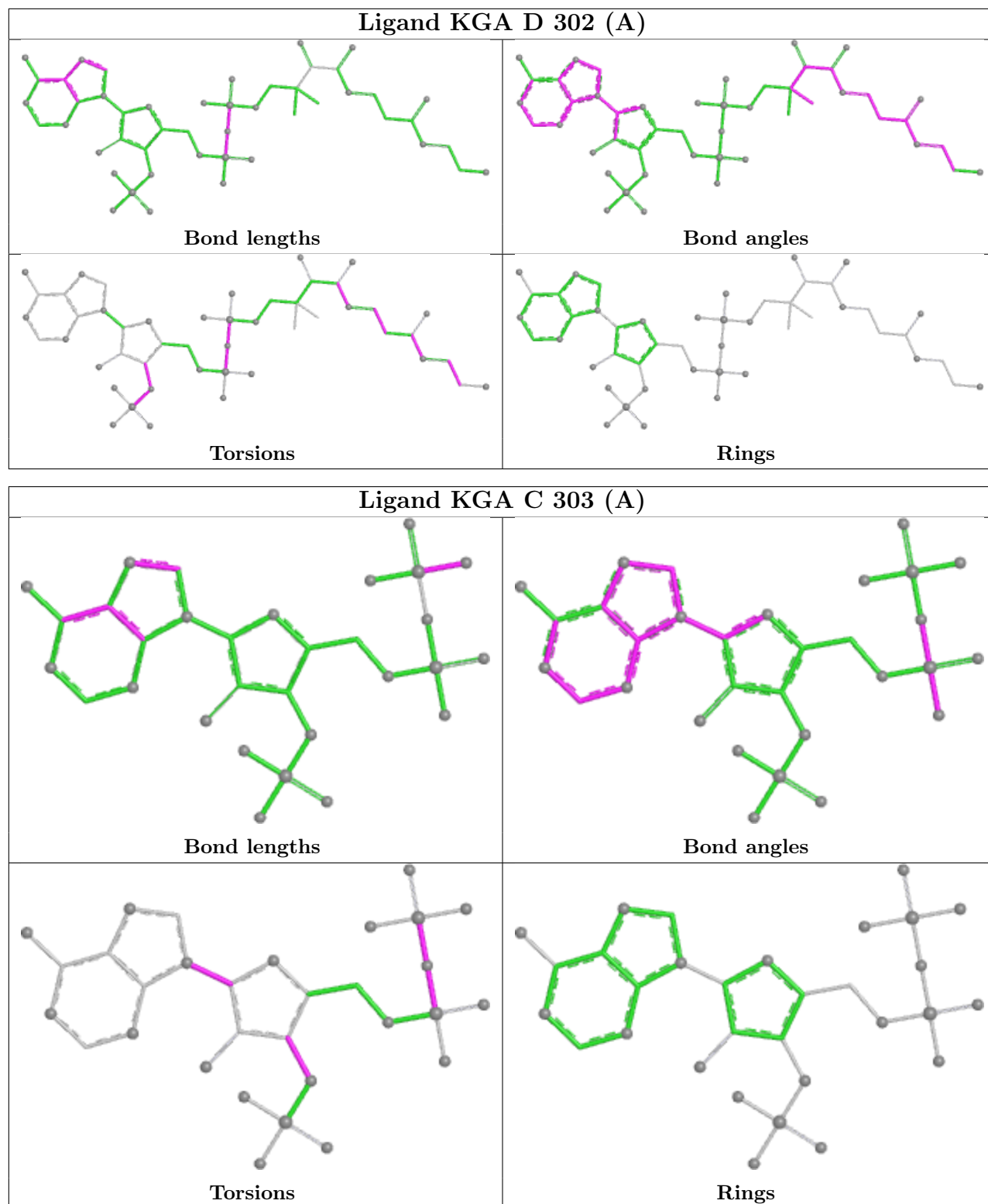
Ligand KGA E 302 (A)



Ligand KGA C 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	260/261 (99%)	-0.52	1 (0%)	88	90	5, 12, 26, 47	24 (9%)
1	B	260/261 (99%)	-0.19	6 (2%)	61	65	5, 14, 33, 62	18 (6%)
1	C	260/261 (99%)	-0.32	9 (3%)	47	52	6, 13, 33, 124	17 (6%)
1	D	260/261 (99%)	-0.31	8 (3%)	51	55	5, 13, 34, 87	16 (6%)
1	E	260/261 (99%)	-0.30	6 (2%)	61	65	5, 13, 35, 93	18 (6%)
1	F	260/261 (99%)	-0.38	4 (1%)	72	76	5, 14, 33, 63	20 (7%)
All	All	1560/1566 (99%)	-0.34	34 (2%)	62	66	5, 13, 33, 124	113 (7%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	LEU	7.4
1	C	71	LEU	7.4
1	B	74	GLY	7.0
1	B	72	PRO	6.5
1	C	72	PRO	6.3
1	B	75	GLY	5.6
1	B	73	SER	4.9
1	E	71	LEU	4.7
1	C	75	GLY	4.7
1	E	75	GLY	4.6
1	D	71	LEU	4.6
1	F	73	SER	4.4
1	B	68	ILE	4.2
1	E	74	GLY	3.8
1	D	72	PRO	3.8
1	C	68	ILE	3.7
1	C	74	GLY	3.7
1	A	23	ARG	3.4
1	E	72	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	73	SER	3.1
1	D	73	SER	3.1
1	D	261	HIS	3.1
1	D	74	GLY	2.9
1	E	73	SER	2.9
1	C	76	ARG	2.8
1	F	72	PRO	2.7
1	D	68	ILE	2.5
1	C	238	TYR	2.5
1	D	76	ARG	2.4
1	C	23	ARG	2.4
1	E	76	ARG	2.3
1	D	238[A]	TYR	2.2
1	F	74	GLY	2.1
1	F	71	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KGA	B	301	48/55	0.78	0.14	29,60,86,90	0
2	KGA	C	303[A]	31/55	0.79	0.18	30,33,41,46	31
2	KGA	F	303[A]	31/55	0.81	0.15	29,37,52,56	31
2	KGA	D	302[B]	48/55	0.82	0.13	28,37,52,57	38
2	KGA	F	301	55/55	0.82	0.13	26,42,69,76	0
2	KGA	D	302[A]	48/55	0.82	0.13	30,42,56,62	38
2	KGA	E	302[A]	31/55	0.85	0.11	23,43,52,58	0
6	PG4	C	304	13/13	0.85	0.14	40,46,53,57	0

Continued on next page...

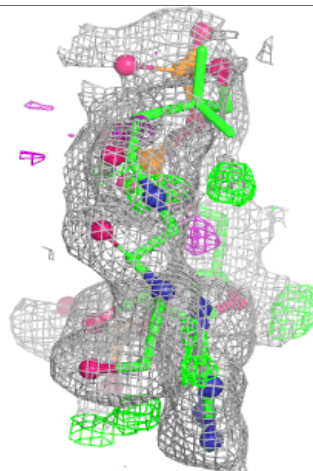
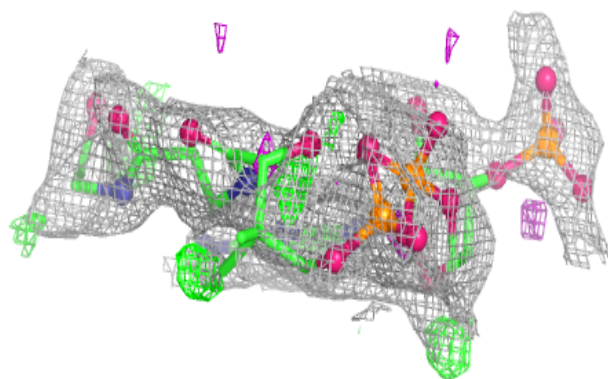
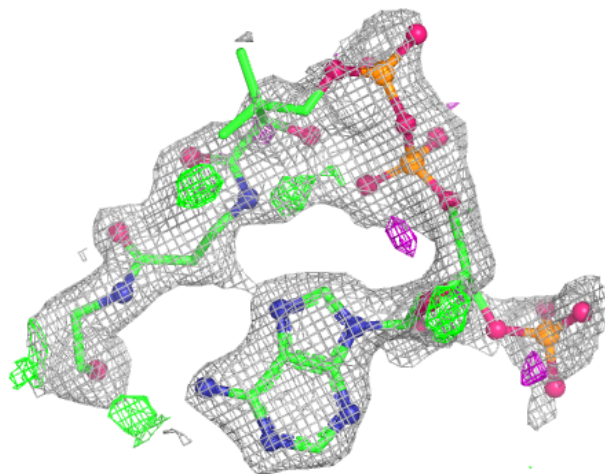
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KGA	C	301	48/55	0.87	0.11	28,41,56,63	0
4	IMD	A	303	5/5	0.90	0.12	38,41,43,43	0
4	IMD	F	305	5/5	0.92	0.12	31,33,33,34	0
2	KGA	A	301	48/55	0.92	0.10	18,36,48,53	0
2	KGA	E	301	55/55	0.93	0.09	23,30,51,57	0
4	IMD	D	303	5/5	0.93	0.15	30,31,33,34	0
7	KG7	F	304	7/7	0.93	0.09	19,21,24,25	0
5	K	C	302	1/1	0.96	0.13	48,48,48,48	0
3	NI	A	302	1/1	0.97	0.04	23,23,23,23	0
3	NI	D	301	1/1	0.98	0.03	21,21,21,21	0
3	NI	F	302	1/1	0.99	0.04	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.

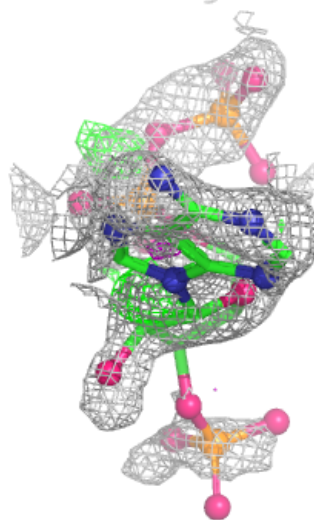
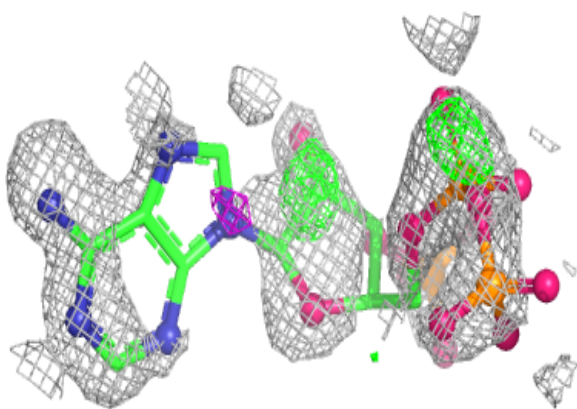
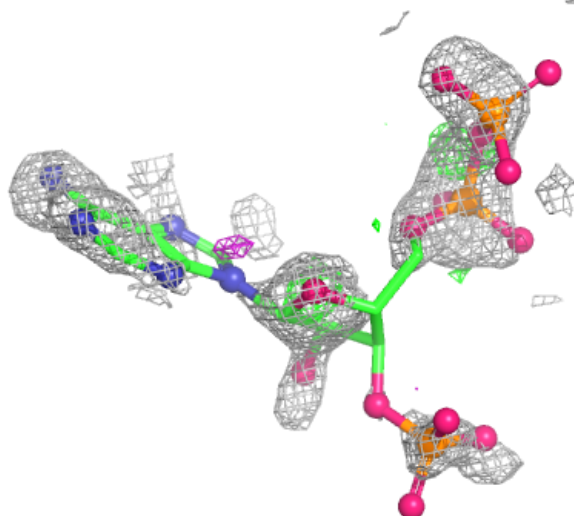
Electron density around KGA B 301:

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



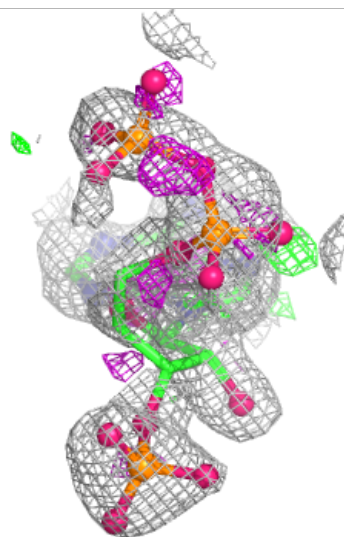
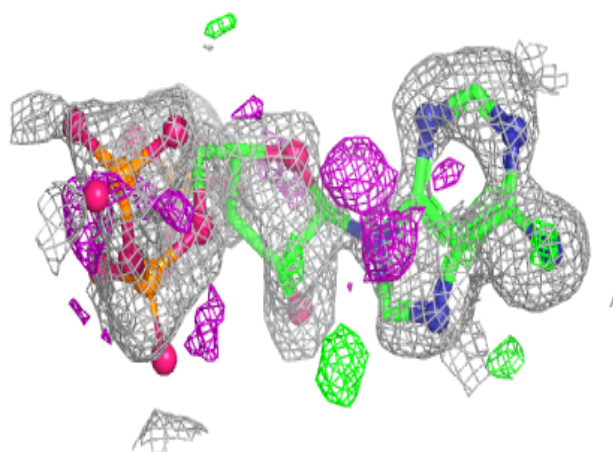
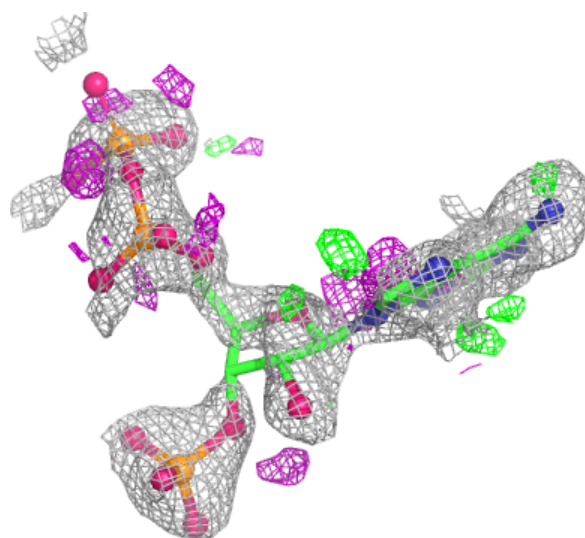
Electron density around KGA C 303 (A):

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



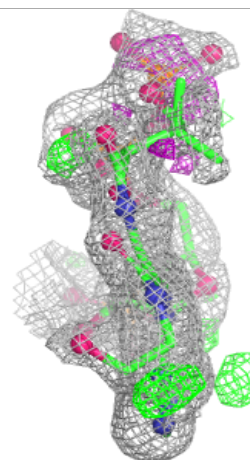
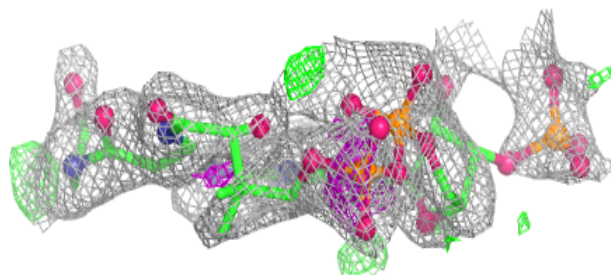
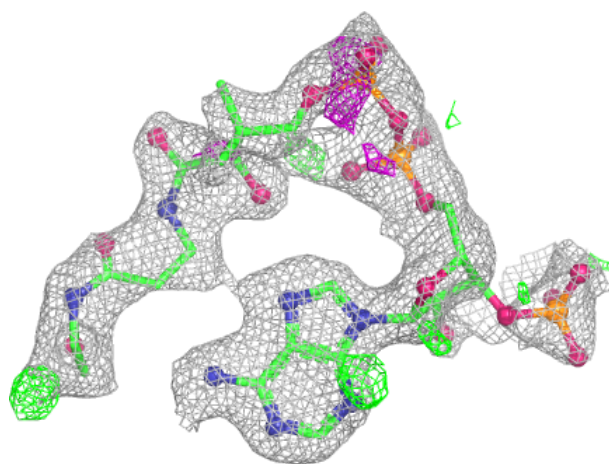
Electron density around KGA F 303 (A):

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



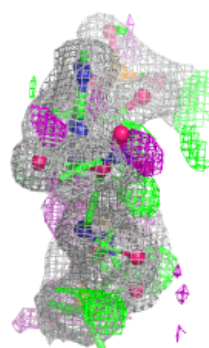
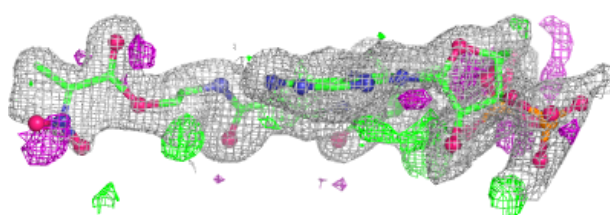
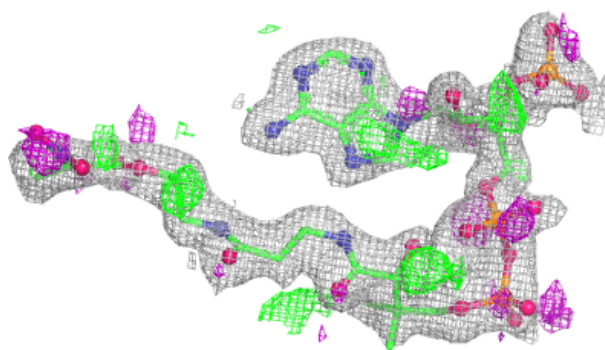
Electron density around KGA D 302 (B):

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

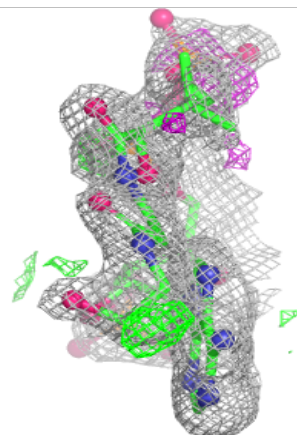
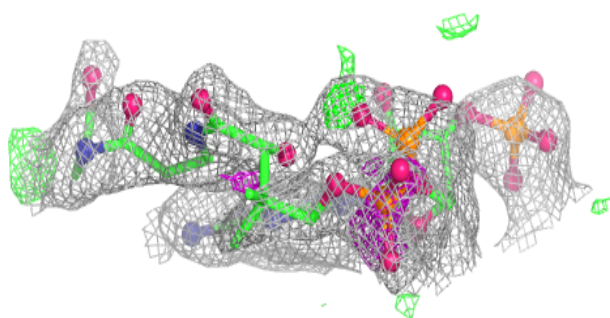
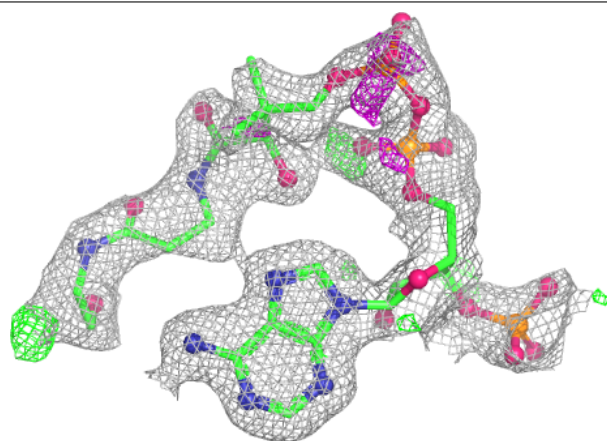


Electron density around KGA F 301:

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

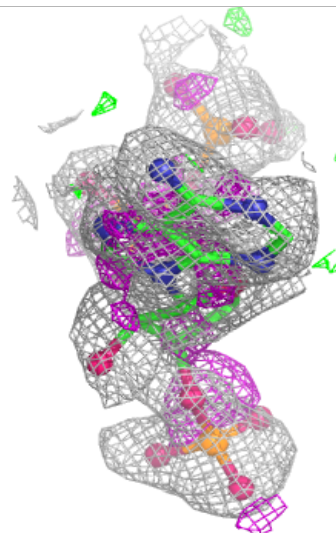
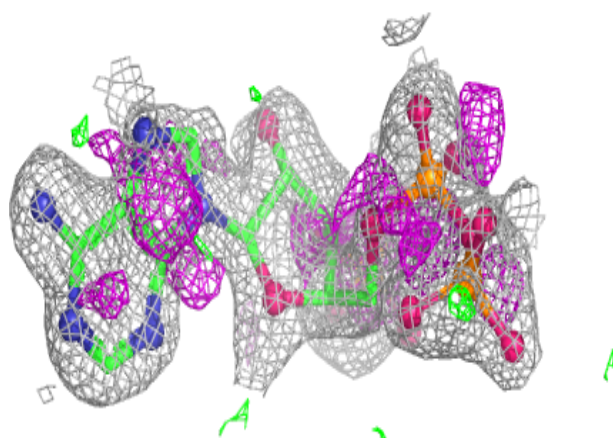
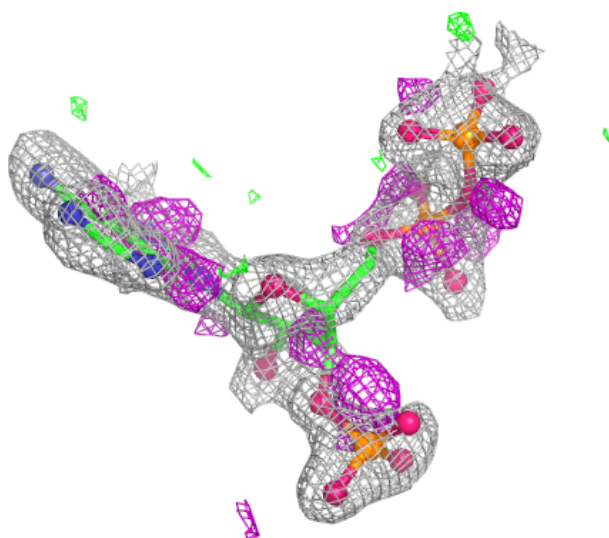
**Electron density around KGA D 302 (A):**

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



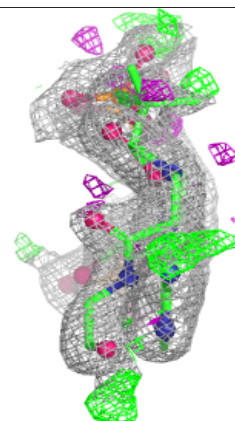
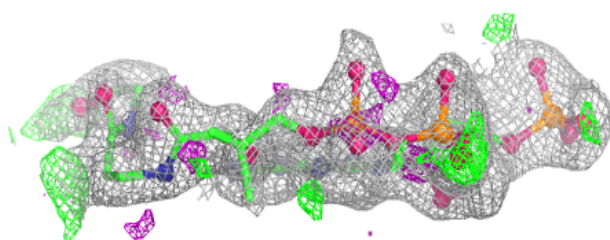
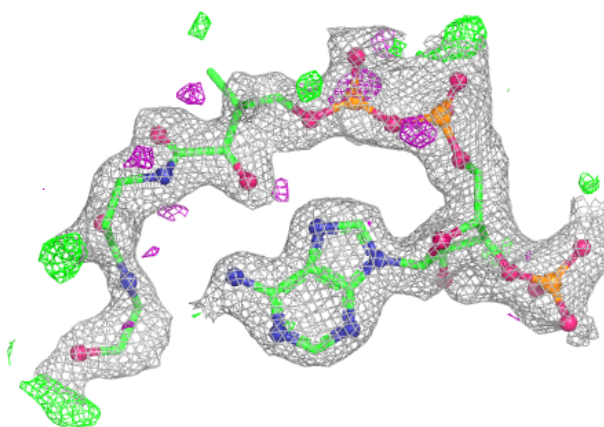
Electron density around KGA E 302 (A):

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

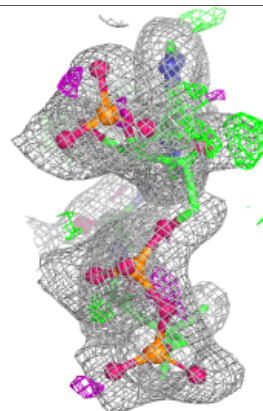
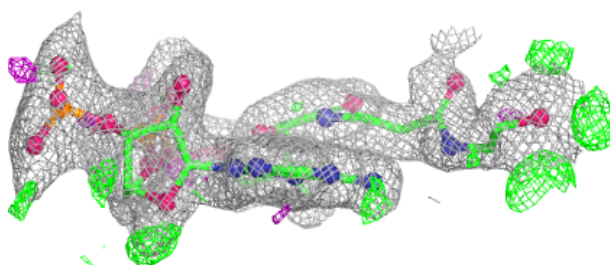
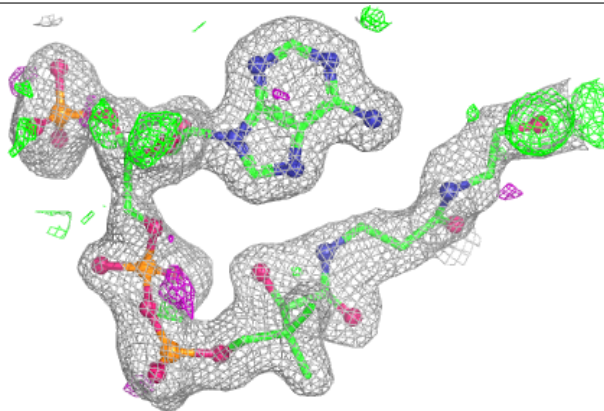


Electron density around KGA C 301:

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

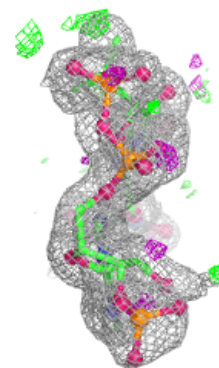
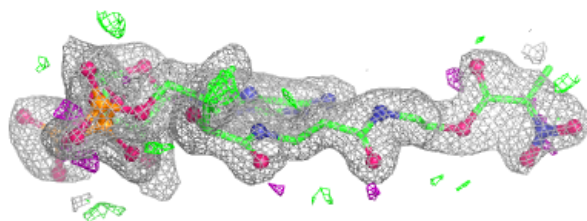
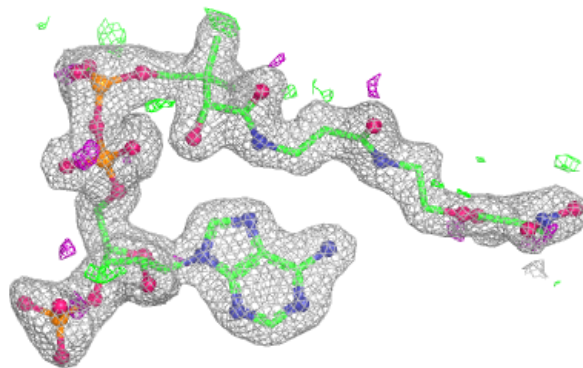
**Electron density around KGA A 301:**

$2mF_o-DF_c$ (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.