



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:32 pm BST

PDB ID : 6N97
Title : Methylmalonyl-CoA decarboxylase in complex with 2-sulfonate-propionyl-amino(dethia)-CoA
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on : 2018-11-30
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

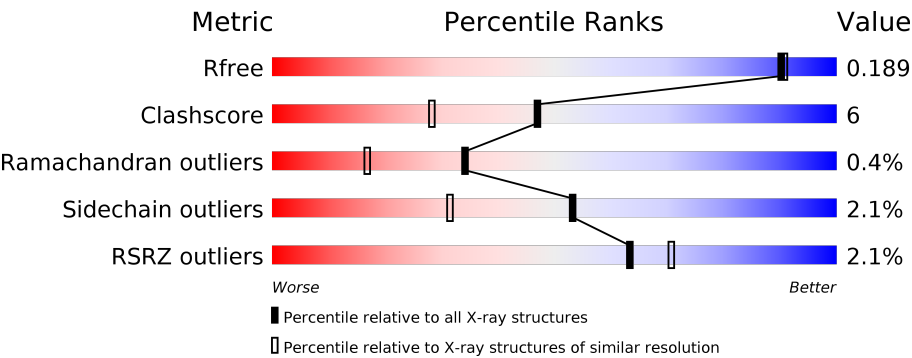
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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></div><div><div></div><div></div><div></div><div></div></div><div>91%8%</div></div>
1	B	261	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>87%13%</div></div>
1	C	261	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>88%11%</div></div>
1	D	261	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>87%13%</div></div>
1	E	261	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>91%8%</div></div>
1	F	261	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%10%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15628 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.

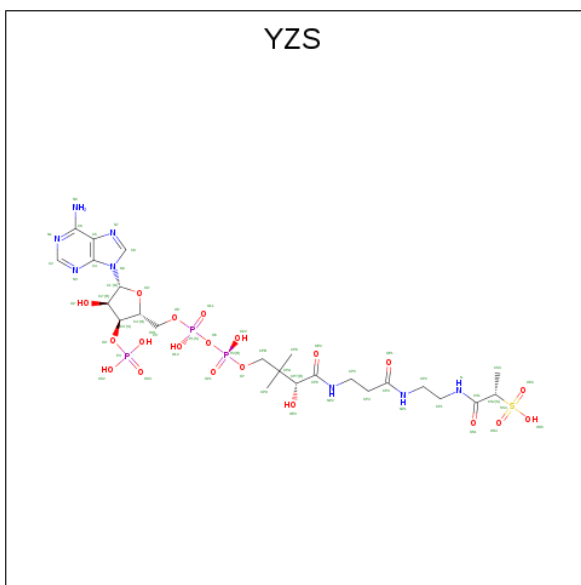
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	18	0
			2142	1373	360	396	13			
1	B	260	Total	C	N	O	S	0	23	0
			2187	1406	372	395	14			
1	C	260	Total	C	N	O	S	0	18	0
			2139	1375	366	386	12			
1	D	260	Total	C	N	O	S	0	23	0
			2170	1395	365	397	13			
1	E	260	Total	C	N	O	S	0	17	0
			2133	1365	364	392	12			
1	F	260	Total	C	N	O	S	0	22	0
			2169	1397	368	391	13			

There are 6 discrepancies between the modelled and reference sequences:

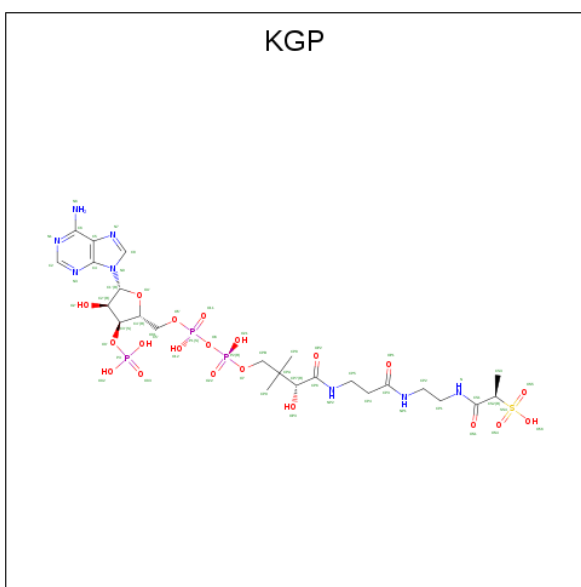
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is (2S)-sulfonatepropionyl-amino(dethia)-CoA (three-letter code: YZS) (formula: C₂₄H₄₁N₈O₂₀P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			56	24	8	20	3	1		
2	B	1	Total	C	N	O	P	S	0	1
			56	24	8	20	3	1		
2	C	1	Total	C	N	O	P	S	0	1
			56	24	8	20	3	1		
2	C	1	Total	C	N	O	P		0	1
			31	10	5	13	3			
2	D	1	Total	C	N	O	P	S	0	1
			56	24	8	20	3	1		
2	E	1	Total	C	N	O	P	S	0	1
			56	24	8	20	3	1		
2	E	1	Total	C	N	O	P		0	1
			31	10	5	13	3			
2	F	1	Total	C	N	O	P	S	0	1
			56	24	8	20	3	1		
2	F	1	Total	C	N	O	P		0	1
			31	10	5	13	3			

- Molecule 3 is (2R)-sulfonatepropionyl-amino(dethia)-CoA (three-letter code: KGP) (formula: C₂₄H₄₁N₈O₂₀P₃S).

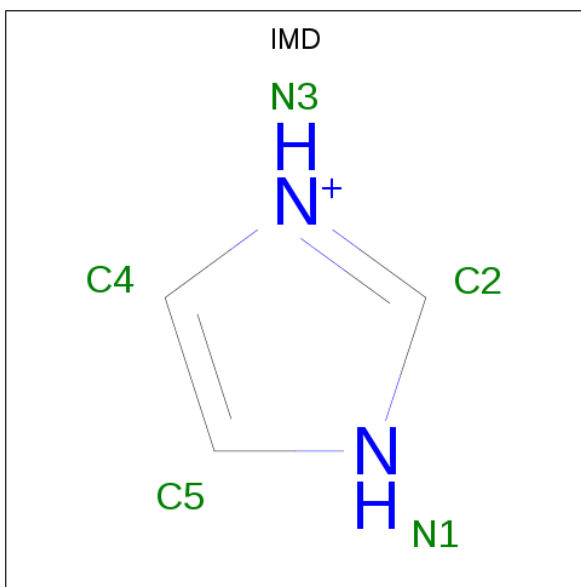


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 56	C 24	N 8	O 20	P 3	S 1	0	1
3	B	1	Total 56	C 24	N 8	O 20	P 3	S 1	0	1
3	C	1	Total 56	C 24	N 8	O 20	P 3	S 1	0	1
3	D	1	Total 56	C 24	N 8	O 20	P 3	S 1	0	1
3	E	1	Total 56	C 24	N 8	O 20	P 3	S 1	0	1
3	F	1	Total 56	C 24	N 8	O 20	P 3	S 1	0	1

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	E	1	Total	Ni	0	0
			1	1		

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	322	Total	O	0	23
			341	341		
6	B	286	Total	O	0	12
			296	296		
6	C	295	Total	O	0	16
			307	307		
6	D	324	Total	O	0	21
			342	342		
6	E	291	Total	O	0	18
			304	304		
6	F	316	Total	O	0	15
			326	326		

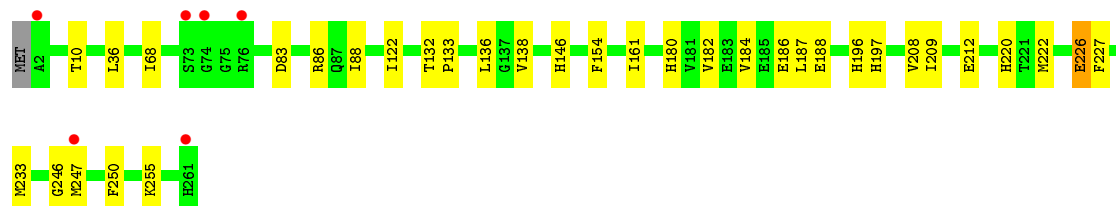
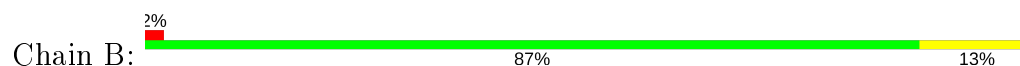
3 Residue-property plots [i](#)

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.

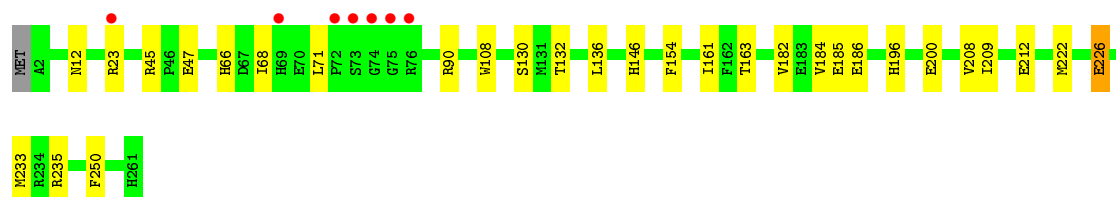
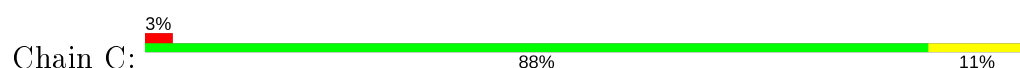
- Molecule 1: Methylmalonyl-CoA decarboxylase



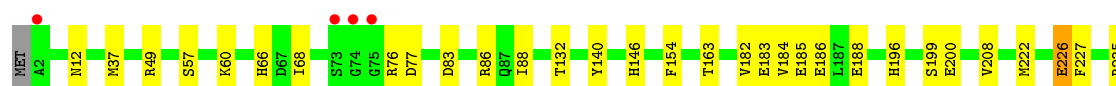
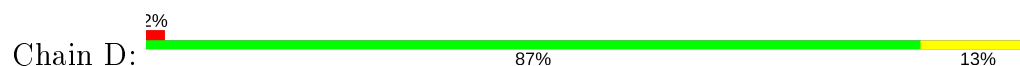
- Molecule 1: Methylmalonyl-CoA decarboxylase

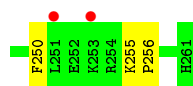


- Molecule 1: Methylmalonyl-CoA decarboxylase



- Molecule 1: Methylmalonyl-CoA decarboxylase

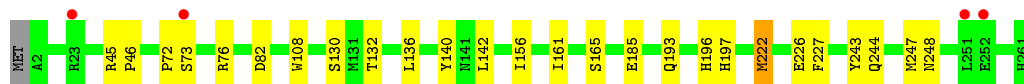
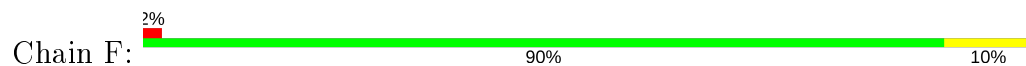




- Molecule 1: Methylmalonyl-CoA decarboxylase



- Molecule 1: Methylmalonyl-CoA decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.96Å 114.61Å 192.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 29.98 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-1.75) 97.0 (29.98-1.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.75Å)	Xtriage
Refinement program	REFMAC refmac_5.8.0238	Depositor
R, R_{free}	0.147 , 0.179 0.161 , 0.189	Depositor DCC
R_{free} test set	9378 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.0	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	0.97	EDS
Total number of atoms	15628	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KGP, YZS, IMD, NI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.82	1/2227 (0.0%)	0.87	1/3012 (0.0%)
1	B	0.77	2/2283 (0.1%)	0.88	1/3088 (0.0%)
1	C	0.83	3/2237 (0.1%)	0.87	1/3026 (0.0%)
1	D	0.85	2/2266 (0.1%)	0.91	3/3065 (0.1%)
1	E	0.79	1/2213 (0.0%)	0.88	3/2994 (0.1%)
1	F	0.77	0/2272	0.89	1/3073 (0.0%)
All	All	0.80	9/13498 (0.1%)	0.88	10/18258 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	226	GLU	CD-OE1	-11.73	1.12	1.25
1	E	226	GLU	CD-OE1	-9.64	1.15	1.25
1	C	226	GLU	CD-OE2	-9.45	1.15	1.25
1	D	185	GLU	CD-OE2	5.78	1.32	1.25
1	B	212	GLU	CD-OE2	-5.66	1.19	1.25
1	C	212	GLU	CD-OE2	-5.52	1.19	1.25
1	A	185	GLU	CD-OE1	5.40	1.31	1.25
1	C	185	GLU	CD-OE1	5.19	1.31	1.25
1	B	212	GLU	CD-OE1	-5.00	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	E	86	ARG	NE-CZ-NH1	-7.71	116.45	120.30
1	D	86	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	86	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	D	235	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	F	82	ASP	CB-CA-C	5.56	121.51	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	E	82	ASP	CB-CA-C	5.39	121.18	110.40
1	C	90	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	E	86	ARG	NE-CZ-NH2	5.03	122.82	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	2142	0	2180	29	0
1	B	2187	0	2245	43	0
1	C	2139	0	2204	26	0
1	D	2170	0	2219	30	0
1	E	2133	0	2165	16	0
1	F	2169	0	2232	41	0
2	A	56	0	0	0	0
2	B	56	0	0	0	0
2	C	87	0	0	8	0
2	D	56	0	0	0	0
2	E	87	0	0	5	0
2	F	87	0	0	17	0
3	A	56	0	0	0	0
3	B	56	0	0	0	0
3	C	56	0	0	1	0
3	D	56	0	0	0	0
3	E	56	0	0	1	0
3	F	56	0	0	1	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
5	D	5	0	5	2	0
6	A	341	0	0	4	0
6	B	296	0	0	8	0
6	C	307	0	0	5	0
6	D	342	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	304	0	0	4	0
6	F	326	0	0	7	0
All	All	15628	0	13250	166	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 (166) 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:D:222[B]:MET:SD	1:D:227[B]:PHE:CE1	2.40	1.14
1:D:222[B]:MET:HG2	1:D:227[B]:PHE:CZ	1.92	1.04
1:F:108:TRP:CH2	2:F:303[A]:YZS:C4	2.41	1.02
1:C:235[A]:ARG:HD2	6:C:461:HOH:O	1.61	0.99
1:F:222[A]:MET:HG2	1:F:227[A]:PHE:CZ	1.97	0.99
1:D:222[B]:MET:CG	1:D:227[B]:PHE:CZ	2.47	0.98
1:F:248:ASN:HB3	6:F:620:HOH:O	1.63	0.96
1:B:222[A]:MET:HE3	1:B:227[A]:PHE:CE1	2.00	0.96
1:F:165:SER:HB3	2:F:303[A]:YZS:O22	1.68	0.94
1:D:222[B]:MET:CG	1:D:227[B]:PHE:CE2	2.51	0.93
1:B:222[A]:MET:CE	1:B:227[A]:PHE:CE1	2.52	0.92
1:F:222[A]:MET:HG2	1:F:227[A]:PHE:CE2	2.03	0.92
1:F:222[A]:MET:SD	1:F:227[A]:PHE:CE1	2.65	0.89
1:D:222[B]:MET:HG3	1:D:227[B]:PHE:CE2	2.09	0.87
1:D:222[B]:MET:SD	1:D:227[B]:PHE:CD1	2.67	0.87
1:F:222[A]:MET:CG	1:F:227[A]:PHE:CE2	2.58	0.86
1:E:215[B]:VAL:HG12	1:F:222[B]:MET:SD	2.16	0.85
1:F:108:TRP:CH2	2:F:303[A]:YZS:C5	2.61	0.83
1:A:222[B]:MET:HE3	1:A:226[B]:GLU:HB3	1.60	0.81
1:B:136:LEU:HD12	1:B:247[A]:MET:CE	2.11	0.81
1:A:215:VAL:HG13	1:B:222[B]:MET:CE	2.12	0.79
1:A:215:VAL:CG1	1:B:222[B]:MET:HE3	2.13	0.78
1:F:108:TRP:CZ3	2:F:303[A]:YZS:C8	2.66	0.78
1:F:222[A]:MET:CG	1:F:227[A]:PHE:CZ	2.67	0.77
1:D:222[B]:MET:SD	1:D:227[B]:PHE:CZ	2.79	0.76
1:F:108:TRP:CZ3	2:F:303[A]:YZS:N7	2.55	0.75
1:C:108:TRP:CZ3	2:C:303[A]:YZS:C8	2.69	0.75
1:B:196[B]:HIS:HD2	6:B:605:HOH:O	1.69	0.74
1:D:222[B]:MET:HG2	1:D:227[B]:PHE:CE2	2.18	0.73
1:A:182[B]:VAL:HG22	6:A:651:HOH:O	1.89	0.72
1:A:215:VAL:CG1	1:B:222[B]:MET:CE	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196[B]:HIS:HD2	6:C:555:HOH:O	1.71	0.72
1:F:196[A]:HIS:HD2	6:F:593:HOH:O	1.71	0.72
1:F:222[A]:MET:SD	1:F:227[A]:PHE:CD1	2.84	0.71
1:A:233[B]:MET:HG2	1:C:208[B]:VAL:HG22	1.72	0.70
1:D:196[B]:HIS:HE1	5:D:303:IMD:HN3	1.37	0.70
1:D:226:GLU:OE2	6:D:401[A]:HOH:O	2.09	0.69
1:D:188[B]:GLU:OE1	6:D:406[B]:HOH:O	2.10	0.68
1:F:73:SER:O	1:F:244[B]:GLN:NE2	2.27	0.68
1:A:222[B]:MET:CE	1:A:226[B]:GLU:HB3	2.22	0.68
1:D:196[B]:HIS:CE1	5:D:303:IMD:HN3	2.12	0.66
1:E:215[B]:VAL:CG1	1:F:222[B]:MET:SD	2.83	0.66
1:B:83:ASP:HB2	6:B:591:HOH:O	1.96	0.66
1:A:215:VAL:HG13	1:B:222[B]:MET:HE3	1.77	0.66
1:F:108:TRP:CZ3	2:F:303[A]:YZS:C5	2.78	0.66
1:A:215:VAL:HG13	1:B:222[B]:MET:HE1	1.76	0.65
1:B:182:VAL:HG11	1:B:187:LEU:HA	1.76	0.65
1:D:146[A]:HIS:HD2	6:D:594:HOH:O	1.79	0.64
1:F:185:GLU:HG3	6:F:406:HOH:O	1.99	0.63
1:B:255[B]:LYS:HG3	6:B:553:HOH:O	1.97	0.63
1:F:108:TRP:HH2	2:F:303[A]:YZS:C4	2.05	0.62
1:B:182:VAL:HG22	1:B:186:GLU:HB2	1.80	0.62
1:C:182[B]:VAL:HG13	1:C:186:GLU:HB2	1.80	0.62
1:D:222[B]:MET:HG3	1:D:227[B]:PHE:CD2	2.34	0.62
1:E:130[A]:SER:HB2	2:E:304[A]:YZS:N7	2.15	0.62
1:B:222[A]:MET:CE	1:B:227[A]:PHE:CZ	2.83	0.61
1:F:130[A]:SER:HB3	2:F:303[A]:YZS:N7	2.15	0.61
1:B:136:LEU:HD12	1:B:247[A]:MET:HE3	1.80	0.61
1:D:66[B]:HIS:HE1	1:D:83:ASP:OD2	1.83	0.61
1:C:108:TRP:CZ3	2:C:303[A]:YZS:N7	2.69	0.60
1:A:182[A]:VAL:HG21	1:A:187:LEU:HA	1.83	0.60
1:A:215:VAL:CG1	1:B:222[A]:MET:SD	2.90	0.59
1:F:130[A]:SER:CB	2:F:303[A]:YZS:N7	2.65	0.59
1:D:66[B]:HIS:CE1	1:D:83:ASP:OD2	2.56	0.59
1:A:226[B]:GLU:HG2	6:A:560:HOH:O	2.03	0.59
1:B:222[A]:MET:HE3	1:B:227[A]:PHE:CZ	2.38	0.58
1:E:10[B]:THR:HG23	6:E:481:HOH:O	2.03	0.58
1:F:222[A]:MET:HG3	1:F:227[A]:PHE:CE2	2.38	0.57
1:D:182[B]:VAL:CG1	1:D:186:GLU:HB2	2.34	0.57
1:F:108:TRP:CH2	2:F:303[A]:YZS:N9	2.72	0.57
1:C:136:LEU:HG	6:C:516:HOH:O	2.05	0.57
1:C:68:ILE:HD12	1:C:250:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:TRP:HZ3	2:F:303[A]:YZS:C8	2.15	0.57
1:C:222[A]:MET:HE3	1:C:226:GLU:HB3	1.88	0.56
1:C:45[A]:ARG:NH2	1:C:47:GLU:OE2	2.36	0.56
1:F:165:SER:CB	2:F:303[A]:YZS:O22	2.51	0.56
1:D:200:GLU:OE2	6:D:402[A]:HOH:O	2.18	0.56
1:F:142[B]:LEU:HD21	1:F:222[B]:MET:CE	2.37	0.55
1:B:188[B]:GLU:HG3	6:B:550[B]:HOH:O	2.07	0.54
1:C:108:TRP:CH2	2:C:303[A]:YZS:C4	2.90	0.54
1:F:243:TYR:CE2	1:F:247:MET:HE1	2.43	0.54
1:E:166:PRO:HB3	2:E:304[A]:YZS:C5	2.38	0.54
1:C:136:LEU:CD1	6:C:516:HOH:O	2.55	0.54
1:E:130[A]:SER:CB	2:E:304[A]:YZS:N7	2.71	0.53
1:E:128:THR:OG1	2:E:304[A]:YZS:N1	2.40	0.53
1:B:136:LEU:HD12	1:B:247[A]:MET:HE2	1.90	0.53
1:F:222[A]:MET:SD	1:F:227[A]:PHE:CZ	3.01	0.53
1:F:222[A]:MET:HG3	1:F:227[A]:PHE:CD2	2.43	0.52
2:F:303[A]:YZS:O7	2:F:303[A]:YZS:O5'	2.27	0.52
1:A:222[B]:MET:HE3	1:A:226[B]:GLU:CB	2.36	0.52
1:E:73:SER:O	1:E:244:GLN:NE2	2.44	0.51
1:B:68:ILE:HD12	1:B:250:PHE:CE2	2.45	0.51
1:D:222[A]:MET:HE3	1:D:226:GLU:HB3	1.93	0.50
1:F:185:GLU:CG	6:F:406:HOH:O	2.57	0.50
1:D:68[B]:ILE:HD12	1:D:250:PHE:CE2	2.47	0.50
1:B:197[B]:HIS:HE1	1:C:163:THR:O	1.95	0.50
1:B:10[A]:THR:HG22	6:B:561:HOH:O	2.11	0.50
1:F:45:ARG:HB3	1:F:46[B]:PRO:HD2	1.93	0.50
1:E:196[B]:HIS:HE1	6:E:571:HOH:O	1.94	0.49
1:B:133:PRO:HB3	1:B:138[B]:VAL:HG22	1.95	0.49
1:D:76:ARG:NH1	6:D:415:HOH:O	2.46	0.48
1:B:247[A]:MET:CE	1:B:247[A]:MET:HA	2.43	0.48
1:A:215:VAL:CG1	1:B:222[B]:MET:HE1	2.39	0.48
1:B:146[B]:HIS:CE1	1:B:220:HIS:ND1	2.81	0.48
1:D:208:VAL:HG23	1:E:233:MET:HE2	1.95	0.47
1:D:68[B]:ILE:HD12	1:D:250:PHE:CZ	2.49	0.47
1:A:215:VAL:HG12	1:B:222[B]:MET:HE3	1.96	0.47
1:B:222[A]:MET:HE2	1:B:227[A]:PHE:CZ	2.48	0.47
1:F:142[B]:LEU:HD21	1:F:222[B]:MET:HE1	1.95	0.47
1:B:222[B]:MET:HE2	1:B:222[B]:MET:HB3	1.24	0.47
1:A:6:VAL:HG11	1:A:36[B]:LEU:HD23	1.97	0.46
1:D:255[A]:LYS:HD2	1:D:256:PRO:HD2	1.96	0.46
1:A:161:ILE:HG21	1:C:209:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TRP:CH2	2:C:303[A]:YZS:C5	2.99	0.46
1:A:215:VAL:HG13	1:B:222[A]:MET:SD	2.55	0.46
1:B:36:LEU:HD23	1:B:88[B]:ILE:CD1	2.46	0.46
1:B:10[B]:THR:HG22	6:B:424:HOH:O	2.16	0.46
6:A:568:HOH:O	1:C:200:GLU:HG2	2.16	0.46
1:A:226[A]:GLU:CD	1:A:229:ARG:HH11	2.20	0.45
1:E:253:LYS:NZ	2:E:302[B]:YZS:O32	2.46	0.45
1:A:40[B]:LEU:HD12	1:A:40[B]:LEU:HA	1.85	0.45
1:D:163:THR:O	1:F:197[B]:HIS:HE1	1.99	0.45
1:B:146[B]:HIS:NE2	1:B:220:HIS:ND1	2.64	0.45
1:A:237:VAL:HG21	1:C:208[B]:VAL:HG21	1.98	0.45
2:F:303[A]:YZS:O12	2:F:303[A]:YZS:C3'	2.65	0.45
1:F:244[A]:GLN:NE2	6:F:403:HOH:O	2.38	0.45
1:C:235[A]:ARG:HD3	6:D:415:HOH:O	2.17	0.45
1:A:211:GLU:HG2	1:B:233[B]:MET:HE1	1.98	0.45
3:F:302[A]:KGP:C4	6:F:563:HOH:O	2.64	0.45
1:C:108:TRP:CH2	2:C:303[A]:YZS:C8	3.00	0.44
2:F:301[B]:YZS:C4	6:F:563:HOH:O	2.64	0.44
1:E:9[B]:VAL:HG12	6:E:572:HOH:O	2.16	0.44
1:F:130[A]:SER:OG	2:F:303[A]:YZS:N7	2.50	0.44
2:C:301[B]:YZS:O5'	2:C:301[B]:YZS:C2'	2.65	0.44
1:E:253:LYS:NZ	3:E:303[A]:KGP:O31	2.49	0.44
3:C:302[A]:KGP:C2'	3:C:302[A]:KGP:O5'	2.66	0.43
1:F:222[A]:MET:CG	1:F:227[A]:PHE:CD2	3.01	0.43
1:A:11:ILE:O	1:A:196[A]:HIS:HE1	2.01	0.43
1:A:233[B]:MET:HE2	1:A:233[B]:MET:HB2	1.77	0.43
1:B:182:VAL:CG1	1:B:187:LEU:HA	2.46	0.43
1:D:182[B]:VAL:HG12	1:D:183:GLU:O	2.18	0.43
1:D:49[A]:ARG:HB2	1:D:199[A]:SER:HB2	2.00	0.43
6:E:596[A]:HOH:O	1:F:156[A]:ILE:HD11	2.18	0.43
1:A:237:VAL:HG21	1:C:208[B]:VAL:CG2	2.48	0.43
1:A:209:ILE:HG21	1:B:161:ILE:HG21	2.01	0.43
1:A:36[B]:LEU:HD23	1:A:36[B]:LEU:HA	1.93	0.43
1:B:136:LEU:O	1:B:246:GLY:HA3	2.19	0.43
1:B:226:GLU:HG2	6:B:508:HOH:O	2.18	0.42
1:D:182[B]:VAL:HG12	1:D:186:GLU:HB2	1.99	0.42
1:E:33:ILE:HD13	1:E:33:ILE:HA	1.92	0.42
1:B:220:HIS:HE1	6:B:574:HOH:O	2.02	0.42
1:D:37:MET:HG2	1:D:88[A]:ILE:HD13	2.02	0.42
1:C:130[A]:SER:OG	2:C:303[A]:YZS:N7	2.53	0.41
1:F:222[A]:MET:HB3	1:F:222[A]:MET:HE3	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122[A]:ILE:HG23	1:B:180:HIS:HB2	2.03	0.41
1:F:72:PRO:HB2	1:F:76:ARG:HB2	2.02	0.41
1:A:215:VAL:HG12	1:B:222[A]:MET:SD	2.58	0.41
1:A:257[B]:ASN:ND2	6:A:418:HOH:O	2.51	0.41
1:E:23[A]:ARG:HB2	1:E:23[A]:ARG:HE	1.81	0.41
1:B:209:ILE:HG21	1:C:161:ILE:HG21	2.02	0.40
1:C:146[A]:HIS:HD2	6:C:549:HOH:O	2.04	0.40
1:C:108:TRP:CH2	2:C:303[A]:YZS:N9	2.89	0.40
1:B:208:VAL:HG23	1:C:233:MET:HE2	2.03	0.40
1:C:235[B]:ARG:HH12	1:D:77:ASP:H	1.68	0.40
1:F:108:TRP:CH2	2:F:303[A]:YZS:C8	3.04	0.40
1:E:209:ILE:HG21	1:F:161:ILE:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	276/261 (106%)	269 (98%)	6 (2%)	1 (0%)	34	17
1	B	281/261 (108%)	274 (98%)	6 (2%)	1 (0%)	34	17
1	C	276/261 (106%)	270 (98%)	5 (2%)	1 (0%)	34	17
1	D	280/261 (107%)	271 (97%)	8 (3%)	1 (0%)	34	17
1	E	274/261 (105%)	265 (97%)	8 (3%)	1 (0%)	34	17
1	F	280/261 (107%)	274 (98%)	5 (2%)	1 (0%)	34	17
All	All	1667/1566 (106%)	1623 (97%)	38 (2%)	6 (0%)	34	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	THR

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Mol	Chain	Res	Type
1	B	132	THR
1	C	132	THR
1	D	132	THR
1	E	132	THR
1	F	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	241/224 (108%)	239 (99%)	2 (1%)	81	72
1	B	246/224 (110%)	242 (98%)	4 (2%)	62	45
1	C	241/224 (108%)	235 (98%)	6 (2%)	47	25
1	D	245/224 (109%)	238 (97%)	7 (3%)	42	19
1	E	239/224 (107%)	231 (97%)	8 (3%)	38	15
1	F	245/224 (109%)	238 (97%)	7 (3%)	42	19
All	All	1457/1344 (108%)	1423 (98%)	34 (2%)	53	28

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	140	TYR
1	B	154	PHE
1	B	184[A]	VAL
1	B	184[B]	VAL
1	B	226	GLU
1	C	12	ASN
1	C	23	ARG
1	C	66	HIS
1	C	71	LEU
1	C	154	PHE
1	C	184	VAL
1	D	12	ASN

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Mol	Chain	Res	Type
1	D	57[A]	SER
1	D	57[B]	SER
1	D	60	LYS
1	D	140	TYR
1	D	154	PHE
1	D	184	VAL
1	E	23[A]	ARG
1	E	23[B]	ARG
1	E	146[A]	HIS
1	E	146[B]	HIS
1	E	154	PHE
1	E	160	LEU
1	E	186	GLU
1	E	261	HIS
1	F	136	LEU
1	F	140	TYR
1	F	193	GLN
1	F	222[A]	MET
1	F	222[B]	MET
1	F	226[A]	GLU
1	F	226[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	69	HIS
1	B	7	ASN
1	B	69	HIS
1	C	12	ASN
1	D	12	ASN
1	E	7	ASN
1	E	20	ASN
1	E	244	GLN
1	F	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\# Z > 2$
3	KGP	D	302[A]	-	47,58,58	1.24	3 (6%)	60,88,88	1.44	7 (11%)
2	YZS	D	301[B]	-	47,58,58	1.25	3 (6%)	60,88,88	1.36	7 (11%)
2	YZS	C	303[A]	-	28,33,58	1.33	3 (10%)	35,52,88	1.46	6 (17%)
2	YZS	F	303[A]	-	28,33,58	1.18	2 (7%)	35,52,88	1.88	10 (28%)
3	KGP	C	302[A]	-	47,58,58	1.28	3 (6%)	60,88,88	1.33	6 (10%)
2	YZS	B	301[B]	-	47,58,58	1.26	3 (6%)	60,88,88	1.39	10 (16%)
2	YZS	C	301[B]	-	47,58,58	1.27	3 (6%)	60,88,88	1.29	8 (13%)
5	IMD	D	303	-	3,5,5	0.22	0	4,5,5	0.72	0
2	YZS	F	301[B]	-	47,58,58	1.23	3 (6%)	60,88,88	3.73	17 (28%)
3	KGP	F	302[A]	-	47,58,58	1.23	3 (6%)	60,88,88	1.84	13 (21%)
2	YZS	E	304[A]	-	28,33,58	1.11	1 (3%)	35,52,88	1.49	6 (17%)
3	KGP	E	303[A]	-	47,58,58	1.24	2 (4%)	60,88,88	3.08	13 (21%)
2	YZS	A	301[B]	-	47,58,58	1.28	3 (6%)	60,88,88	3.27	12 (20%)
2	YZS	E	302[B]	-	47,58,58	1.19	2 (4%)	60,88,88	3.19	11 (18%)
3	KGP	A	302[A]	-	47,58,58	1.29	3 (6%)	60,88,88	3.26	13 (21%)
3	KGP	B	302[A]	-	47,58,58	1.30	3 (6%)	60,88,88	1.56	9 (15%)

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
3	KGP	D	302[A]	-	-	4/54/77/77	0/3/3/3
2	YZS	D	301[B]	-	-	6/54/77/77	0/3/3/3
2	YZS	C	303[A]	-	-	0/17/37/77	0/3/3/3
2	YZS	F	303[A]	-	-	9/17/37/77	0/3/3/3
3	KGP	C	302[A]	-	-	0/54/77/77	0/3/3/3
2	YZS	B	301[B]	-	-	3/54/77/77	0/3/3/3
2	YZS	C	301[B]	-	-	2/54/77/77	0/3/3/3
5	IMD	D	303	-	-	-	0/1/1/1
2	YZS	F	301[B]	-	-	14/54/77/77	0/3/3/3
3	KGP	F	302[A]	-	-	10/54/77/77	0/3/3/3
2	YZS	E	304[A]	-	-	4/17/37/77	0/3/3/3
3	KGP	E	303[A]	-	-	11/54/77/77	0/3/3/3
2	YZS	A	301[B]	-	-	6/54/77/77	0/3/3/3
2	YZS	E	302[B]	-	-	13/54/77/77	0/3/3/3
3	KGP	A	302[A]	-	-	4/54/77/77	0/3/3/3
3	KGP	B	302[A]	-	-	2/54/77/77	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[A]	KGP	CS1-N	6.97	1.48	1.33
3	E	303[A]	KGP	CS1-N	6.55	1.47	1.33
2	B	301[B]	YZS	CS1-N	6.49	1.47	1.33
3	C	302[A]	KGP	CS1-N	6.44	1.47	1.33
2	C	301[B]	YZS	CS1-N	6.29	1.47	1.33
2	D	301[B]	YZS	CS1-N	6.24	1.47	1.33
3	D	302[A]	KGP	CS1-N	6.21	1.47	1.33
3	A	302[A]	KGP	CS1-N	6.12	1.47	1.33
3	F	302[A]	KGP	CS1-N	6.10	1.46	1.33
2	E	302[B]	YZS	CS1-N	6.06	1.46	1.33
2	A	301[B]	YZS	CS1-N	6.03	1.46	1.33
2	F	301[B]	YZS	CS1-N	5.87	1.46	1.33
2	C	303[A]	YZS	C2-N3	3.97	1.38	1.32
2	F	303[A]	YZS	C5-C4	3.26	1.49	1.40
2	C	303[A]	YZS	C5-C4	3.03	1.48	1.40
2	E	304[A]	YZS	C5-C4	2.66	1.48	1.40
2	A	301[B]	YZS	O4'-C1'	2.62	1.44	1.41
3	A	302[A]	KGP	O4'-C1'	2.57	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303[A]	YZS	P2-O7	2.52	1.64	1.54
3	C	302[A]	KGP	O4'-C1'	2.49	1.44	1.41
3	C	302[A]	KGP	C5-C4	2.47	1.47	1.40
2	C	301[B]	YZS	C5-C4	2.47	1.47	1.40
2	C	301[B]	YZS	O4'-C1'	2.45	1.44	1.41
2	D	301[B]	YZS	O4'-C1'	2.37	1.44	1.41
3	D	302[A]	KGP	O4'-C1'	2.36	1.44	1.41
2	E	302[B]	YZS	C5-C4	2.32	1.47	1.40
3	E	303[A]	KGP	C5-C4	2.32	1.47	1.40
2	F	301[B]	YZS	O4'-C1'	2.25	1.44	1.41
3	F	302[A]	KGP	O4'-C1'	2.25	1.44	1.41
2	B	301[B]	YZS	C2-N3	2.22	1.35	1.32
3	B	302[A]	KGP	C2-N3	2.20	1.35	1.32
2	A	301[B]	YZS	C5-C4	2.19	1.46	1.40
3	A	302[A]	KGP	C5-C4	2.19	1.46	1.40
2	F	303[A]	YZS	C8-N7	2.18	1.38	1.34
3	B	302[A]	KGP	C5-C4	2.15	1.46	1.40
2	B	301[B]	YZS	C5-C4	2.11	1.46	1.40
3	F	302[A]	KGP	C5-C4	2.09	1.46	1.40
2	F	301[B]	YZS	C5-C4	2.08	1.46	1.40
3	D	302[A]	KGP	C5-C4	2.05	1.46	1.40
2	D	301[B]	YZS	C5-C4	2.02	1.46	1.40

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302[B]	YZS	CP8-CPA-CPB	-14.03	85.35	108.23
3	E	303[A]	KGP	CP8-CPA-CPB	-13.96	85.47	108.23
2	F	301[B]	YZS	CP8-CPA-CP7	-13.15	86.02	108.82
2	A	301[B]	YZS	CP8-CPA-CPB	-12.64	87.62	108.23
3	A	302[A]	KGP	CP8-CPA-CPB	-12.63	87.63	108.23
2	F	301[B]	YZS	CP9-CPA-CP7	12.56	130.59	108.82
2	F	301[B]	YZS	CP8-CPA-CPB	-11.59	89.33	108.23
2	A	301[B]	YZS	CP8-CPA-CP7	-10.74	90.19	108.82
3	A	302[A]	KGP	CP8-CPA-CP7	-10.73	90.22	108.82
2	F	301[B]	YZS	CP8-CPA-CP9	-9.97	88.85	109.17
2	F	301[B]	YZS	OS4-SS4-CS2	-9.83	102.89	109.43
2	E	302[B]	YZS	CP8-CPA-CP7	-9.47	92.41	108.82
3	E	303[A]	KGP	CP8-CPA-CP7	-9.42	92.49	108.82
3	A	302[A]	KGP	CP8-CPA-CP9	-9.40	90.00	109.17
2	A	301[B]	YZS	CP8-CPA-CP9	-9.39	90.03	109.17
2	A	301[B]	YZS	O56-SS4-CS2	-9.10	103.37	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[A]	KGP	OS4-SS4-CS2	-8.82	103.56	109.43
2	E	302[B]	YZS	OS4-SS4-CS2	-8.66	103.66	109.43
3	B	302[A]	KGP	OS4-SS4-CS2	-7.40	104.50	109.43
3	A	302[A]	KGP	CP9-CPA-CPB	7.21	119.99	108.23
2	A	301[B]	YZS	CP9-CPA-CPB	7.20	119.97	108.23
3	E	303[A]	KGP	CP8-CPA-CP9	-7.16	94.57	109.17
2	E	302[B]	YZS	CP8-CPA-CP9	-7.14	94.61	109.17
3	E	303[A]	KGP	CP9-CPA-CP7	6.77	120.55	108.82
2	E	302[B]	YZS	CP9-CPA-CP7	6.76	120.54	108.82
3	C	302[A]	KGP	OS5-SS4-CS2	-6.47	105.12	109.43
3	A	302[A]	KGP	OP3-CP7-CPA	-5.88	96.41	110.25
2	A	301[B]	YZS	OP3-CP7-CPA	-5.87	96.42	110.25
3	E	303[A]	KGP	CP9-CPA-CPB	5.78	117.67	108.23
2	E	302[B]	YZS	CP9-CPA-CPB	5.62	117.40	108.23
3	D	302[A]	KGP	OS5-SS4-CS2	-5.62	105.69	109.43
3	E	303[A]	KGP	OS4-SS4-CS2	-5.47	105.79	109.43
2	C	301[B]	YZS	O56-SS4-CS2	-5.38	105.85	109.43
3	F	302[A]	KGP	OS5-SS4-CS2	-5.30	105.90	109.43
3	A	302[A]	KGP	CP9-CPA-CP7	5.17	117.79	108.82
2	A	301[B]	YZS	CP9-CPA-CP7	5.17	117.78	108.82
2	F	301[B]	YZS	P2-O6-P1	-5.13	115.22	132.83
3	E	303[A]	KGP	OS5-SS4-CS2	-5.10	106.03	109.43
3	F	302[A]	KGP	P2-O6-P1	-5.01	115.65	132.83
2	E	302[B]	YZS	P2-O6-P1	-4.84	116.23	132.83
3	E	303[A]	KGP	P2-O6-P1	-4.80	116.37	132.83
2	F	301[B]	YZS	O56-SS4-CS2	-4.77	106.25	109.43
3	E	303[A]	KGP	OP3-CP7-CPA	-4.73	99.12	110.25
3	F	302[A]	KGP	OS4-SS4-CS2	-4.60	106.37	109.43
2	E	302[B]	YZS	OP3-CP7-CPA	-4.59	99.44	110.25
2	E	302[B]	YZS	O56-SS4-CS2	-4.41	106.49	109.43
2	B	301[B]	YZS	O56-SS4-CS2	-4.26	106.59	109.43
2	D	301[B]	YZS	OS4-SS4-CS2	-4.21	106.63	109.43
2	F	303[A]	YZS	P1-O6-P2	-4.11	118.71	132.83
2	D	301[B]	YZS	P2-O6-P1	-4.07	118.85	132.83
3	D	302[A]	KGP	P2-O6-P1	-4.04	118.96	132.83
2	C	303[A]	YZS	N3-C2-N1	-4.01	122.41	128.68
2	E	304[A]	YZS	P1-O6-P2	-3.88	119.52	132.83
3	D	302[A]	KGP	N3-C2-N1	-3.84	122.68	128.68
2	D	301[B]	YZS	N3-C2-N1	-3.81	122.72	128.68
3	F	302[A]	KGP	C5'-C4'-C3'	-3.80	101.82	114.40
3	E	303[A]	KGP	N3-C2-N1	-3.74	122.83	128.68
2	E	302[B]	YZS	N3-C2-N1	-3.74	122.83	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[B]	YZS	CP5-CP4-CP3	-3.74	106.13	112.36
3	B	302[A]	KGP	CP5-CP4-CP3	-3.72	106.16	112.36
2	E	304[A]	YZS	N3-C2-N1	-3.72	122.87	128.68
3	F	302[A]	KGP	O7-CPB-CPA	-3.71	104.59	110.55
3	F	302[A]	KGP	N3-C2-N1	-3.66	122.96	128.68
2	F	301[B]	YZS	N3-C2-N1	-3.64	123.00	128.68
2	F	301[B]	YZS	C5'-C4'-C3'	-3.61	102.43	114.40
2	F	301[B]	YZS	OP3-CP7-CPA	-3.57	101.84	110.25
2	F	303[A]	YZS	N3-C2-N1	-3.52	123.18	128.68
2	B	301[B]	YZS	N3-C2-N1	-3.46	123.26	128.68
2	F	303[A]	YZS	C1'-N9-C4	-3.46	120.56	126.64
2	F	303[A]	YZS	O7-P2-O6	3.43	116.15	104.64
3	B	302[A]	KGP	N3-C2-N1	-3.42	123.34	128.68
2	A	301[B]	YZS	N3-C2-N1	-3.34	123.46	128.68
3	A	302[A]	KGP	N3-C2-N1	-3.26	123.58	128.68
2	F	301[B]	YZS	P1-O5'-C5'	-3.15	103.20	121.68
2	B	301[B]	YZS	OS4-SS4-CS2	-3.13	107.34	109.43
2	E	304[A]	YZS	C4-C5-N7	-3.08	106.19	109.40
2	C	303[A]	YZS	C1'-N9-C4	-3.08	121.24	126.64
3	F	302[A]	KGP	P1-O5'-C5'	-3.07	103.68	121.68
3	A	302[A]	KGP	P2-O6-P1	-3.05	122.34	132.83
2	A	301[B]	YZS	P2-O6-P1	-3.05	122.37	132.83
2	F	303[A]	YZS	O4'-C4'-C5'	-3.01	99.47	109.37
2	F	301[B]	YZS	CP5-CP4-CP3	-3.01	107.35	112.36
2	A	301[B]	YZS	C1'-N9-C4	-3.00	121.37	126.64
3	A	302[A]	KGP	C1'-N9-C4	-2.98	121.40	126.64
3	A	302[A]	KGP	OS5-SS4-CS2	2.96	111.40	109.43
3	F	302[A]	KGP	OP3-CP7-CPA	-2.95	103.32	110.25
3	F	302[A]	KGP	C1'-N9-C4	-2.94	121.47	126.64
3	C	302[A]	KGP	N3-C2-N1	-2.92	124.11	128.68
2	D	301[B]	YZS	CP5-CP4-CP3	-2.91	107.50	112.36
2	C	301[B]	YZS	N3-C2-N1	-2.91	124.13	128.68
2	E	304[A]	YZS	O4'-C1'-C2'	2.85	111.08	106.93
2	F	301[B]	YZS	C1'-N9-C4	-2.81	121.70	126.64
2	F	303[A]	YZS	C4-C5-N7	-2.78	106.50	109.40
3	D	302[A]	KGP	CP5-CP4-CP3	-2.78	107.73	112.36
2	F	303[A]	YZS	O7-P2-O22	-2.78	97.03	107.64
2	E	304[A]	YZS	C1'-N9-C4	-2.75	121.81	126.64
2	F	303[A]	YZS	O3'-C3'-C2'	-2.71	101.85	111.68
2	C	301[B]	YZS	OS4-SS4-CS2	-2.69	107.64	109.43
3	F	302[A]	KGP	CP5-CP4-CP3	-2.66	107.93	112.36
3	B	302[A]	KGP	N6-C6-N1	2.63	124.03	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301[B]	YZS	CP7-CP6-NP2	-2.63	111.35	116.58
2	F	301[B]	YZS	CP2-NP1-CP3	-2.62	117.97	122.84
2	B	301[B]	YZS	N6-C6-N1	2.62	124.01	118.57
2	C	303[A]	YZS	O5'-P1-O11	-2.61	98.86	109.07
3	B	302[A]	KGP	C5-C6-N6	-2.55	116.48	120.35
2	B	301[B]	YZS	C5-C6-N6	-2.55	116.48	120.35
3	D	302[A]	KGP	CP9-CPA-CP7	2.51	113.18	108.82
2	D	301[B]	YZS	CP9-CPA-CP7	2.51	113.17	108.82
3	C	302[A]	KGP	CP5-NP2-CP6	-2.48	118.16	122.59
2	F	303[A]	YZS	C2-N1-C6	2.46	122.97	118.75
2	A	301[B]	YZS	CP5-CP4-CP3	-2.43	108.30	112.36
2	C	303[A]	YZS	O22-P2-O6	2.43	112.79	104.64
2	F	301[B]	YZS	CP4-CP5-NP2	-2.41	107.04	111.90
3	F	302[A]	KGP	CP2-NP1-CP3	-2.40	118.38	122.84
3	A	302[A]	KGP	CP5-CP4-CP3	-2.39	108.37	112.36
3	B	302[A]	KGP	O7-CPB-CPA	-2.34	106.78	110.55
2	B	301[B]	YZS	O7-CPB-CPA	-2.33	106.79	110.55
3	D	302[A]	KGP	N6-C6-N1	2.33	123.41	118.57
2	C	301[B]	YZS	C4-C5-N7	-2.31	106.99	109.40
2	D	301[B]	YZS	N6-C6-N1	2.31	123.36	118.57
3	C	302[A]	KGP	C4-C5-N7	-2.29	107.02	109.40
2	B	301[B]	YZS	C1'-N9-C4	-2.27	122.64	126.64
2	C	301[B]	YZS	P2-O6-P1	-2.27	125.04	132.83
3	C	302[A]	KGP	P2-O6-P1	-2.26	125.09	132.83
2	B	301[B]	YZS	OP3-CP7-CPA	-2.22	105.04	110.25
3	B	302[A]	KGP	OP3-CP7-CPA	-2.21	105.05	110.25
2	C	303[A]	YZS	C2-N1-C6	2.18	122.48	118.75
2	C	301[B]	YZS	CP5-NP2-CP6	-2.17	118.72	122.59
3	E	303[A]	KGP	C4-C5-N7	-2.17	107.14	109.40
2	F	303[A]	YZS	O4'-C1'-C2'	2.15	110.07	106.93
2	E	302[B]	YZS	C4-C5-N7	-2.13	107.18	109.40
3	B	302[A]	KGP	C1'-N9-C4	-2.12	122.91	126.64
2	C	301[B]	YZS	OS4-SS4-O56	-2.11	108.18	116.52
3	A	302[A]	KGP	N6-C6-N1	2.11	122.96	118.57
2	A	301[B]	YZS	N6-C6-N1	2.11	122.96	118.57
2	E	304[A]	YZS	C2-N1-C6	2.11	122.36	118.75
3	D	302[A]	KGP	C5-C6-N6	-2.09	117.17	120.35
2	C	303[A]	YZS	C4-C5-N7	-2.07	107.24	109.40
2	B	301[B]	YZS	O3'-C3'-C4'	-2.06	102.62	110.08
3	C	302[A]	KGP	C5'-C4'-C3'	-2.06	107.57	114.40
3	E	303[A]	KGP	CP5-CP4-CP3	-2.05	108.94	112.36
3	F	302[A]	KGP	O4'-C4'-C3'	2.05	109.26	104.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301[B]	YZS	C5-C6-N6	-2.04	117.25	120.35
2	F	301[B]	YZS	CP1-N-CS1	-2.04	118.95	122.59
2	C	301[B]	YZS	C5'-C4'-C3'	-2.03	107.68	114.40
3	B	302[A]	KGP	P2-O6-P1	-2.01	125.92	132.83
3	F	302[A]	KGP	C4-C5-N7	-2.01	107.31	109.40
3	E	303[A]	KGP	C1'-N9-C4	-2.00	123.12	126.64

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302[A]	KGP	C3'-O3'-P3-O31
2	D	301[B]	YZS	N-CS1-CS2-CS3
2	D	301[B]	YZS	OS1-CS1-CS2-CS3
2	F	303[A]	YZS	C5'-O5'-P1-O11
2	F	303[A]	YZS	C5'-O5'-P1-O12
2	F	303[A]	YZS	P1-O6-P2-O7
2	B	301[B]	YZS	C3'-O3'-P3-O31
2	B	301[B]	YZS	N-CS1-CS2-CS3
2	B	301[B]	YZS	OS1-CS1-CS2-CS3
2	C	301[B]	YZS	N-CS1-CS2-CS3
2	C	301[B]	YZS	OS1-CS1-CS2-CS3
2	F	301[B]	YZS	C5'-O5'-P1-O11
2	F	301[B]	YZS	C5'-O5'-P1-O12
2	F	301[B]	YZS	C5'-O5'-P1-O6
2	F	301[B]	YZS	CP7-CPA-CPB-O7
2	F	301[B]	YZS	OP3-CP7-CPA-CP9
2	F	301[B]	YZS	CP6-CP7-CPA-CP9
2	F	301[B]	YZS	N-CS1-CS2-CS3
2	F	301[B]	YZS	OS1-CS1-CS2-CS3
3	F	302[A]	KGP	C5'-O5'-P1-O11
3	F	302[A]	KGP	C5'-O5'-P1-O12
3	F	302[A]	KGP	C5'-O5'-P1-O6
3	F	302[A]	KGP	CP6-CP7-CPA-CPB
2	E	304[A]	YZS	O4'-C4'-C5'-O5'
3	E	303[A]	KGP	C5'-O5'-P1-O11
3	E	303[A]	KGP	C5'-O5'-P1-O6
3	E	303[A]	KGP	CP7-CPA-CPB-O7
3	E	303[A]	KGP	OP3-CP7-CPA-CP9
3	E	303[A]	KGP	CP6-CP7-CPA-CP9
2	A	301[B]	YZS	CP7-CPA-CPB-O7
2	A	301[B]	YZS	OP3-CP7-CPA-CP9

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Mol	Chain	Res	Type	Atoms
2	A	301[B]	YZS	CP6-CP7-CPA-CP9
2	A	301[B]	YZS	N-CS1-CS2-CS3
2	E	302[B]	YZS	C5'-O5'-P1-O6
2	E	302[B]	YZS	CP7-CPA-CPB-O7
2	E	302[B]	YZS	OP3-CP7-CPA-CP9
2	E	302[B]	YZS	CP6-CP7-CPA-CP9
2	E	302[B]	YZS	N-CS1-CS2-CS3
2	E	302[B]	YZS	OS1-CS1-CS2-CS3
3	A	302[A]	KGP	CP7-CPA-CPB-O7
3	A	302[A]	KGP	OP3-CP7-CPA-CP9
3	A	302[A]	KGP	CP6-CP7-CPA-CP9
3	B	302[A]	KGP	C3'-O3'-P3-O33
2	F	301[B]	YZS	C3'-C4'-C5'-O5'
3	F	302[A]	KGP	C3'-C4'-C5'-O5'
3	E	303[A]	KGP	CP8-CPA-CPB-O7
2	E	302[B]	YZS	CP8-CPA-CPB-O7
2	A	301[B]	YZS	OS1-CS1-CS2-CS3
3	F	302[A]	KGP	O4'-C4'-C5'-O5'
2	F	303[A]	YZS	C4'-C5'-O5'-P1
2	F	301[B]	YZS	O4'-C4'-C5'-O5'
2	F	303[A]	YZS	O4'-C4'-C5'-O5'
2	F	303[A]	YZS	P2-O6-P1-O5'
2	F	301[B]	YZS	P1-O6-P2-O7
2	E	304[A]	YZS	P2-O6-P1-O5'
3	D	302[A]	KGP	O4'-C4'-C5'-O5'
2	D	301[B]	YZS	O4'-C4'-C5'-O5'
2	D	301[B]	YZS	C3'-O3'-P3-O31
2	D	301[B]	YZS	C5'-O5'-P1-O6
2	F	303[A]	YZS	C5'-O5'-P1-O6
3	D	302[A]	KGP	C3'-C4'-C5'-O5'
2	D	301[B]	YZS	C3'-C4'-C5'-O5'
3	E	303[A]	KGP	OP3-CP7-CPA-CPB
2	E	302[B]	YZS	OP3-CP7-CPA-CPB
2	F	301[B]	YZS	CP4-CP5-NP2-CP6
2	E	302[B]	YZS	C3'-C4'-C5'-O5'
2	F	301[B]	YZS	CP8-CPA-CPB-O7
2	A	301[B]	YZS	CP8-CPA-CPB-O7
3	A	302[A]	KGP	CP8-CPA-CPB-O7
3	E	303[A]	KGP	C3'-C4'-C5'-O5'
2	E	304[A]	YZS	C3'-C4'-C5'-O5'
2	F	303[A]	YZS	P1-O6-P2-O21
3	E	303[A]	KGP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	E	302[B]	YZS	O4'-C4'-C5'-O5'
2	F	303[A]	YZS	P1-O6-P2-O22
2	F	301[B]	YZS	CP6-CP7-CPA-CP8
3	F	302[A]	KGP	CP6-CP7-CPA-CP9
3	F	302[A]	KGP	CP4-CP5-NP2-CP6
3	D	302[A]	KGP	C5'-O5'-P1-O6
3	E	303[A]	KGP	CPB-O7-P2-O6
2	E	302[B]	YZS	CPB-O7-P2-O6
3	B	302[A]	KGP	C3'-O3'-P3-O31
2	E	304[A]	YZS	C4'-C5'-O5'-P1
3	F	302[A]	KGP	C2'-C3'-O3'-P3
3	F	302[A]	KGP	CPB-O7-P2-O22
3	E	303[A]	KGP	CPB-O7-P2-O21
2	E	302[B]	YZS	C5'-O5'-P1-O12
2	E	302[B]	YZS	CPB-O7-P2-O21

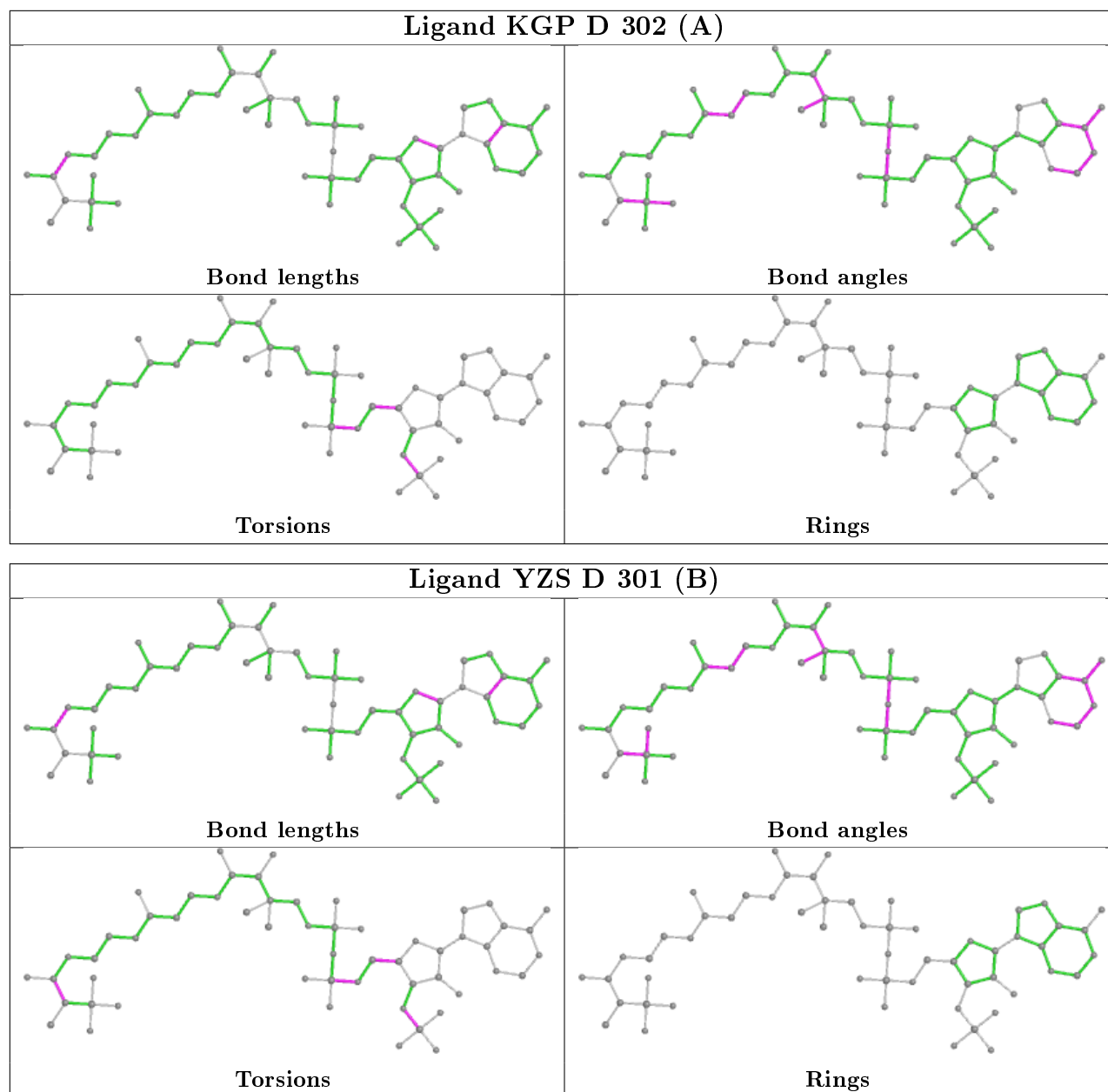
There are no ring outliers.

10 monomers are involved in 35 short contacts:

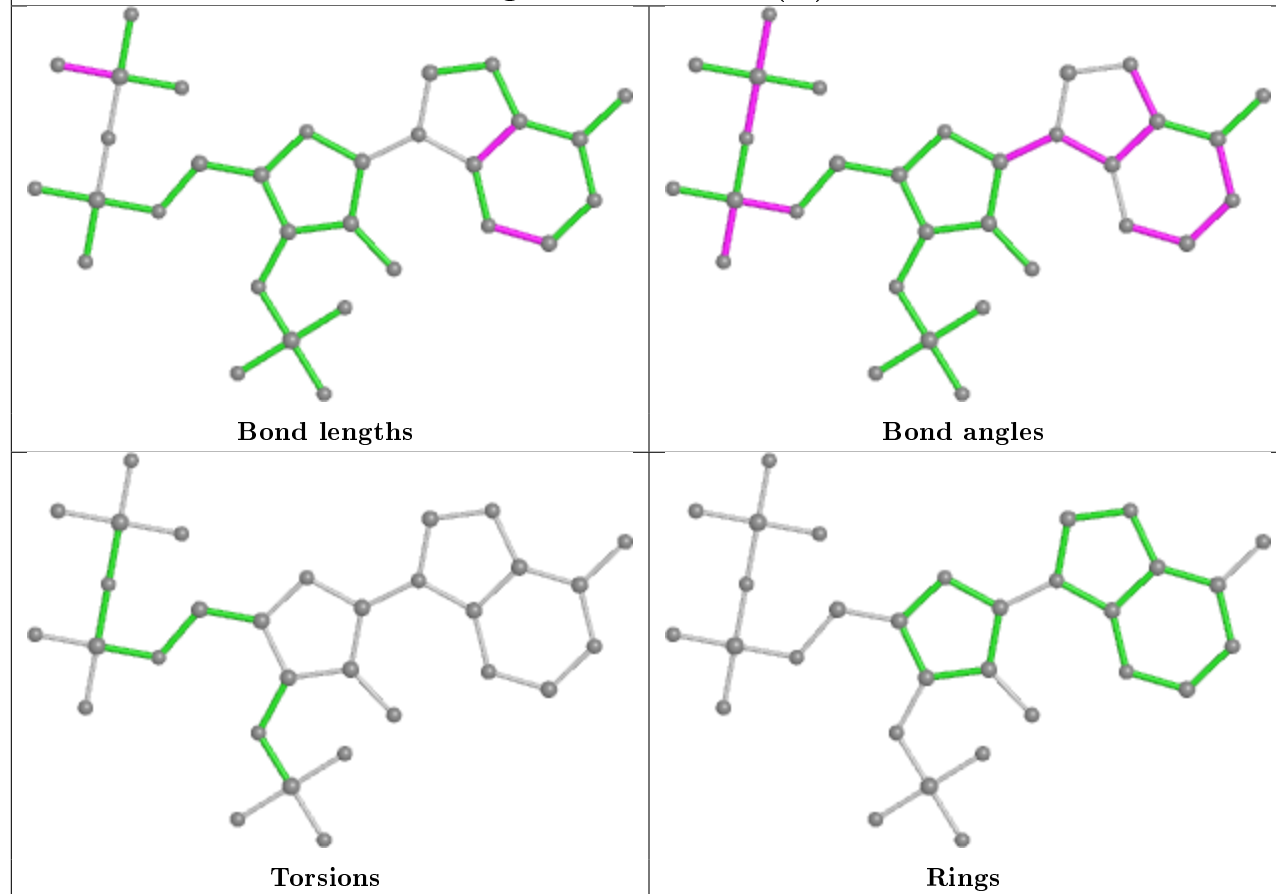
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303[A]	YZS	7	0
2	F	303[A]	YZS	16	0
3	C	302[A]	KGP	1	0
2	C	301[B]	YZS	1	0
5	D	303	IMD	2	0
2	F	301[B]	YZS	1	0
3	F	302[A]	KGP	1	0
2	E	304[A]	YZS	4	0
3	E	303[A]	KGP	1	0
2	E	302[B]	YZS	1	0

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

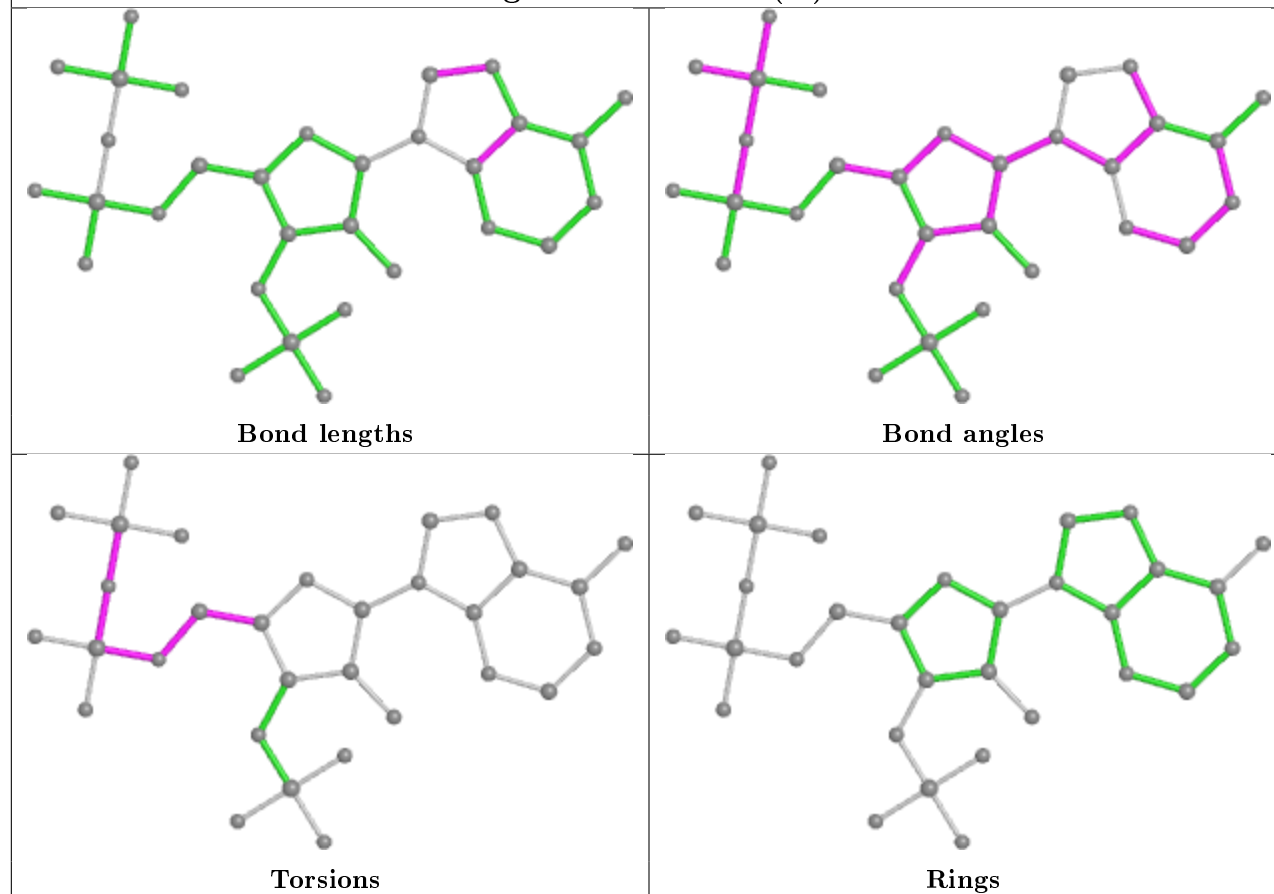
equivalents in the CSD to analyse the geometry.



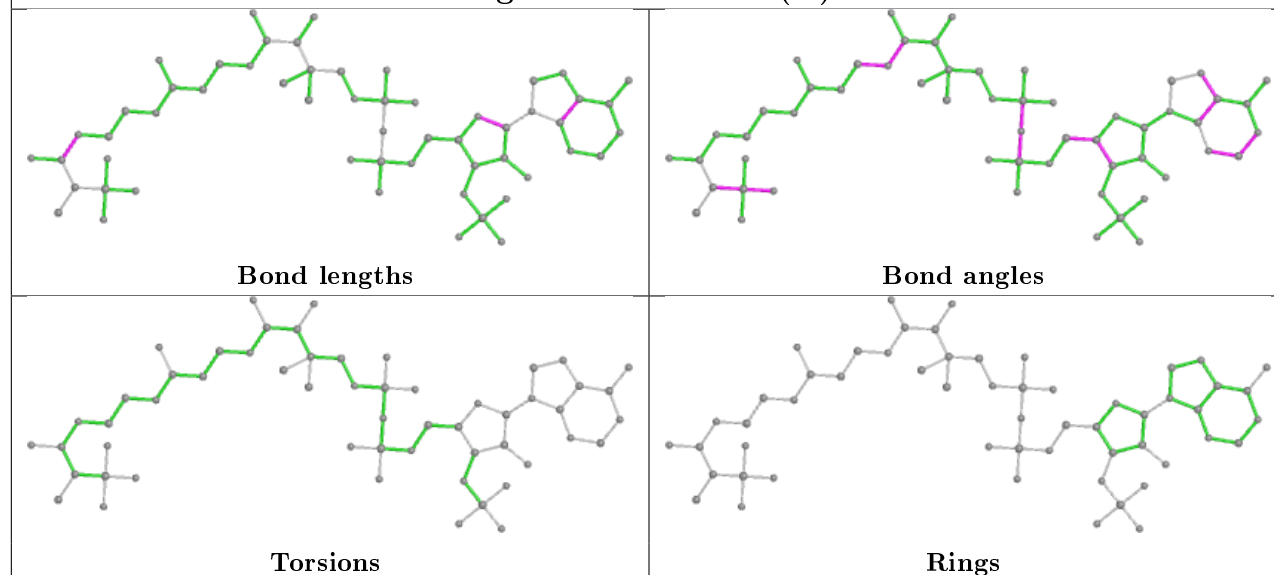
Ligand YZS C 303 (A)

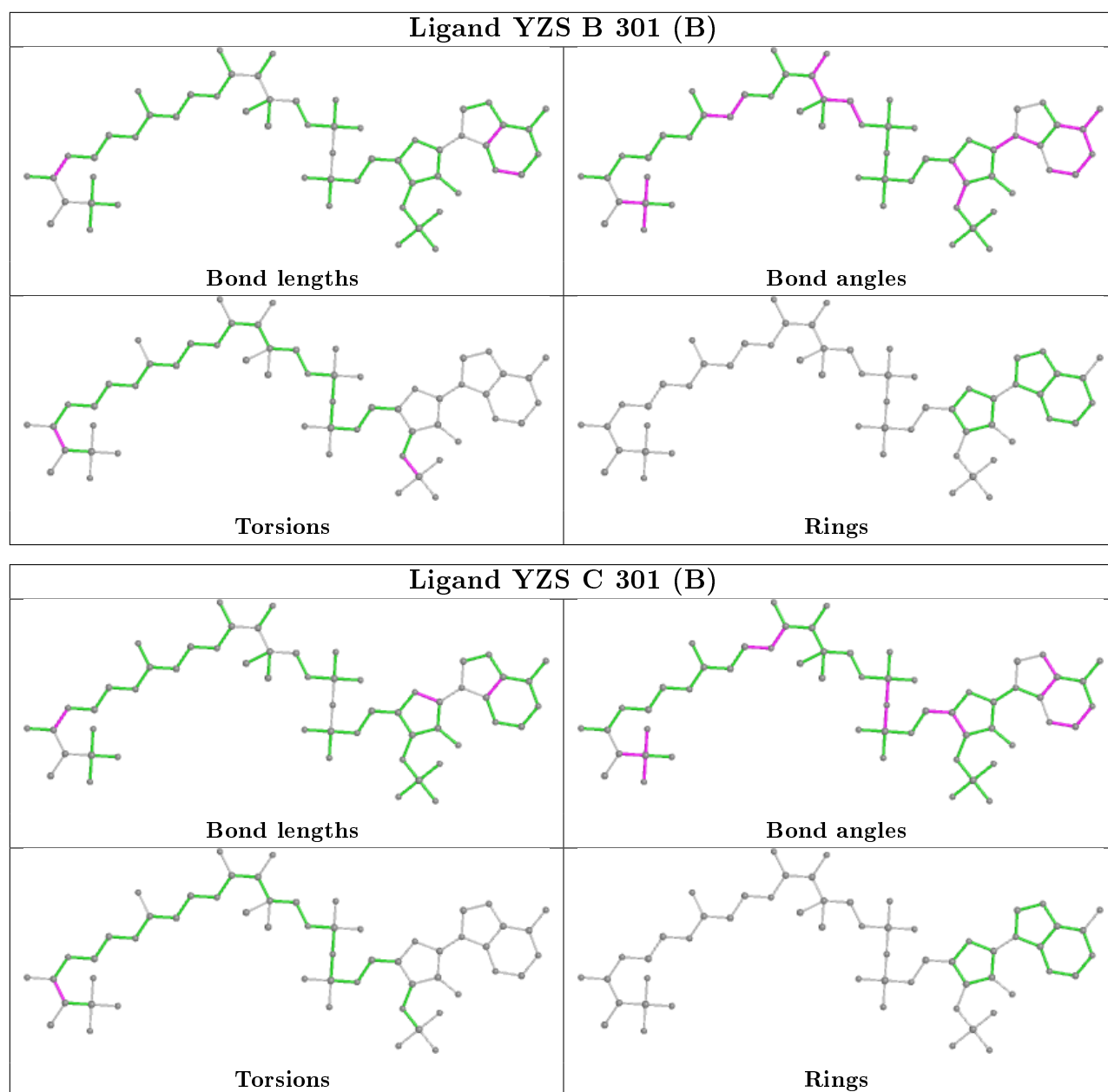


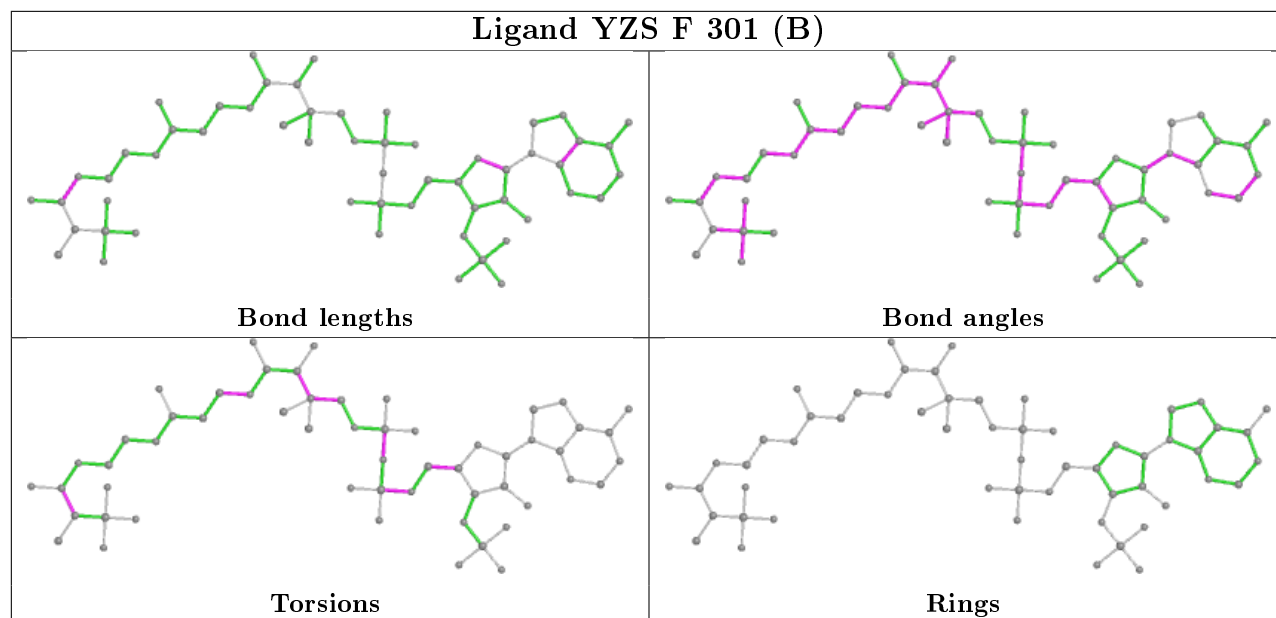
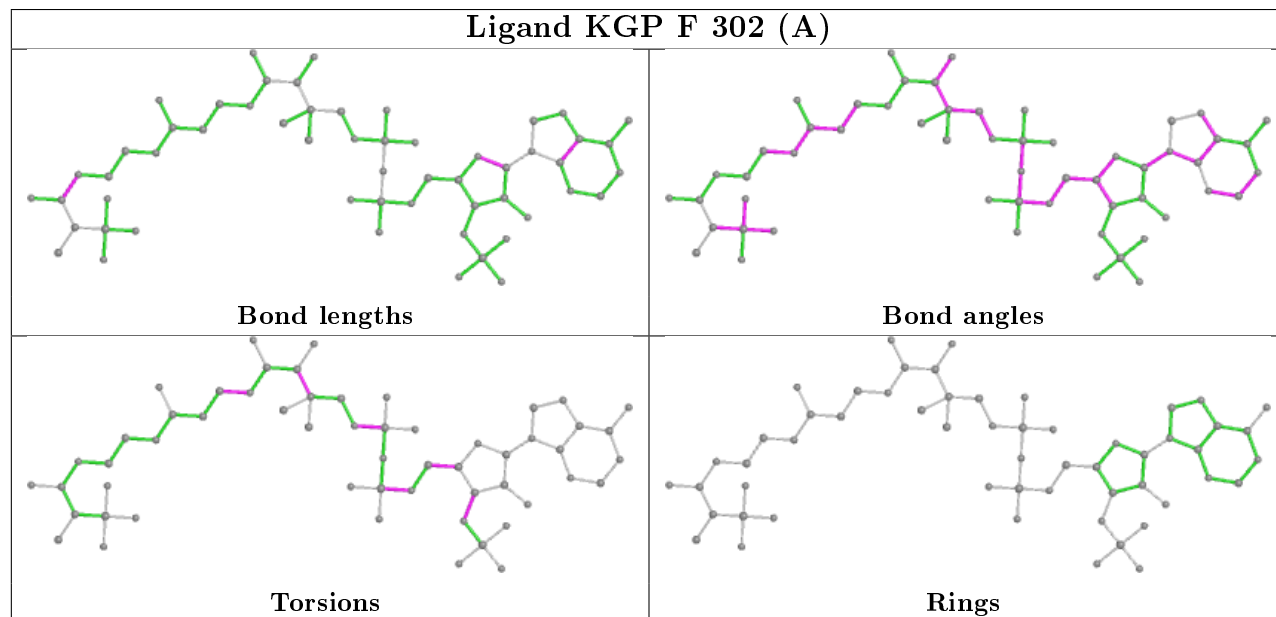
Ligand YZS F 303 (A)



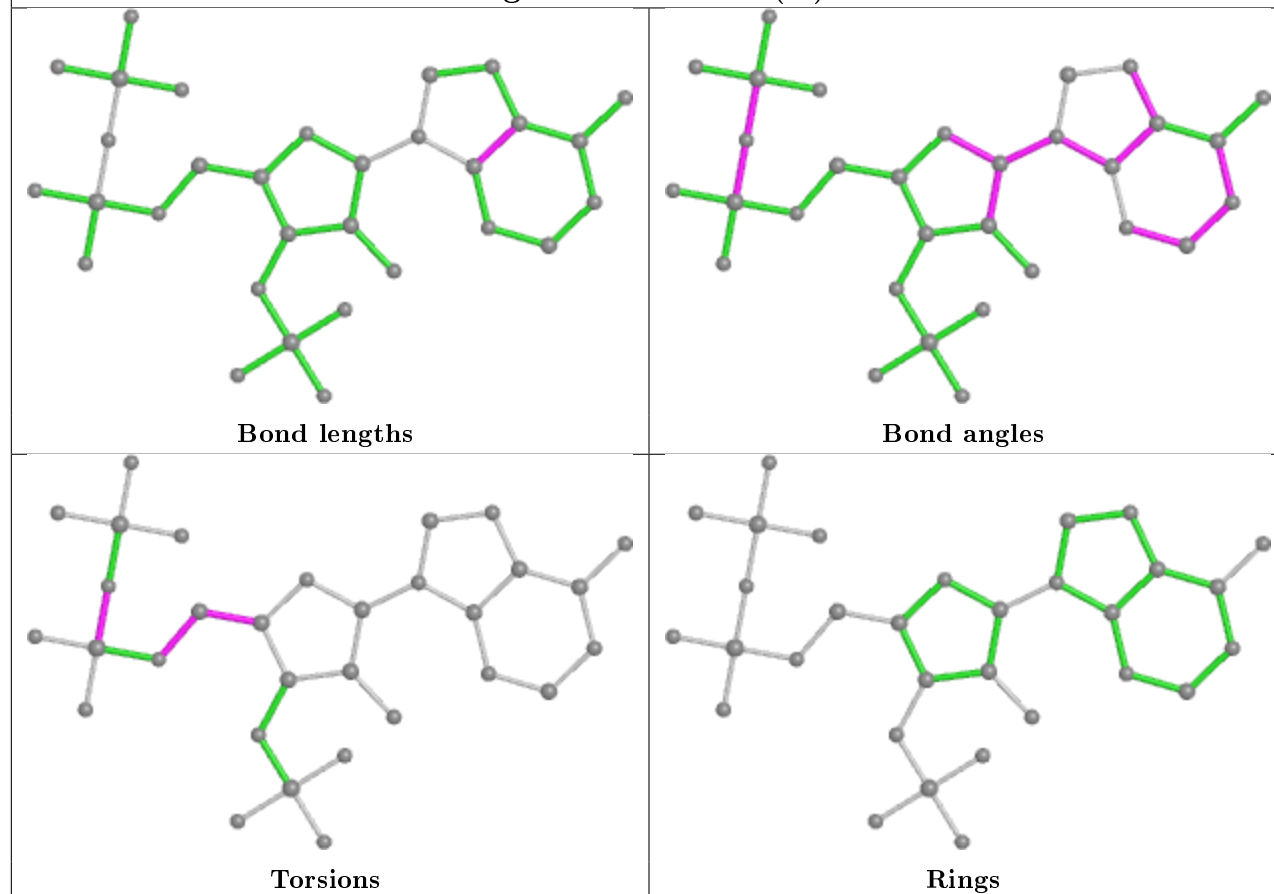
Ligand KGP C 302 (A)



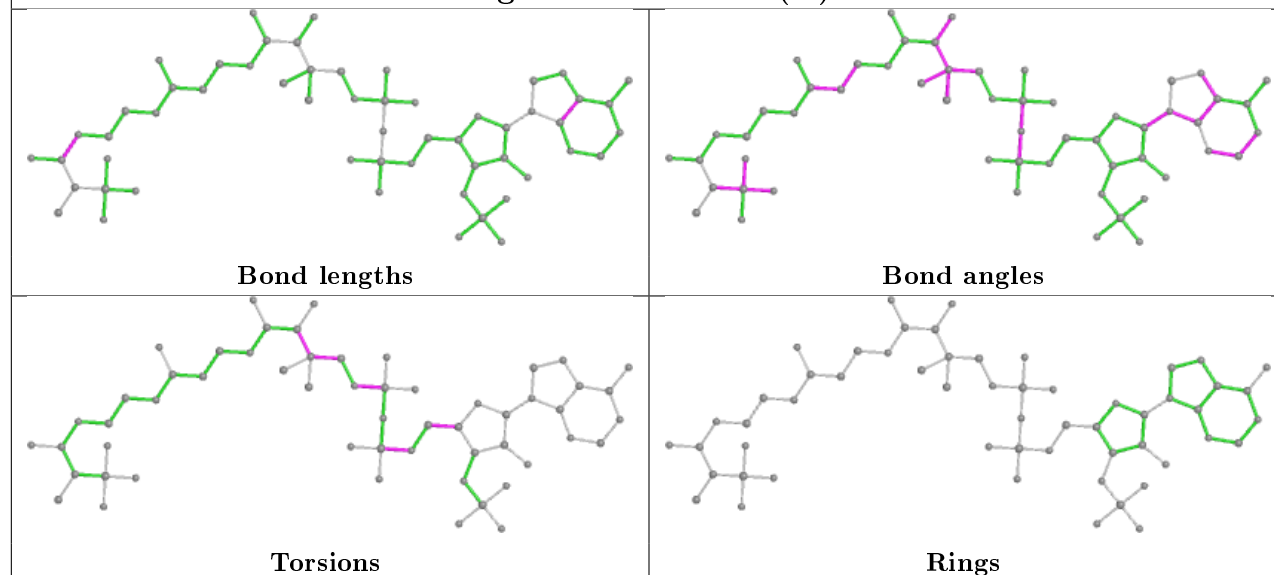


Ligand YZS F 301 (B)**Ligand KGP F 302 (A)**

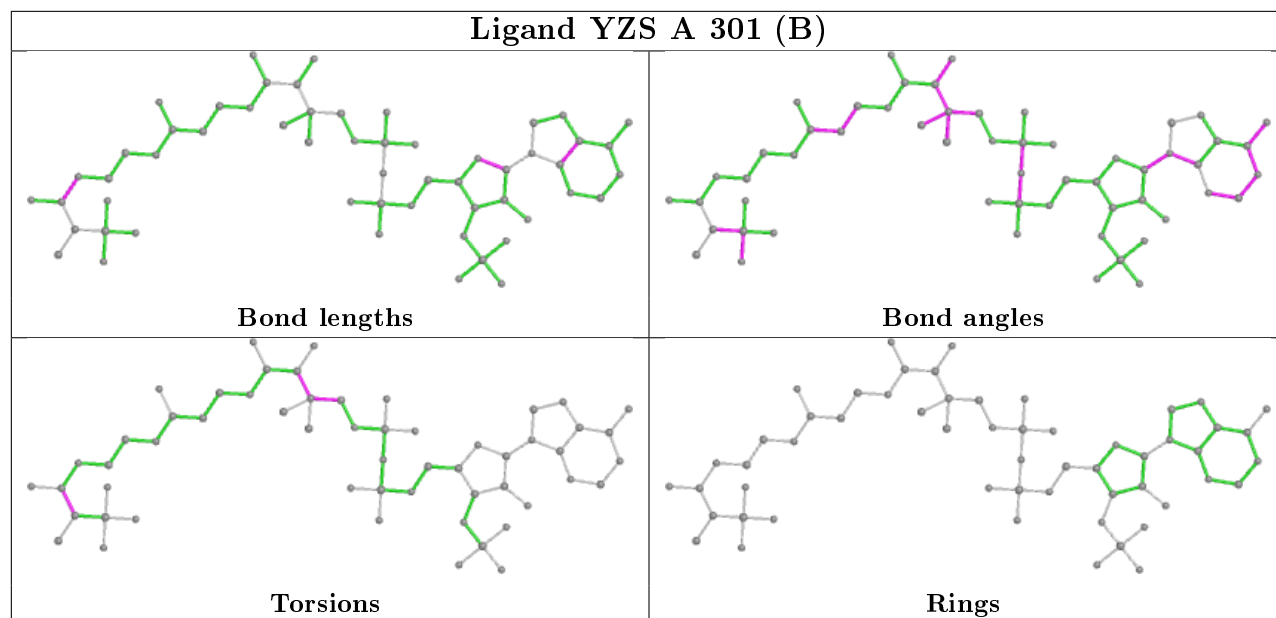
Ligand YZS E 304 (A)



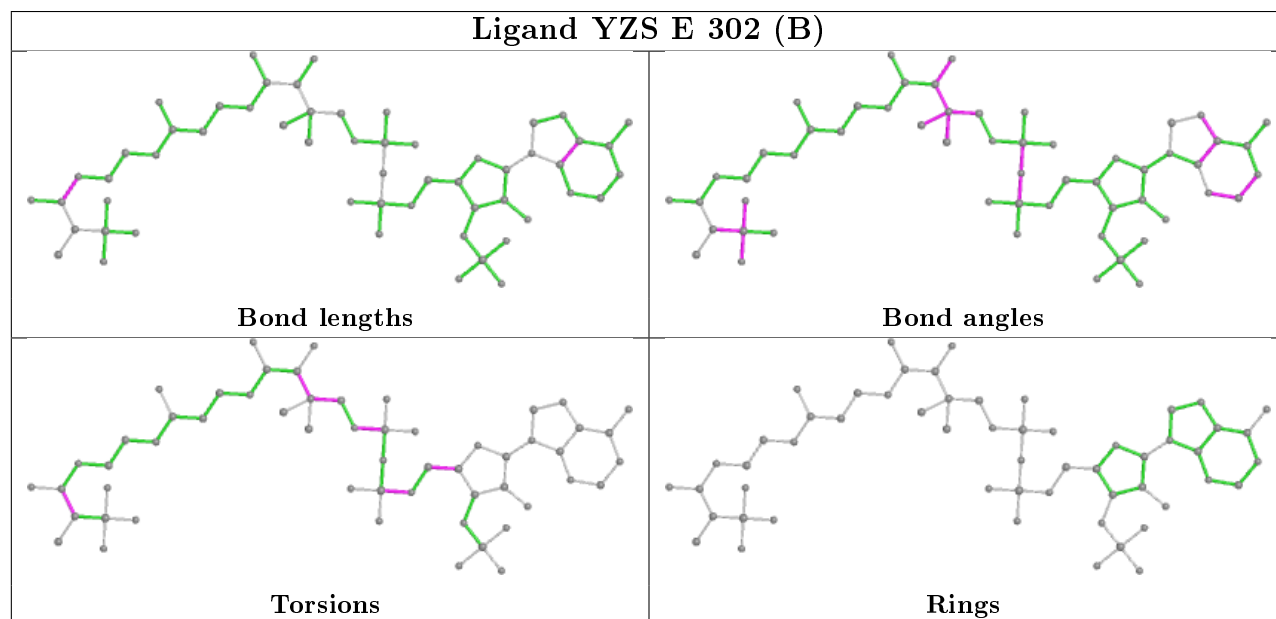
Ligand KGP E 303 (A)

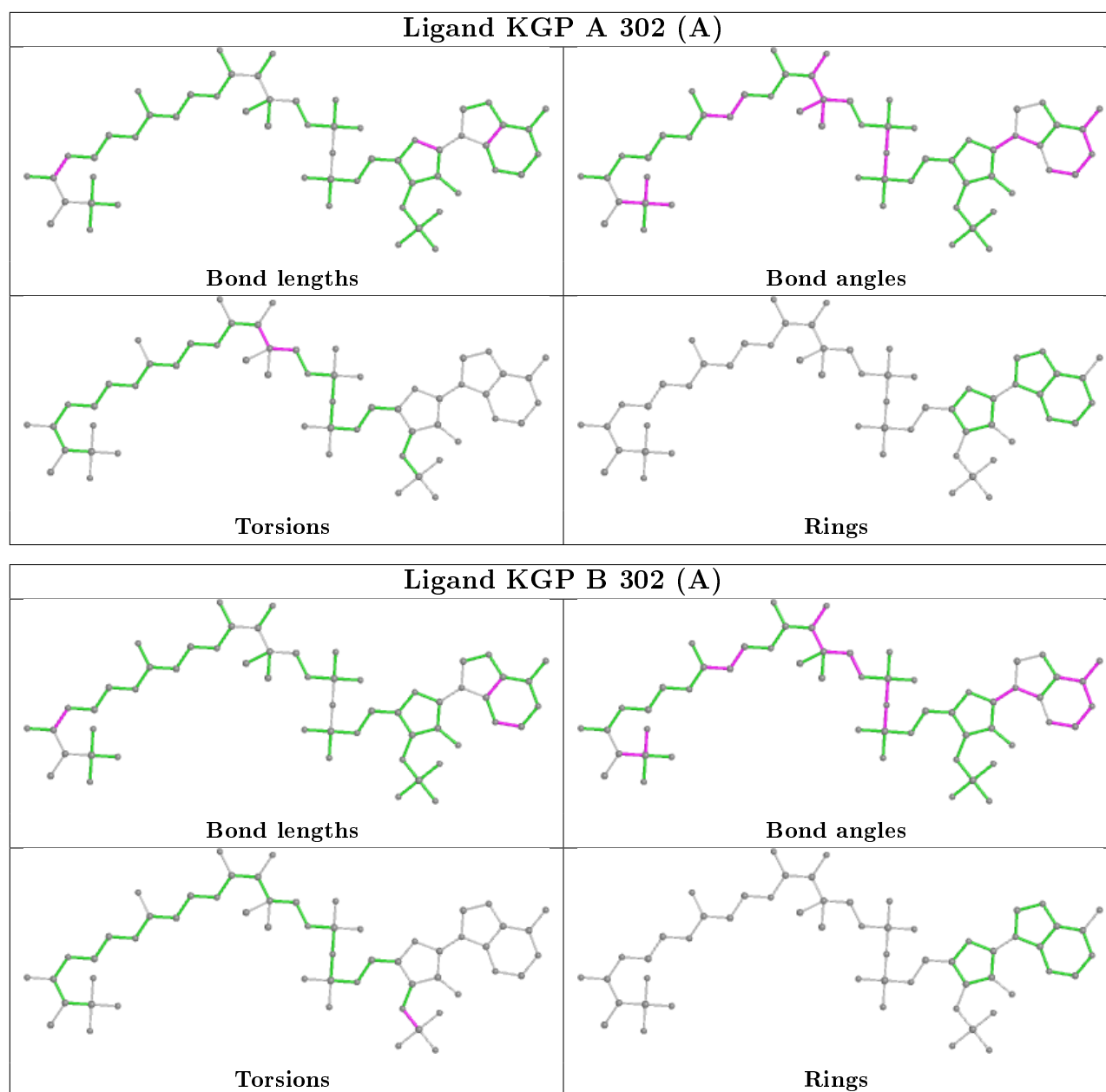


Ligand YZS A 301 (B)



Ligand YZS E 302 (B)





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%)	-0.29	2 (0%) 86 90	17, 22, 36, 67	0
1	B	260/261 (99%)	-0.15	6 (2%) 60 67	17, 23, 45, 84	0
1	C	260/261 (99%)	-0.12	7 (2%) 54 60	16, 21, 45, 89	0
1	D	260/261 (99%)	-0.24	6 (2%) 60 67	17, 21, 43, 80	0
1	E	260/261 (99%)	-0.08	8 (3%) 49 55	17, 23, 45, 107	0
1	F	260/261 (99%)	-0.16	4 (1%) 73 80	17, 23, 44, 65	0
All	All	1560/1566 (99%)	-0.17	33 (2%) 63 71	16, 22, 44, 107	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	73	SER	9.4
1	C	73	SER	7.2
1	D	74	GLY	7.1
1	E	74	GLY	6.4
1	C	74	GLY	5.5
1	B	73	SER	5.4
1	C	75	GLY	4.7
1	E	2	ALA	4.1
1	C	23	ARG	3.9
1	E	251	LEU	3.9
1	C	72	PRO	3.5
1	B	2	ALA	3.4
1	F	73	SER	3.4
1	C	76	ARG	3.3
1	F	251	LEU	3.3
1	D	251	LEU	3.3
1	B	74	GLY	3.0
1	E	75	GLY	2.9
1	A	261	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	261	HIS	2.8
1	F	23	ARG	2.6
1	E	261	HIS	2.6
1	C	69	HIS	2.5
1	E	76	ARG	2.5
1	D	2	ALA	2.5
1	A	23	ARG	2.4
1	B	76	ARG	2.3
1	D	75	GLY	2.3
1	D	253	LYS	2.0
1	B	247[A]	MET	2.0
1	D	73	SER	2.0
1	F	252	GLU	2.0
1	E	250	PHE	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(Å ²)	Q<0.9
2	YZS	E	304[A]	31/56	0.79	0.36	36,53,62,65	31
2	YZS	F	303[A]	31/56	0.83	0.28	31,41,52,59	31
2	YZS	C	303[A]	31/56	0.85	0.20	31,40,58,60	31
3	KGP	F	302[A]	56/56	0.87	0.15	24,41,64,70	56
2	YZS	F	301[B]	56/56	0.87	0.15	24,42,64,70	56
2	YZS	D	301[B]	56/56	0.89	0.14	24,36,53,58	56
3	KGP	D	302[A]	56/56	0.89	0.14	23,36,53,58	56
3	KGP	E	303[A]	56/56	0.91	0.13	23,38,54,57	56
2	YZS	E	302[B]	56/56	0.91	0.13	23,38,54,56	56

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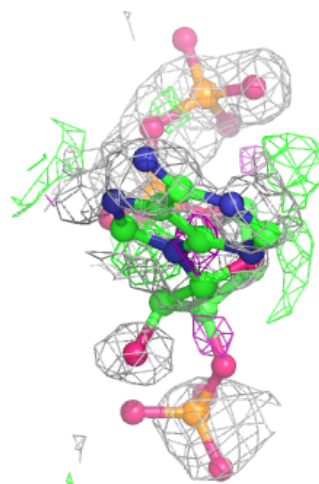
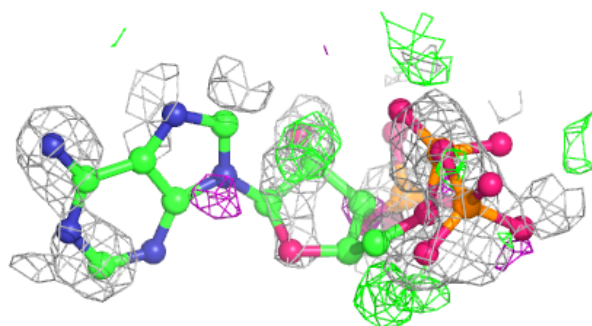
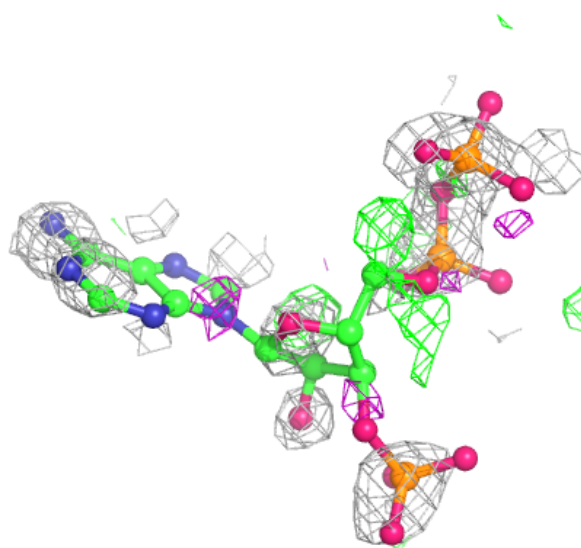
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	YZS	C	301[B]	56/56	0.93	0.12	23,39,58,61	56
3	KGP	C	302[A]	56/56	0.93	0.12	24,39,58,60	56
2	YZS	A	301[B]	56/56	0.94	0.09	23,33,48,57	56
2	YZS	B	301[B]	56/56	0.94	0.09	25,34,56,61	56
3	KGP	A	302[A]	56/56	0.94	0.09	22,32,48,57	56
3	KGP	B	302[A]	56/56	0.94	0.09	23,34,55,62	56
5	IMD	D	303	5/5	0.96	0.08	22,23,24,24	0
4	NI	A	303	1/1	0.97	0.03	66,66,66,66	0
4	NI	E	301	1/1	0.98	0.04	59,59,59,59	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.

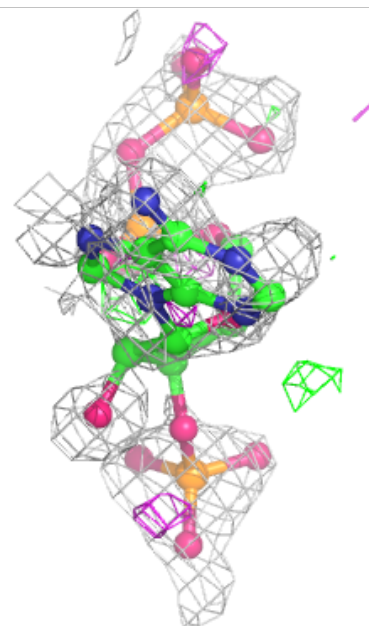
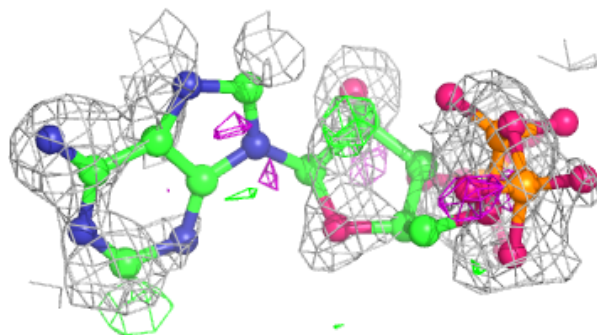
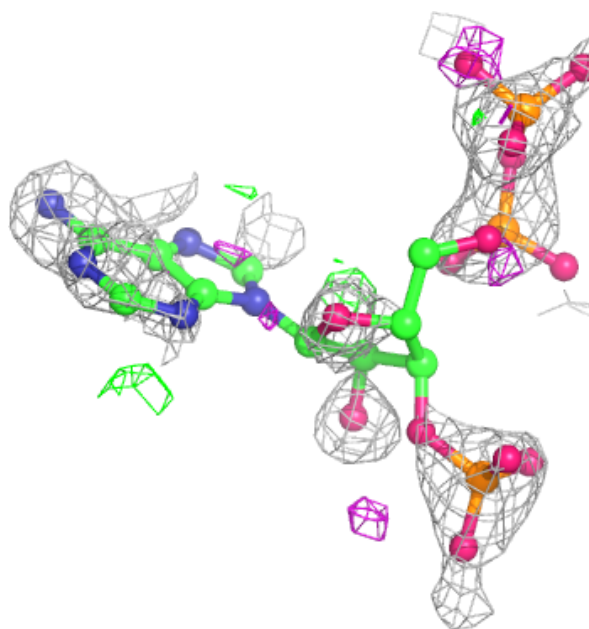
Electron density around YZS E 304 (A):

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



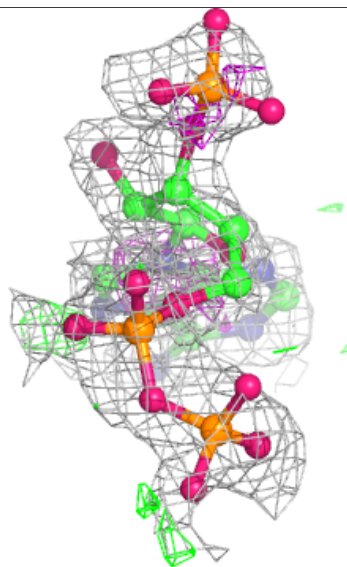
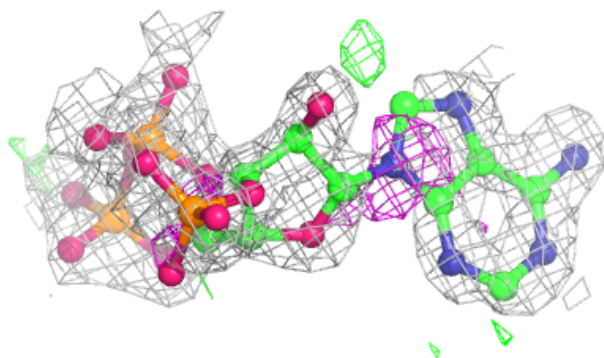
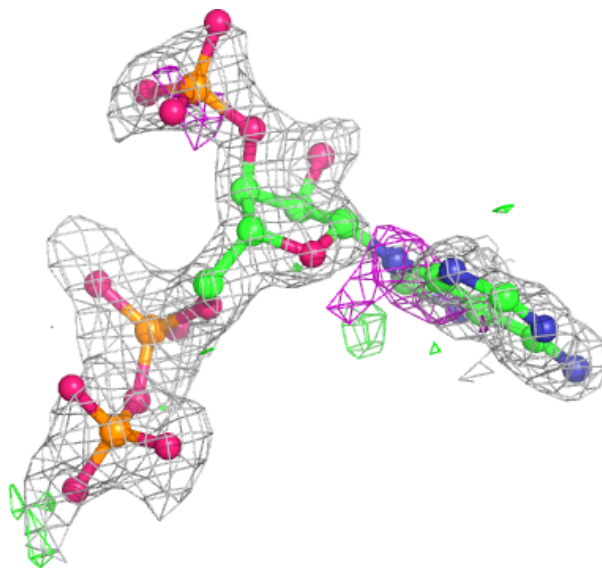
Electron density around YZS F 303 (A):

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



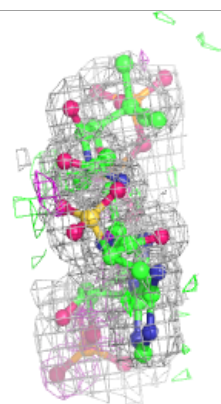
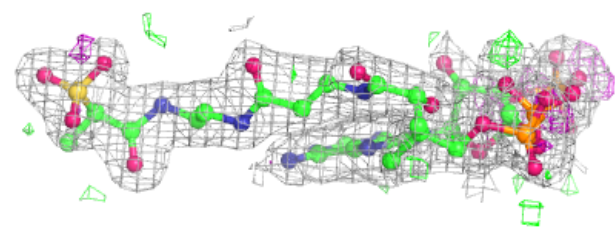
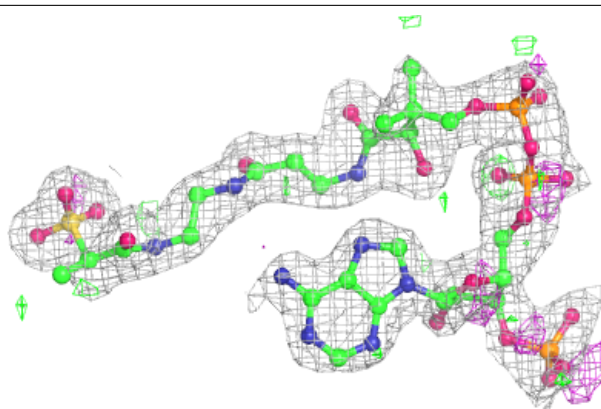
Electron density around YZS C 303 (A):

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

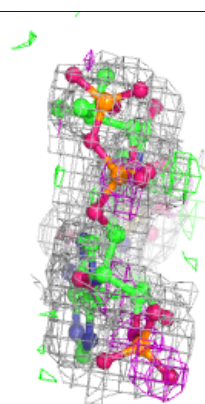
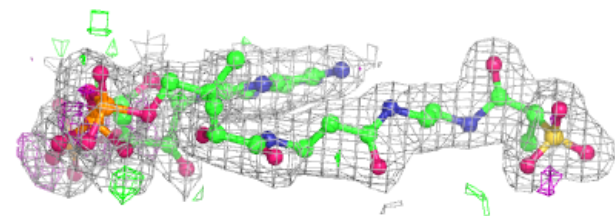
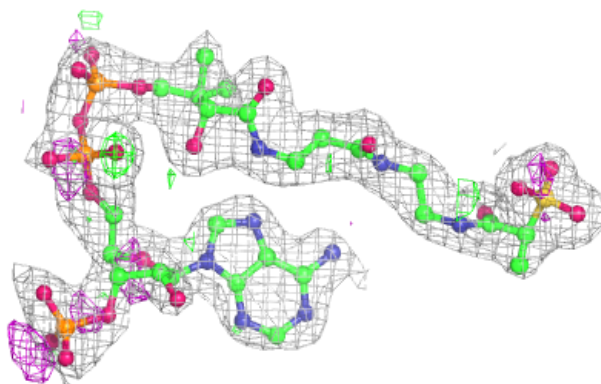


Electron density around KGP F 302 (A):

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

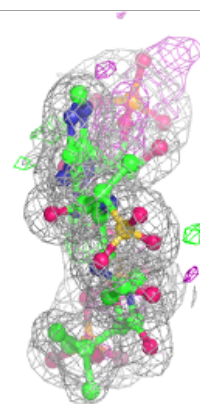
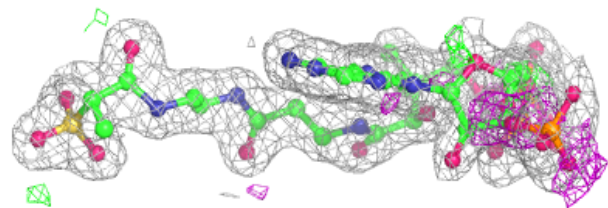
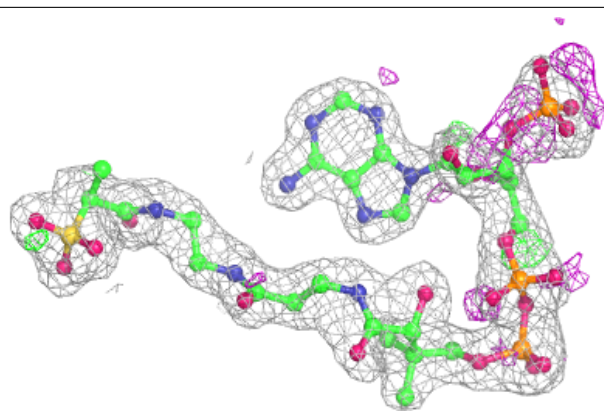
**Electron density around YZS F 301 (B):**

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and green (positive)

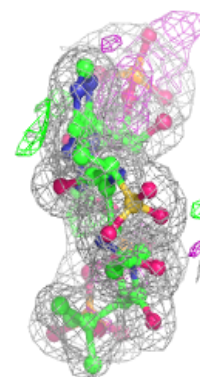
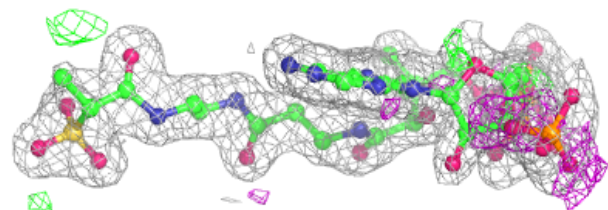
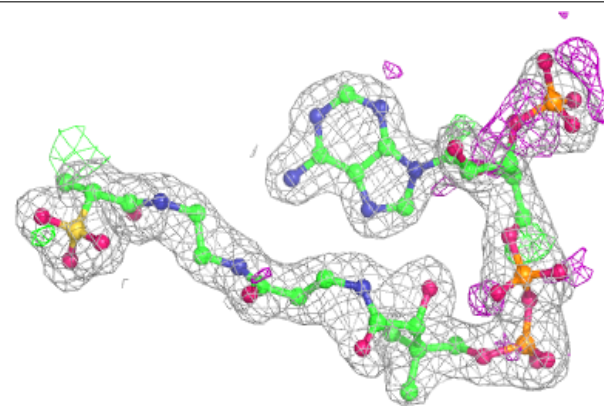


Electron density around YZS D 301 (B):

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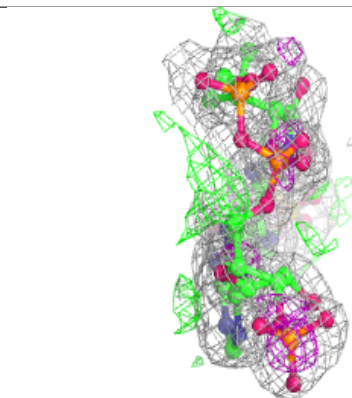
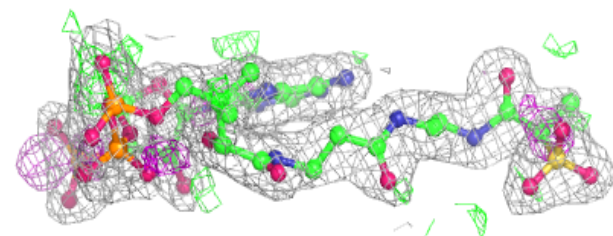
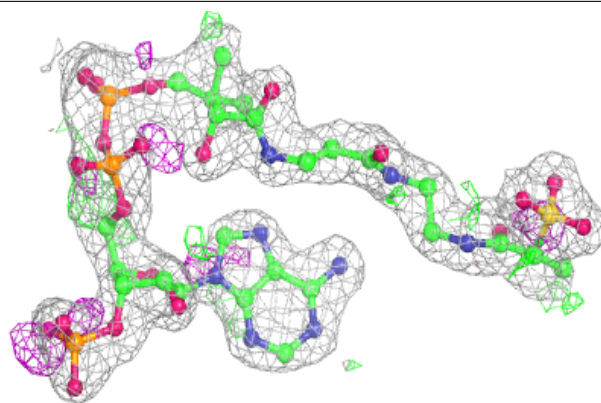
**Electron density around KGP D 302 (A):**

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

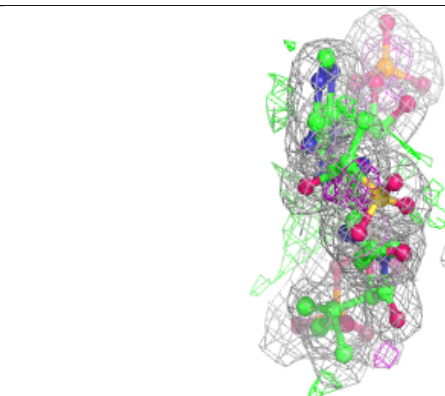
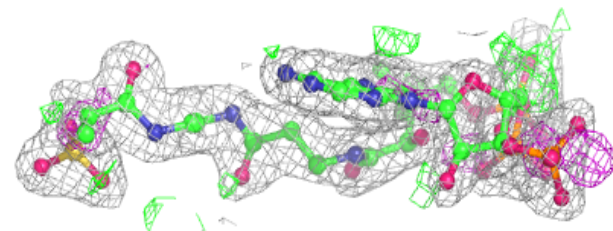
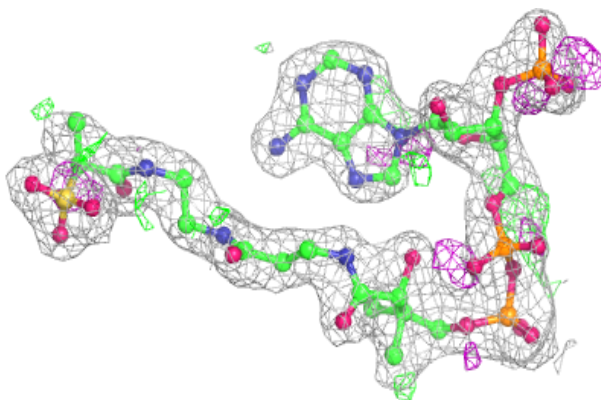


Electron density around KGP E 303 (A):

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and green (positive)

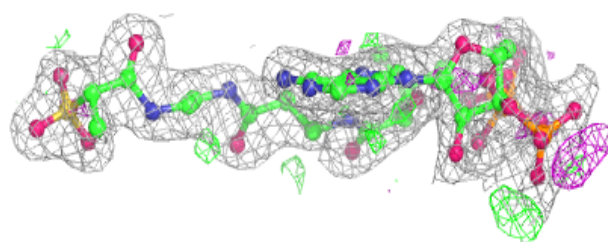
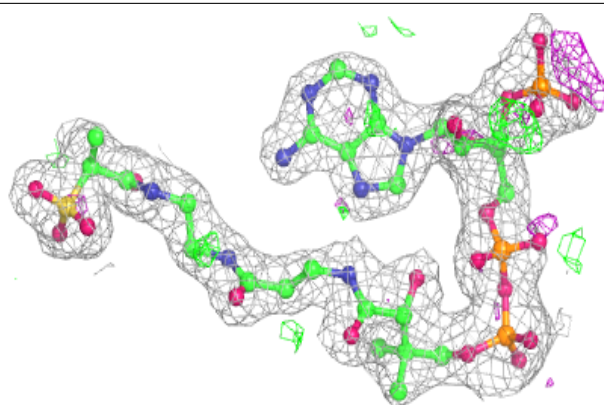
**Electron density around YZS E 302 (B):**

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and green (positive)

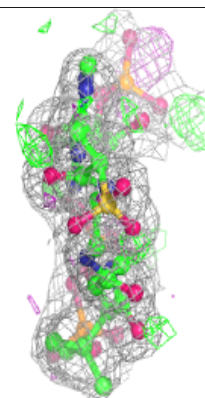
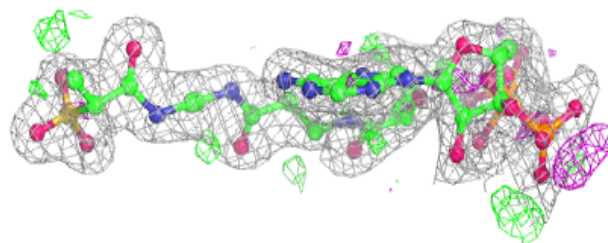
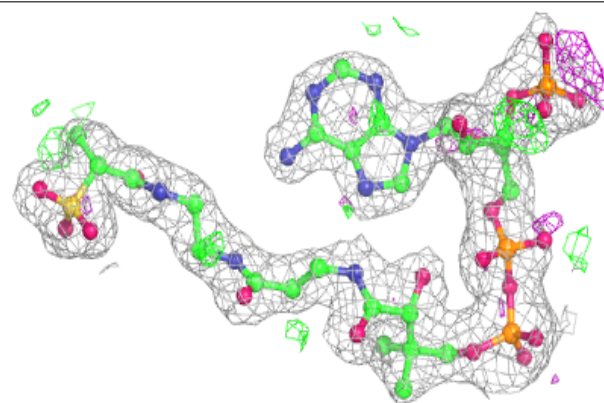


Electron density around YZS C 301 (B):

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

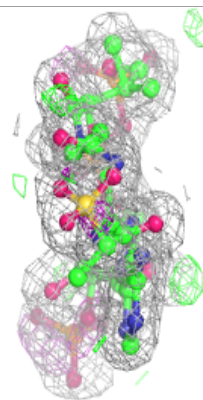
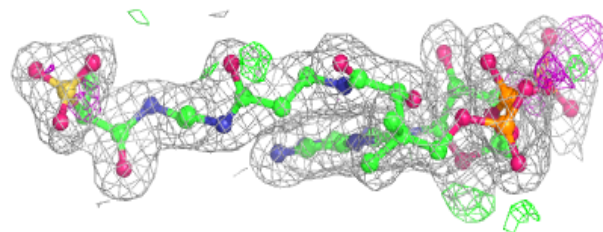
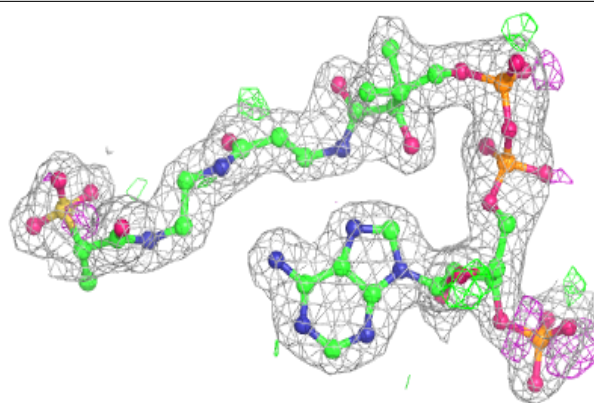
**Electron density around KGP C 302 (A):**

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

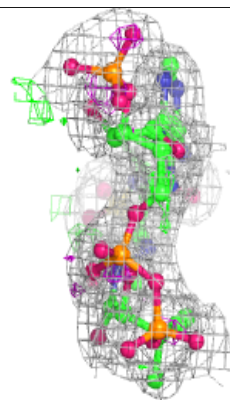
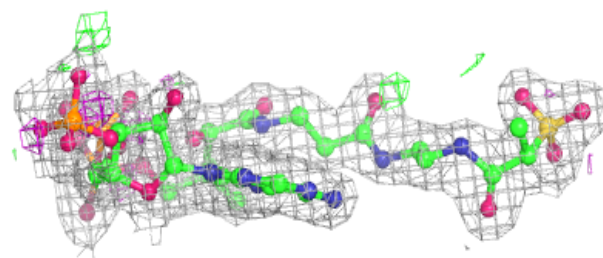
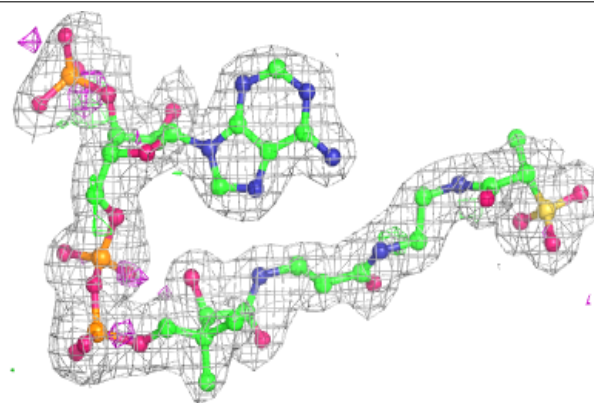


Electron density around YZS A 301 (B):

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and green (positive)

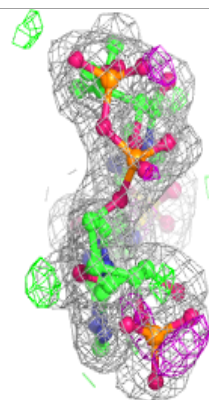
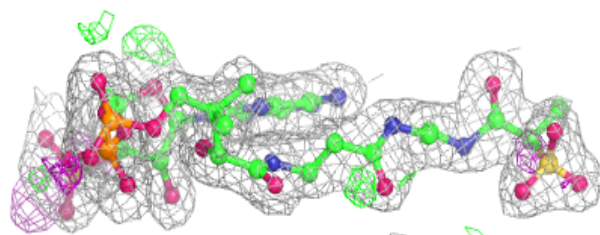
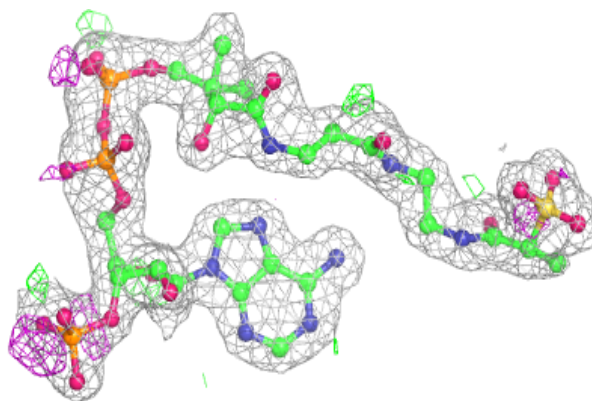
**Electron density around YZS B 301 (B):**

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and green (positive)

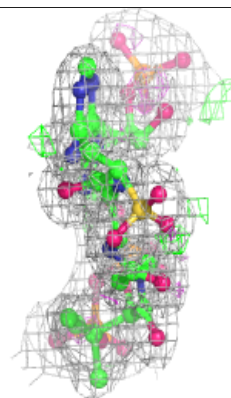
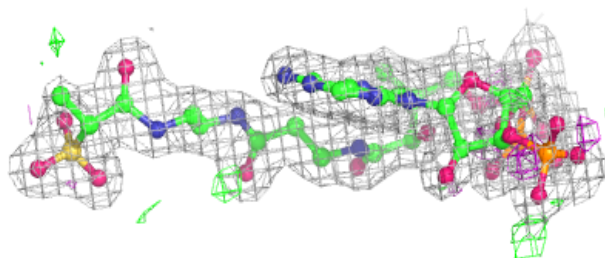
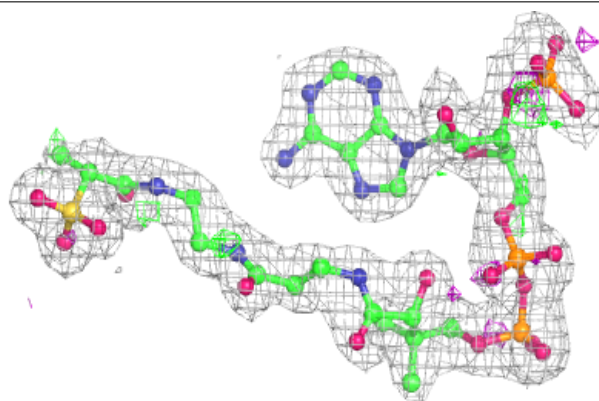


Electron density around KGP A 302 (A):

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

**Electron density around KGP B 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.