Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 02:45 AM EDT

PDB ID	:	6S74
Title	:	Crystal structure of CARM1 in complex with inhibitor UM305
Authors	:	Gunnell, E.A.; Muhsen, U.; Dowden, J.; Dreveny, I.
Deposited on	:	2019-07-04
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

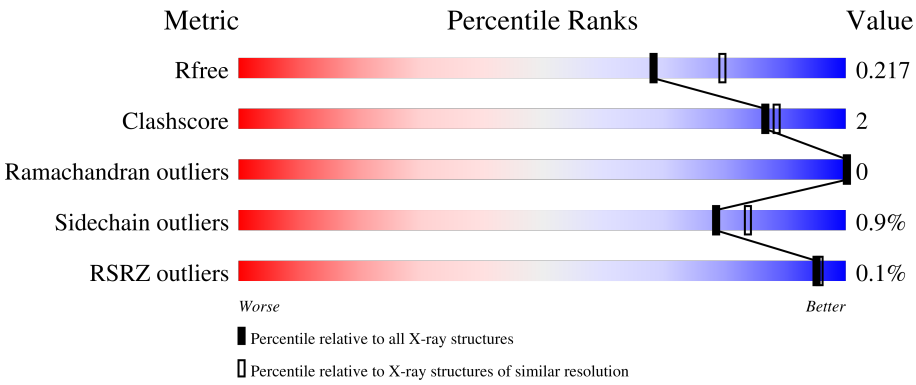
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	351	93% 5% •
1	B	351	91% 6% •
1	C	351	89% 8% • •
1	D	351	92% 5% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11804 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 Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2763	1786	455	507	15	0	2	0
1	B	342	2744	1772	453	505	14	0	0	0
1	C	342	2775	1791	462	508	14	0	4	0
1	D	342	2753	1777	454	508	14	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	480	HIS	-	expression tag	UNP Q86X55
A	481	HIS	-	expression tag	UNP Q86X55
A	482	HIS	-	expression tag	UNP Q86X55
A	483	HIS	-	expression tag	UNP Q86X55
A	484	HIS	-	expression tag	UNP Q86X55
A	485	HIS	-	expression tag	UNP Q86X55
B	480	HIS	-	expression tag	UNP Q86X55
B	481	HIS	-	expression tag	UNP Q86X55
B	482	HIS	-	expression tag	UNP Q86X55
B	483	HIS	-	expression tag	UNP Q86X55
B	484	HIS	-	expression tag	UNP Q86X55
B	485	HIS	-	expression tag	UNP Q86X55
C	480	HIS	-	expression tag	UNP Q86X55
C	481	HIS	-	expression tag	UNP Q86X55
C	482	HIS	-	expression tag	UNP Q86X55
C	483	HIS	-	expression tag	UNP Q86X55
C	484	HIS	-	expression tag	UNP Q86X55
C	485	HIS	-	expression tag	UNP Q86X55
D	480	HIS	-	expression tag	UNP Q86X55
D	481	HIS	-	expression tag	UNP Q86X55
D	482	HIS	-	expression tag	UNP Q86X55

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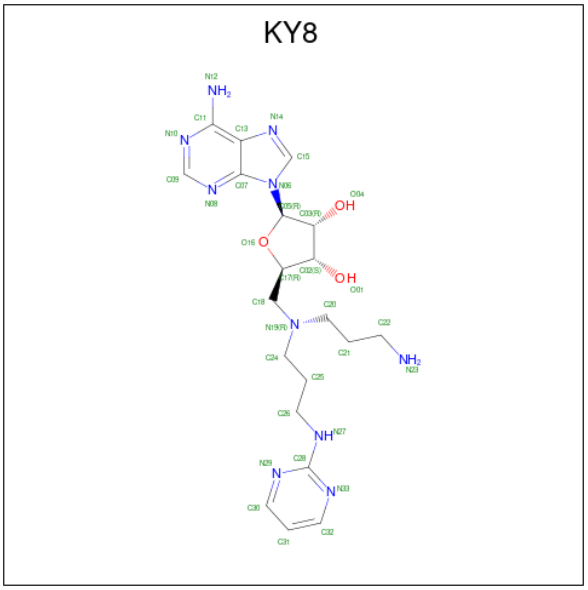
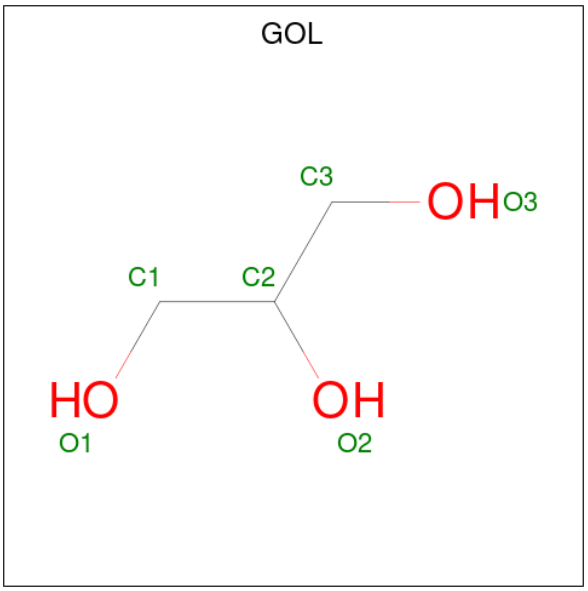
Chain	Residue	Modelled	Actual	Comment	Reference
D	483	HIS	-	expression tag	UNP Q86X55
D	484	HIS	-	expression tag	UNP Q86X55
D	485	HIS	-	expression tag	UNP Q86X55

- Molecule 2 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-[[3-azanylpropyl-[3-(pyrimidin-2-ylamino)propyl]amino]methyl]oxolane-3,4-diol (three-letter code: KY8) (formula: $C_{20}H_{30}N_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	66	40	20	6	0	1
			Total	C	N	O		
2	B	1	66	40	20	6	0	1
			Total	C	N	O		
2	C	1	33	20	10	3	0	0
			Total	C	N	O		
2	D	1	33	20	10	3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0
			Total	C	O		
3	C	1	6	3	3	0	0

- Molecule 4 is water.

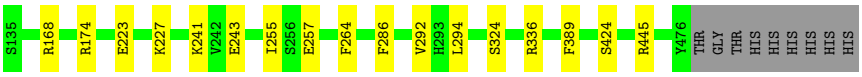
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	175	175	175	0	0
			Total	O		
4	B	138	138	138	0	0
			Total	O		
4	C	131	131	131	0	0
			Total	O		
4	D	109	109	109	0	0

3 Residue-property plots (i)

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

• Molecule 1: Histone-arginine methyltransferase CARM1

Chain A:



• Molecule 1: Histone-arginine methyltransferase CARM1

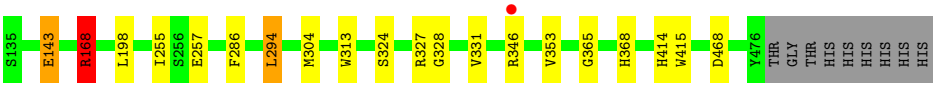
Chain B:

• Molecule 1: Histone-arginine methyltransferase CARM1

Chain C:

• Molecule 1: Histone-arginine methyltransferase CARM1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.39Å 99.03Å 207.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.10 48.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.4 (48.17-2.10) 87.5 (48.17-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.192 , 0.216 0.194 , 0.217	Depositor DCC
R_{free} test set	4029 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11804	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.8419e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KY8, GOL

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	0.99	3/2834 (0.1%)	0.84	5/3839 (0.1%)
1	B	0.92	2/2814 (0.1%)	0.80	5/3813 (0.1%)
1	C	0.95	2/2854 (0.1%)	0.83	4/3865 (0.1%)
1	D	0.92	1/2823 (0.0%)	0.81	5/3826 (0.1%)
All	All	0.95	8/11325 (0.1%)	0.82	19/15343 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	GLU	CD-OE1	9.27	1.35	1.25
1	A	324	SER	CB-OG	-7.66	1.32	1.42
1	A	445	ARG	CZ-NH1	6.87	1.42	1.33
1	D	143	GLU	CD-OE1	6.48	1.32	1.25
1	C	314	TYR	CE1-CZ	5.79	1.46	1.38
1	A	243	GLU	CD-OE1	5.35	1.31	1.25
1	B	244	GLU	CD-OE1	5.33	1.31	1.25
1	B	464	SER	CB-OG	-5.06	1.35	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	344	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	174	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	445	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	D	168	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	168	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	D	468	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	168	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	C	142	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	168	ARG	NE-CZ-NH2	-5.99	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	244	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	B	336	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	445[A]	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	445[B]	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	234	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	D	327	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	336	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	445	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	168	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	D	304	MET	CG-SD-CE	5.16	108.46	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2763	0	2708	5	0
1	B	2744	0	2692	12	0
1	C	2775	0	2733	14	0
1	D	2753	0	2698	10	0
2	A	66	0	0	1	0
2	B	66	0	0	6	0
2	C	33	0	0	0	0
2	D	33	0	0	1	0
3	A	6	0	8	0	0
3	C	12	0	16	0	0
4	A	175	0	0	0	0
4	B	138	0	0	3	0
4	C	131	0	0	3	0
4	D	109	0	0	1	0
All	All	11804	0	10855	46	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 2.

All (46) 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)
2:B:501[B]:KY8:N06	2:B:501[B]:KY8:C07	1.67	1.56
2:B:501[B]:KY8:C13	2:B:501[B]:KY8:N14	1.67	1.51
2:B:501[B]:KY8:C13	2:B:501[B]:KY8:C15	2.53	0.86
2:B:501[B]:KY8:C07	2:B:501[B]:KY8:C15	2.60	0.80
1:B:187:ILE:HD11	1:B:208:ARG:HH21	1.54	0.73
2:B:501[B]:KY8:N06	2:B:501[B]:KY8:C13	2.52	0.73
1:B:410:GLU:OE2	4:B:601:HOH:O	2.17	0.58
1:D:198:LEU:HD11	1:D:257[B]:GLU:HG3	1.86	0.57
1:B:189:LEU:HD13	1:B:247:LEU:HD21	1.89	0.55
1:B:188:VAL:HB	1:B:210:ILE:HD13	1.90	0.53
1:B:336:ARG:NH1	4:B:609:HOH:O	2.42	0.53
1:B:207:ALA:HB3	1:B:210:ILE:HD11	1.91	0.52
1:B:223:GLU:OE2	1:B:227:LYS:HE3	2.09	0.51
1:C:294:LEU:HG	1:C:389:PHE:CE2	2.46	0.51
1:B:264:PHE:CE2	1:B:292:VAL:HG21	2.45	0.51
1:C:336[A]:ARG:HG2	1:C:466:LEU:O	2.12	0.50
1:B:168:ARG:HD3	2:B:501[A]:KY8:C31	2.42	0.49
1:A:223:GLU:OE2	1:A:227:LYS:HE3	2.13	0.49
1:C:189:LEU:HD13	1:C:247:LEU:HD11	1.95	0.47
1:A:294:LEU:HG	1:A:389:PHE:CE2	2.51	0.46
1:C:223:GLU:OE2	1:C:227:LYS:HE2	2.15	0.46
1:D:257[A]:GLU:OE2	1:D:415:TRP:HZ2	1.99	0.46
1:D:328:GLY:O	1:D:331:VAL:HG22	2.17	0.45
1:C:148:GLN:NE2	4:C:607:HOH:O	2.41	0.45
1:D:294:LEU:HD12	1:D:353:VAL:HB	1.99	0.45
1:D:168:ARG:NH2	2:D:501:KY8:N33	2.58	0.44
1:B:433:THR:HG23	4:B:659:HOH:O	2.16	0.44
1:C:168:ARG:NH2	1:C:257:GLU:OE1	2.51	0.44
1:D:255:ILE:HG22	1:D:286:PHE:HB2	2.00	0.44
1:D:414:HIS:NE2	4:D:602:HOH:O	2.35	0.43
1:C:151:GLN:HG3	4:C:669:HOH:O	2.19	0.43
1:C:135:SER:O	1:C:139:GLU:HG2	2.20	0.42
1:C:255:ILE:HG22	1:C:286:PHE:HB2	2.02	0.42
1:C:365:GLY:HA2	1:C:368:HIS:NE2	2.34	0.42
1:D:294:LEU:CD1	1:D:353:VAL:HB	2.50	0.42
1:A:264:PHE:CE2	1:A:292:VAL:HG21	2.55	0.42
1:D:313:TRP:O	1:D:324:SER:HA	2.20	0.42
1:B:207:ALA:CB	1:B:210:ILE:HD11	2.50	0.41
1:D:365:GLY:HA2	1:D:368:HIS:CD2	2.56	0.41
1:A:255:ILE:HG22	1:A:286:PHE:HB2	2.03	0.41
1:B:365:GLY:HA2	1:B:368:HIS:ND1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:TRP:O	1:C:324:SER:HA	2.20	0.41
1:C:257:GLU:OE2	1:C:415:TRP:HZ2	2.03	0.40
1:C:337:GLN:NE2	4:C:620:HOH:O	2.54	0.40
1:A:241:LYS:HA	2:A:501[A]:KY8:N10	2.36	0.40
1:C:183:PHE:O	1:C:207:ALA:HA	2.22	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	342/351 (97%)	331 (97%)	11 (3%)	0	100	100
1	B	340/351 (97%)	328 (96%)	12 (4%)	0	100	100
1	C	344/351 (98%)	333 (97%)	11 (3%)	0	100	100
1	D	341/351 (97%)	331 (97%)	10 (3%)	0	100	100
All	All	1367/1404 (97%)	1323 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/306 (98%)	298 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	298/306 (97%)	296 (99%)	2 (1%)	84	88
1	C	302/306 (99%)	299 (99%)	3 (1%)	76	82
1	D	299/306 (98%)	295 (99%)	4 (1%)	69	75
All	All	1199/1224 (98%)	1188 (99%)	11 (1%)	78	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	GLU
1	A	424	SER
1	B	168	ARG
1	B	257	GLU
1	C	148	GLN
1	C	337	GLN
1	C	424	SER
1	D	143	GLU
1	D	168	ARG
1	D	294	LEU
1	D	346	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	337	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KY8	B	501[B]	-	32,36,36	5.00	26 (81%)	34,49,49	3.03	8 (23%)
2	KY8	A	501[B]	-	32,36,36	4.18	19 (59%)	34,49,49	2.86	15 (44%)
2	KY8	D	501	-	32,36,36	4.35	21 (65%)	34,49,49	2.72	13 (38%)
2	KY8	B	501[A]	-	32,36,36	4.56	21 (65%)	34,49,49	2.69	14 (41%)
2	KY8	C	501	-	32,36,36	4.27	20 (62%)	34,49,49	3.04	17 (50%)
3	GOL	C	502	-	5,5,5	0.23	0	5,5,5	0.37	0
3	GOL	A	502	-	5,5,5	0.21	0	5,5,5	1.01	0
3	GOL	C	503	-	5,5,5	0.12	0	5,5,5	0.59	0
2	KY8	A	501[A]	-	32,36,36	4.75	24 (75%)	34,49,49	2.33	15 (44%)

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	KY8	B	501[B]	-	-	9/15/35/35	0/4/4/4
2	KY8	A	501[B]	-	-	5/15/35/35	0/4/4/4
2	KY8	D	501	-	-	8/15/35/35	0/4/4/4
2	KY8	B	501[A]	-	-	6/15/35/35	0/4/4/4
2	KY8	C	501	-	-	5/15/35/35	0/4/4/4
3	GOL	C	502	-	-	3/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
2	KY8	A	501[A]	-	-	7/15/35/35	0/4/4/4

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501[A]	KY8	C28-N33	10.24	1.48	1.34
2	D	501	KY8	O16-C17	-10.14	1.22	1.45
2	A	501[A]	KY8	C28-N29	10.09	1.48	1.34
2	D	501	KY8	C03-C02	-9.97	1.26	1.53
2	B	501[B]	KY8	O16-C17	-9.84	1.23	1.45
2	B	501[B]	KY8	C28-N29	9.77	1.48	1.34
2	B	501[B]	KY8	C03-C02	-9.70	1.27	1.53
2	B	501[A]	KY8	C28-N29	9.67	1.48	1.34
2	C	501	KY8	C28-N33	9.45	1.47	1.34
2	B	501[B]	KY8	C28-N33	9.42	1.47	1.34
2	A	501[A]	KY8	C03-C02	-9.33	1.28	1.53
2	A	501[B]	KY8	C03-C02	-9.02	1.28	1.53
2	A	501[B]	KY8	C28-N33	9.00	1.47	1.34
2	C	501	KY8	O16-C17	-8.99	1.25	1.45
2	C	501	KY8	C07-N08	-8.99	1.23	1.35
2	A	501[A]	KY8	O16-C17	-8.97	1.25	1.45
2	B	501[A]	KY8	C03-C02	-8.92	1.29	1.53
2	B	501[A]	KY8	O16-C17	-8.89	1.25	1.45
2	A	501[A]	KY8	O16-C05	-8.67	1.29	1.40
2	D	501	KY8	O16-C05	-8.64	1.29	1.40
2	A	501[B]	KY8	C07-N08	-8.48	1.24	1.35
2	B	501[A]	KY8	C07-N08	-8.44	1.24	1.35
2	A	501[B]	KY8	O16-C17	-8.24	1.26	1.45
2	C	501	KY8	C03-C02	-8.16	1.31	1.53
2	C	501	KY8	C28-N29	7.96	1.45	1.34
2	B	501[B]	KY8	C13-N14	7.69	1.67	1.39
2	A	501[B]	KY8	C28-N29	7.63	1.45	1.34
2	A	501[A]	KY8	C13-N14	7.40	1.66	1.39
2	D	501	KY8	C28-N29	7.38	1.44	1.34
2	B	501[B]	KY8	O16-C05	-7.32	1.31	1.40
2	D	501	KY8	C28-N33	6.92	1.44	1.34
2	A	501[A]	KY8	C28-N33	6.71	1.44	1.34
2	D	501	KY8	C13-N14	6.16	1.62	1.39
2	A	501[A]	KY8	C28-N27	-5.87	1.25	1.34
2	B	501[B]	KY8	C15-N14	5.75	1.45	1.34
2	B	501[A]	KY8	C30-N29	5.66	1.46	1.34
2	B	501[B]	KY8	C11-N12	5.55	1.53	1.34
2	B	501[A]	KY8	O04-C03	5.44	1.56	1.43
2	B	501[B]	KY8	C30-N29	5.34	1.45	1.34
2	B	501[B]	KY8	C20-N19	5.30	1.59	1.47
2	A	501[A]	KY8	C11-N12	5.28	1.53	1.34
2	C	501	KY8	C11-N12	5.16	1.52	1.34
2	A	501[B]	KY8	C30-N29	5.06	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	KY8	O04-C03	4.94	1.55	1.43
2	A	501[A]	KY8	C30-N29	4.92	1.44	1.34
2	A	501[A]	KY8	C15-N14	4.91	1.43	1.34
2	B	501[B]	KY8	C32-N33	4.89	1.44	1.34
2	C	501	KY8	C20-N19	4.88	1.58	1.47
2	B	501[A]	KY8	C11-N12	4.83	1.51	1.34
2	B	501[A]	KY8	C32-N33	4.71	1.44	1.34
2	D	501	KY8	C28-N27	-4.70	1.27	1.34
2	A	501[B]	KY8	O04-C03	4.67	1.54	1.43
2	A	501[A]	KY8	C32-N33	4.56	1.44	1.34
2	B	501[B]	KY8	C05-N06	4.54	1.61	1.49
2	C	501	KY8	C30-N29	4.49	1.44	1.34
2	A	501[B]	KY8	C11-N12	4.47	1.50	1.34
2	D	501	KY8	C11-N12	4.44	1.50	1.34
2	A	501[B]	KY8	C32-N33	4.41	1.43	1.34
2	B	501[A]	KY8	C31-C30	4.35	1.50	1.37
2	B	501[B]	KY8	C18-N19	4.27	1.55	1.47
2	A	501[A]	KY8	C05-N06	4.24	1.60	1.49
2	A	501[B]	KY8	C20-N19	4.22	1.57	1.47
2	C	501	KY8	C32-N33	4.22	1.43	1.34
2	B	501[B]	KY8	C24-N19	4.16	1.56	1.47
2	C	501	KY8	C13-N14	4.08	1.54	1.39
2	D	501	KY8	C32-N33	4.00	1.43	1.34
2	A	501[B]	KY8	C13-N14	3.94	1.54	1.39
2	A	501[A]	KY8	C20-N19	3.94	1.56	1.47
2	D	501	KY8	C15-N14	3.92	1.41	1.34
2	A	501[A]	KY8	C31-C30	3.87	1.48	1.37
2	B	501[A]	KY8	C13-N14	3.86	1.53	1.39
2	D	501	KY8	C30-N29	3.85	1.42	1.34
2	D	501	KY8	C24-N19	3.78	1.56	1.47
2	A	501[A]	KY8	C09-N10	3.74	1.40	1.33
2	B	501[B]	KY8	C31-C30	3.71	1.48	1.37
2	D	501	KY8	C02-C17	-3.62	1.43	1.53
2	A	501[A]	KY8	C31-C32	3.61	1.48	1.37
2	B	501[B]	KY8	C09-N08	3.58	1.37	1.32
2	A	501[A]	KY8	C24-N19	3.54	1.55	1.47
2	B	501[B]	KY8	C09-N10	3.53	1.40	1.33
2	B	501[A]	KY8	C31-C32	3.53	1.47	1.37
2	C	501	KY8	C31-C30	3.50	1.47	1.37
2	B	501[A]	KY8	C24-N19	3.42	1.55	1.47
2	A	501[B]	KY8	C09-N08	3.42	1.37	1.32
2	B	501[B]	KY8	C31-C32	3.31	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	KY8	C09-N08	3.21	1.37	1.32
2	B	501[A]	KY8	C09-N08	3.18	1.37	1.32
2	B	501[B]	KY8	C26-N27	3.18	1.52	1.45
2	B	501[A]	KY8	C28-N27	-3.15	1.29	1.34
2	D	501	KY8	C31-C30	3.12	1.46	1.37
2	B	501[A]	KY8	C18-N19	3.05	1.53	1.47
2	A	501[B]	KY8	C09-N10	3.04	1.39	1.33
2	A	501[A]	KY8	C26-N27	3.02	1.51	1.45
2	A	501[A]	KY8	C02-C17	-3.00	1.45	1.53
2	B	501[B]	KY8	C25-C26	2.98	1.63	1.51
2	B	501[B]	KY8	C02-C17	-2.90	1.45	1.53
2	C	501	KY8	C18-N19	2.83	1.53	1.47
2	B	501[B]	KY8	O04-C03	2.81	1.49	1.43
2	D	501	KY8	C20-N19	2.79	1.53	1.47
2	A	501[A]	KY8	C09-N08	2.77	1.36	1.32
2	A	501[A]	KY8	O04-C03	2.74	1.49	1.43
2	D	501	KY8	C05-N06	2.73	1.56	1.49
2	A	501[B]	KY8	C24-N19	2.70	1.53	1.47
2	A	501[B]	KY8	C31-C30	2.69	1.45	1.37
2	C	501	KY8	C31-C32	2.69	1.45	1.37
2	B	501[B]	KY8	C21-C22	2.65	1.64	1.51
2	C	501	KY8	C28-N27	-2.64	1.30	1.34
2	A	501[B]	KY8	C31-C32	2.63	1.45	1.37
2	C	501	KY8	C09-N08	2.58	1.36	1.32
2	C	501	KY8	O01-C02	2.57	1.49	1.43
2	B	501[B]	KY8	C07-N08	2.50	1.39	1.35
2	B	501[A]	KY8	C20-N19	2.47	1.53	1.47
2	B	501[A]	KY8	C09-N10	2.45	1.38	1.33
2	D	501	KY8	C31-C32	2.41	1.44	1.37
2	C	501	KY8	C24-N19	2.40	1.52	1.47
2	A	501[B]	KY8	C21-C22	2.38	1.62	1.51
2	B	501[B]	KY8	C28-N27	-2.37	1.30	1.34
2	A	501[B]	KY8	C26-N27	2.34	1.50	1.45
2	A	501[A]	KY8	C18-N19	2.34	1.52	1.47
2	B	501[A]	KY8	O16-C05	-2.33	1.37	1.40
2	A	501[A]	KY8	C25-C26	2.33	1.60	1.51
2	D	501	KY8	C25-C26	2.32	1.60	1.51
2	B	501[B]	KY8	C21-C20	2.29	1.60	1.51
2	B	501[A]	KY8	C26-N27	2.25	1.50	1.45
2	B	501[A]	KY8	C21-C22	2.20	1.62	1.51
2	A	501[B]	KY8	O16-C05	-2.17	1.38	1.40
2	A	501[A]	KY8	C07-N08	2.17	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	KY8	C21-C22	2.13	1.61	1.51
2	D	501	KY8	O04-C03	2.09	1.48	1.43
2	C	501	KY8	C26-N27	2.08	1.50	1.45
2	D	501	KY8	C09-N10	2.08	1.37	1.33

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[B]	KY8	C30-N29-C28	9.79	123.60	115.42
2	B	501[B]	KY8	C32-N33-C28	9.49	123.35	115.42
2	B	501[B]	KY8	N33-C28-N29	-9.21	117.10	126.43
2	C	501	KY8	N33-C28-N29	-8.45	117.87	126.43
2	C	501	KY8	C30-N29-C28	7.46	121.65	115.42
2	A	501[B]	KY8	N33-C28-N29	-7.45	118.88	126.43
2	B	501[A]	KY8	N33-C28-N29	-7.24	119.09	126.43
2	B	501[A]	KY8	C32-N33-C28	6.74	121.05	115.42
2	D	501	KY8	C32-N33-C28	6.48	120.84	115.42
2	C	501	KY8	C32-N33-C28	6.30	120.68	115.42
2	D	501	KY8	N33-C28-N29	-6.08	120.28	126.43
2	D	501	KY8	C17-O16-C05	-5.99	104.44	109.92
2	B	501[B]	KY8	C30-N29-C28	5.98	120.42	115.42
2	B	501[A]	KY8	C30-N29-C28	5.90	120.35	115.42
2	A	501[A]	KY8	C17-O16-C05	-5.61	104.79	109.92
2	B	501[B]	KY8	N27-C28-N29	5.36	124.42	117.21
2	B	501[B]	KY8	N08-C09-N10	-5.02	121.86	128.67
2	D	501	KY8	C30-N29-C28	4.93	119.54	115.42
2	A	501[A]	KY8	C30-N29-C28	4.85	119.47	115.42
2	C	501	KY8	C24-N19-C20	-4.82	99.96	111.44
2	A	501[A]	KY8	N08-C09-N10	-4.53	122.52	128.67
2	D	501	KY8	N08-C09-N10	-4.35	122.77	128.67
2	A	501[B]	KY8	C31-C30-N29	-4.22	116.74	123.42
2	C	501	KY8	N08-C09-N10	-4.20	122.97	128.67
2	D	501	KY8	N27-C28-N33	4.19	122.84	117.21
2	A	501[A]	KY8	N27-C28-N29	4.00	122.59	117.21
2	B	501[A]	KY8	N08-C09-N10	-3.91	123.37	128.67
2	D	501	KY8	O16-C17-C18	-3.72	102.79	108.88
2	A	501[B]	KY8	N08-C09-N10	-3.61	123.78	128.67
2	D	501	KY8	C24-N19-C20	-3.60	102.87	111.44
2	C	501	KY8	C26-N27-C28	-3.45	117.84	123.82
2	C	501	KY8	C17-O16-C05	-3.36	106.85	109.92
2	C	501	KY8	N27-C28-N29	3.30	121.65	117.21
2	A	501[A]	KY8	C31-C30-N29	-3.30	118.20	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501[A]	KY8	C25-C24-N19	-3.29	104.70	113.93
2	B	501[A]	KY8	N27-C28-N33	3.28	121.62	117.21
2	A	501[B]	KY8	C17-O16-C05	-3.27	106.93	109.92
2	A	501[A]	KY8	N33-C28-N29	-3.21	123.18	126.43
2	A	501[B]	KY8	N27-C28-N33	3.19	121.50	117.21
2	C	501	KY8	O16-C05-N06	3.10	112.85	108.75
2	B	501[A]	KY8	C17-O16-C05	-3.07	107.12	109.92
2	B	501[A]	KY8	C24-N19-C20	-3.02	104.25	111.44
2	A	501[A]	KY8	C21-C20-N19	-2.95	105.64	113.93
2	A	501[B]	KY8	C13-C11-N12	2.94	124.79	120.31
2	B	501[A]	KY8	C13-C11-N12	2.92	124.76	120.31
2	B	501[B]	KY8	C24-N19-C20	-2.91	104.50	111.44
2	C	501	KY8	C13-C11-N12	2.90	124.73	120.31
2	B	501[B]	KY8	C31-C32-N33	-2.82	118.96	123.42
2	D	501	KY8	C32-C31-C30	2.77	120.22	116.63
2	A	501[B]	KY8	C32-C31-C30	2.75	120.20	116.63
2	D	501	KY8	C31-C32-N33	-2.72	119.11	123.42
2	A	501[B]	KY8	C24-N19-C20	-2.69	105.03	111.44
2	A	501[B]	KY8	C11-C13-C07	2.59	122.94	117.90
2	A	501[A]	KY8	C32-C31-C30	2.57	119.97	116.63
2	A	501[B]	KY8	C32-N33-C28	2.55	117.55	115.42
2	C	501	KY8	C05-N06-C07	-2.52	122.22	126.64
2	C	501	KY8	C24-N19-C18	-2.45	106.18	111.89
2	B	501[A]	KY8	C11-C13-C07	2.41	122.59	117.90
2	C	501	KY8	N27-C28-N33	2.40	120.44	117.21
2	A	501[B]	KY8	C13-C11-N10	-2.38	114.56	120.23
2	C	501	KY8	C13-C11-N10	-2.37	114.58	120.23
2	B	501[A]	KY8	C13-C11-N10	-2.36	114.59	120.23
2	B	501[A]	KY8	C31-C30-N29	-2.34	119.72	123.42
2	A	501[A]	KY8	O16-C05-N06	-2.34	105.65	108.75
2	A	501[B]	KY8	C21-C20-N19	-2.32	107.41	113.93
2	A	501[A]	KY8	C20-N19-C18	-2.31	106.52	111.89
2	A	501[A]	KY8	C24-N19-C20	-2.29	106.00	111.44
2	C	501	KY8	C11-C13-C07	2.27	122.31	117.90
2	C	501	KY8	C31-C30-N29	-2.22	119.90	123.42
2	A	501[A]	KY8	N27-C28-N33	-2.22	114.22	117.21
2	B	501[A]	KY8	C32-C31-C30	2.20	119.49	116.63
2	D	501	KY8	C31-C30-N29	-2.20	119.94	123.42
2	D	501	KY8	C21-C20-N19	-2.19	107.77	113.93
2	A	501[B]	KY8	C25-C26-N27	-2.19	105.53	111.46
2	A	501[A]	KY8	C25-C26-N27	-2.15	105.64	111.46
2	C	501	KY8	C20-N19-C18	-2.15	106.89	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[A]	KY8	N12-C11-N10	2.14	122.91	118.33
2	A	501[B]	KY8	C05-N06-C07	-2.14	122.89	126.64
2	D	501	KY8	C24-N19-C18	-2.06	107.10	111.89
2	A	501[A]	KY8	C32-N33-C28	2.04	117.13	115.42
2	B	501[B]	KY8	C17-O16-C05	-2.03	108.07	109.92
2	B	501[A]	KY8	C31-C32-N33	-2.01	120.24	123.42

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[A]	KY8	C02-C17-C18-N19
2	A	501[A]	KY8	O16-C17-C18-N19
2	A	501[B]	KY8	C02-C17-C18-N19
2	A	501[B]	KY8	O16-C17-C18-N19
2	B	501[A]	KY8	C02-C17-C18-N19
2	B	501[A]	KY8	O16-C17-C18-N19
2	B	501[B]	KY8	C02-C17-C18-N19
2	B	501[B]	KY8	O16-C17-C18-N19
2	B	501[B]	KY8	C25-C24-N19-C18
2	C	501	KY8	C02-C17-C18-N19
2	C	501	KY8	O16-C17-C18-N19
2	D	501	KY8	C02-C17-C18-N19
2	D	501	KY8	O16-C17-C18-N19
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	C	502	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-C3
2	A	501[A]	KY8	C24-C25-C26-N27
3	A	502	GOL	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-O2
2	A	501[B]	KY8	C21-C20-N19-C24
2	D	501	KY8	C21-C20-N19-C24
2	C	501	KY8	C21-C20-N19-C24
2	A	501[A]	KY8	C25-C24-N19-C18
2	B	501[B]	KY8	C25-C24-N19-C20
2	B	501[A]	KY8	C25-C24-N19-C20
2	B	501[B]	KY8	N19-C20-C21-C22
3	A	502	GOL	O2-C2-C3-O3
2	A	501[A]	KY8	N19-C24-C25-C26
2	A	501[A]	KY8	C25-C24-N19-C20
2	A	501[B]	KY8	C21-C20-N19-C18

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Mol	Chain	Res	Type	Atoms
2	B	501[A]	KY8	C20-C21-C22-N23
2	C	501	KY8	C20-C21-C22-N23
3	C	502	GOL	O2-C2-C3-O3
2	B	501[A]	KY8	C17-C18-N19-C24
2	D	501	KY8	C24-C25-C26-N27
2	D	501	KY8	C25-C24-N19-C18
2	A	501[A]	KY8	C20-C21-C22-N23
2	B	501[B]	KY8	C20-C21-C22-N23
2	D	501	KY8	C20-C21-C22-N23
3	C	502	GOL	O1-C1-C2-C3
2	D	501	KY8	C21-C20-N19-C18
2	B	501[A]	KY8	C25-C24-N19-C18
2	B	501[B]	KY8	C21-C20-N19-C24
2	D	501	KY8	C17-C18-N19-C20
2	A	501[B]	KY8	C25-C26-N27-C28
2	B	501[B]	KY8	C25-C26-N27-C28
2	C	501	KY8	N19-C24-C25-C26
2	B	501[B]	KY8	C17-C18-N19-C24

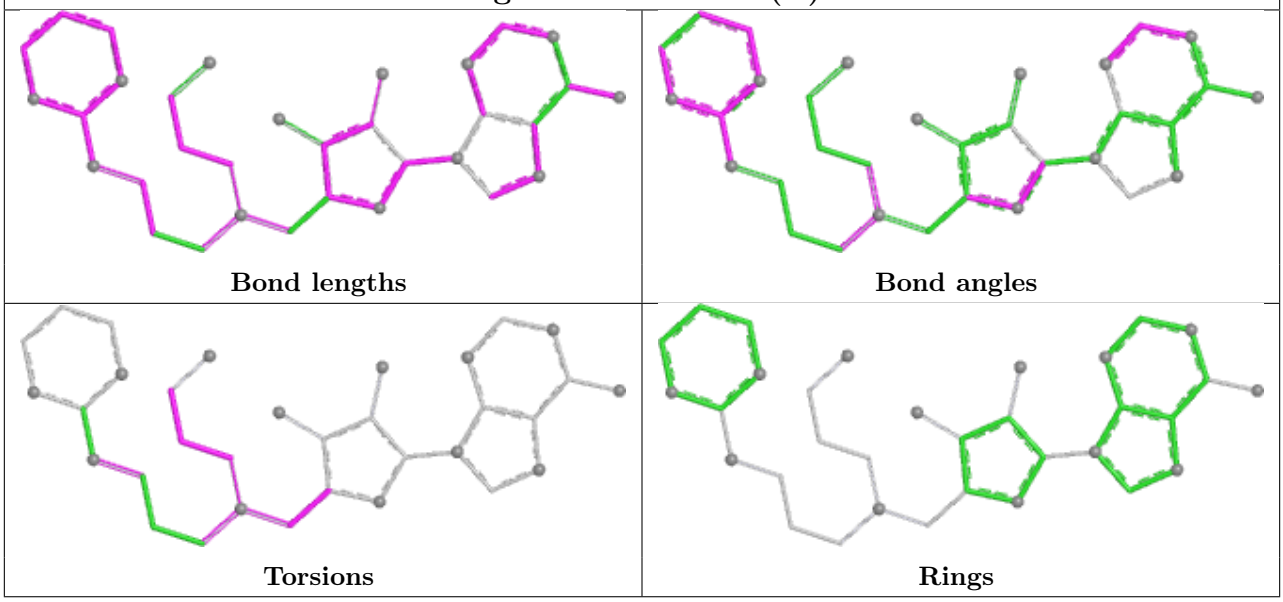
There are no ring outliers.

4 monomers are involved in 8 short contacts:

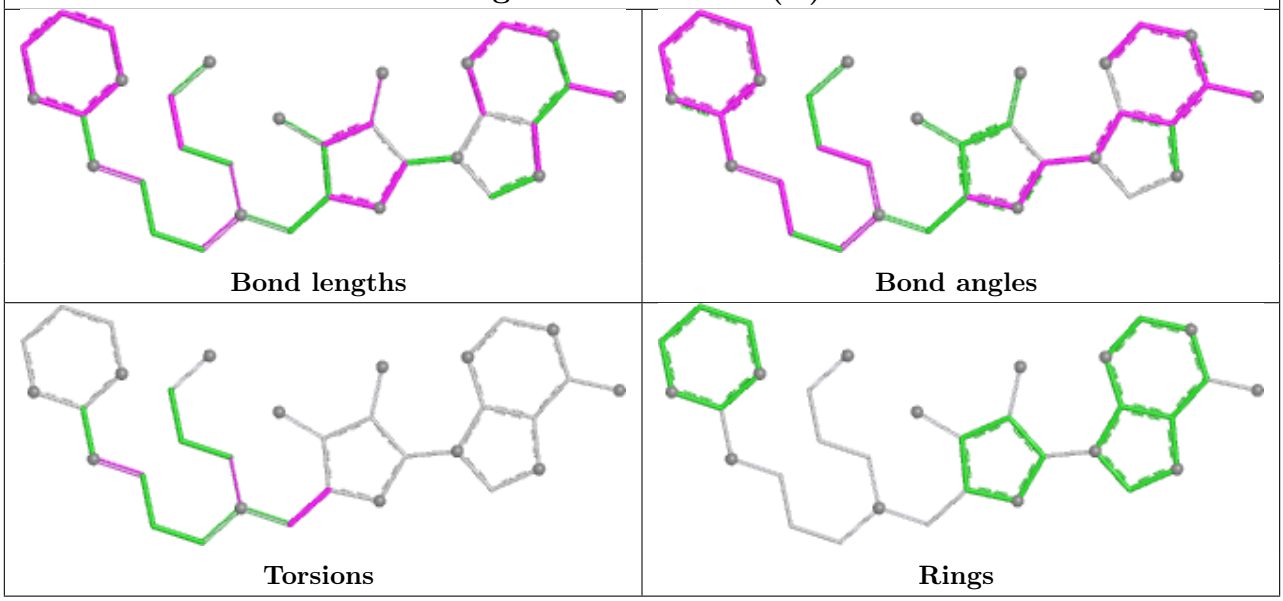
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501[B]	KY8	5	0
2	D	501	KY8	1	0
2	B	501[A]	KY8	1	0
2	A	501[A]	KY8	1	0

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

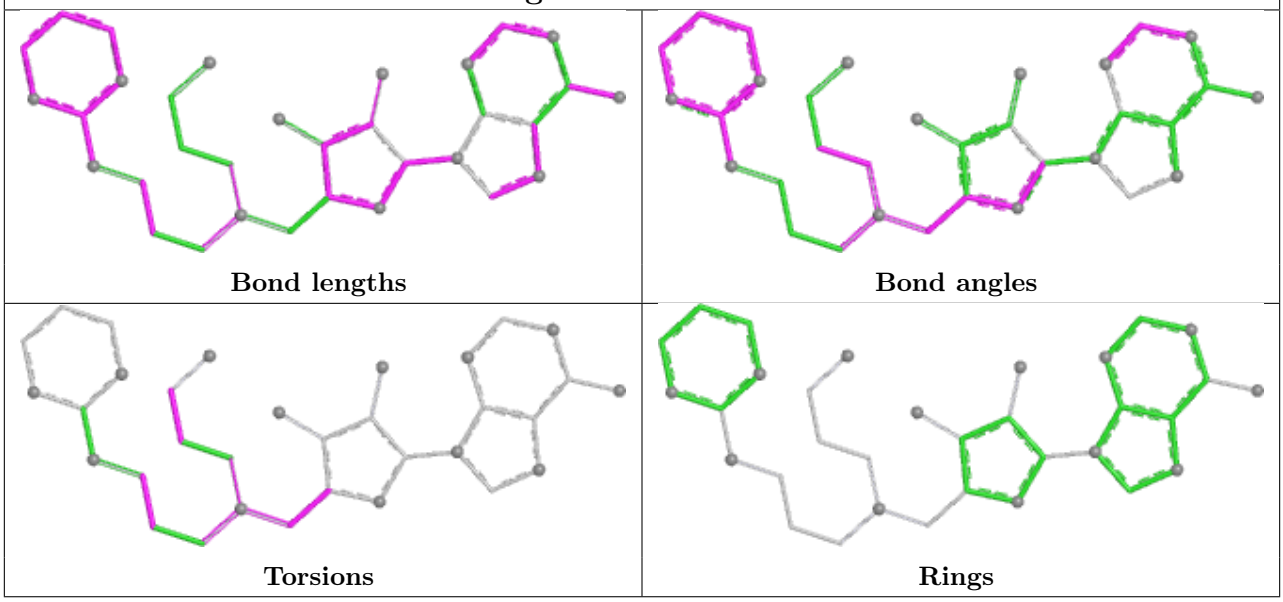
Ligand KY8 B 501 (B)



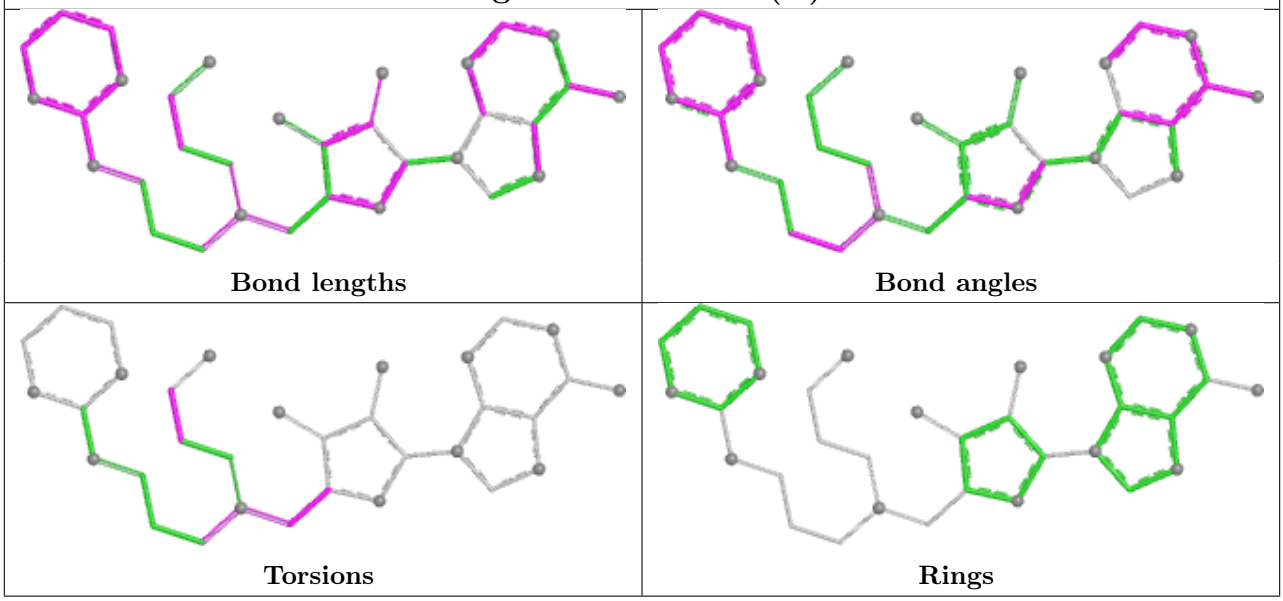
Ligand KY8 A 501 (B)



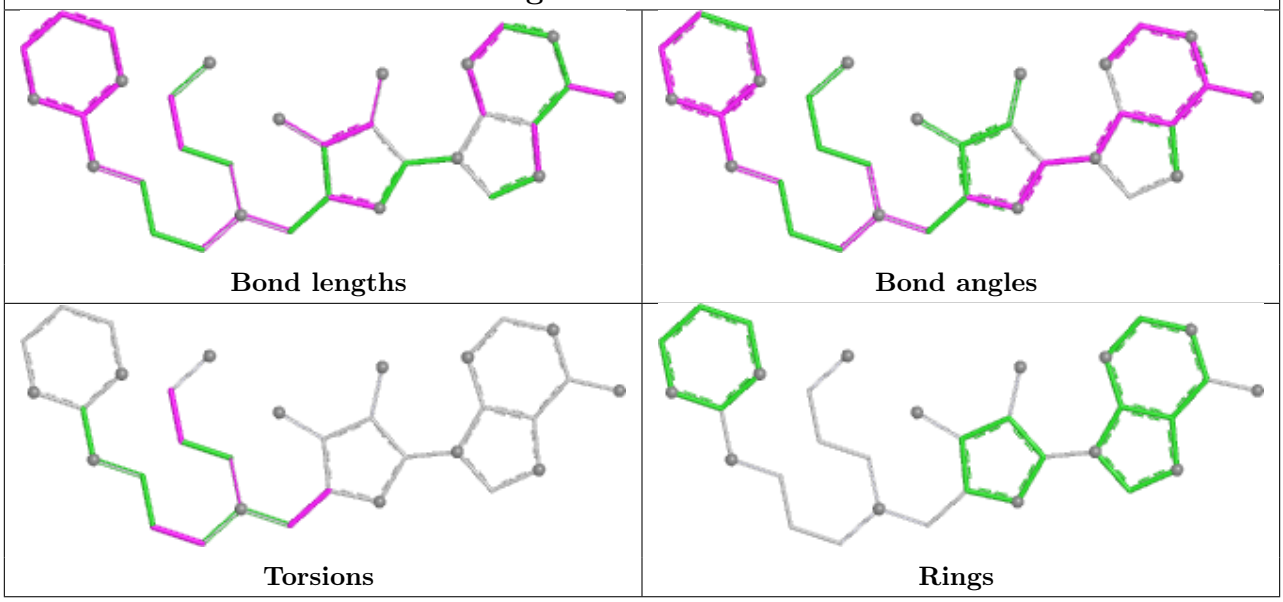
Ligand KY8 D 501



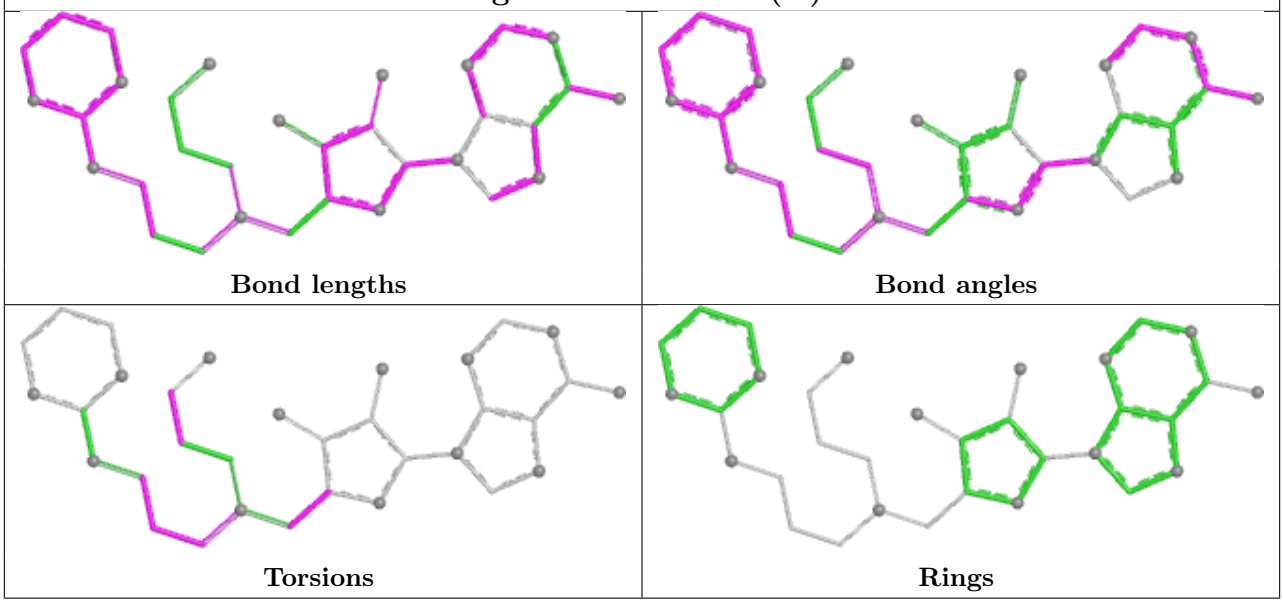
Ligand KY8 B 501 (A)



Ligand KY8 C 501



Ligand KY8 A 501 (A)



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	342/351 (97%)	-0.57	0	100	100	19, 30, 44, 57	0
1	B	342/351 (97%)	-0.39	0	100	100	26, 40, 57, 70	0
1	C	342/351 (97%)	-0.49	0	100	100	20, 33, 46, 56	0
1	D	342/351 (97%)	-0.45	1 (0%)	94	94	27, 37, 51, 84	0
All	All	1368/1404 (97%)	-0.47	1 (0%)	95	96	19, 35, 51, 84	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	346	ARG	2.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	502	6/6	0.82	0.15	58,59,62,70	0

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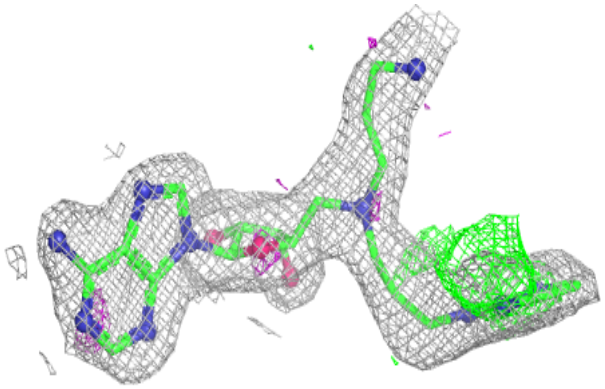
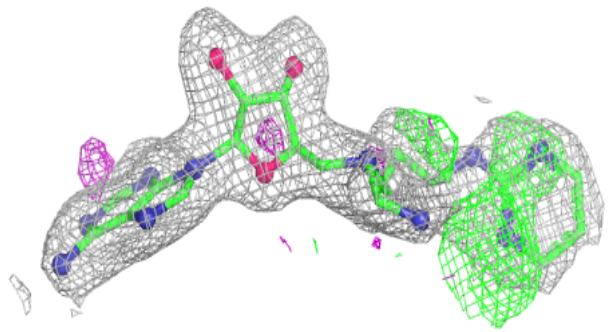
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	503	6/6	0.88	0.13	50,55,56,58	0
2	KY8	A	501[A]	33/33	0.89	0.15	20,25,35,36	33
2	KY8	A	501[B]	33/33	0.89	0.15	21,25,33,34	33
2	KY8	B	501[A]	33/33	0.90	0.15	28,32,40,43	33
2	KY8	B	501[B]	33/33	0.90	0.15	35,41,45,46	33
2	KY8	D	501	33/33	0.92	0.12	29,37,47,52	0
2	KY8	C	501	33/33	0.93	0.12	25,29,43,46	0
3	GOL	A	502	6/6	0.95	0.12	43,46,48,49	0

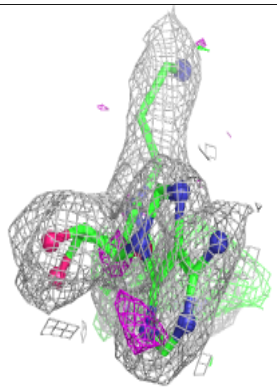
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KY8 A 501 (A):

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

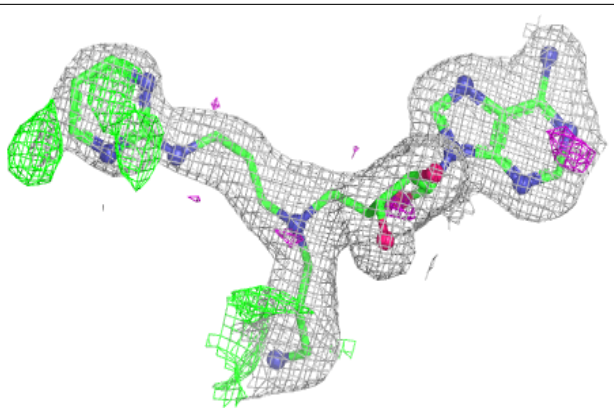


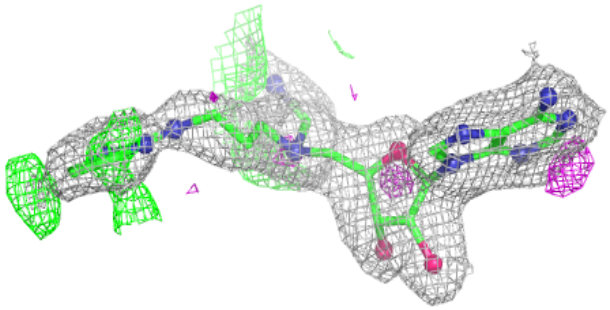


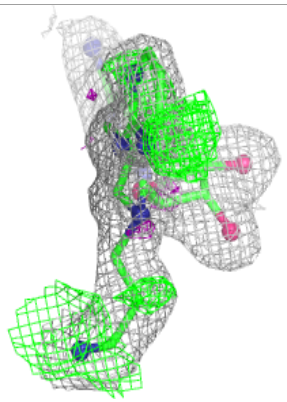


Electron density around KY8 A 501 (B):

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

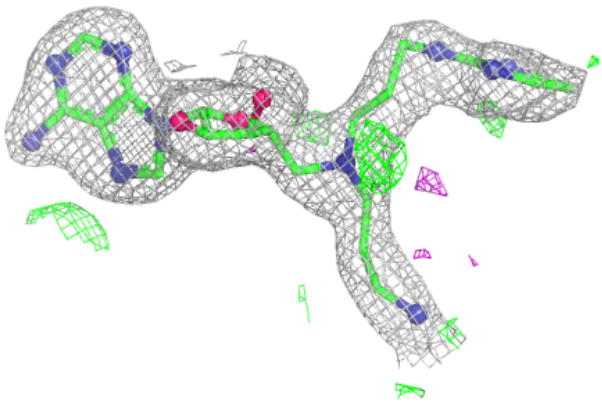


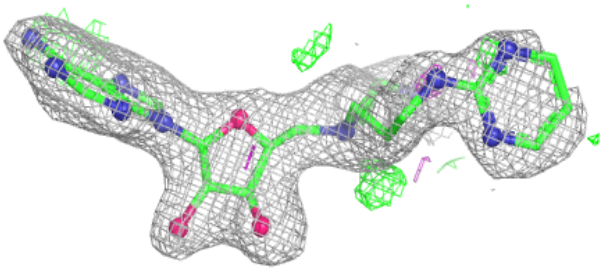


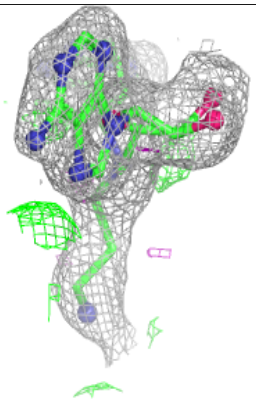


Electron density around KY8 B 501 (A):

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

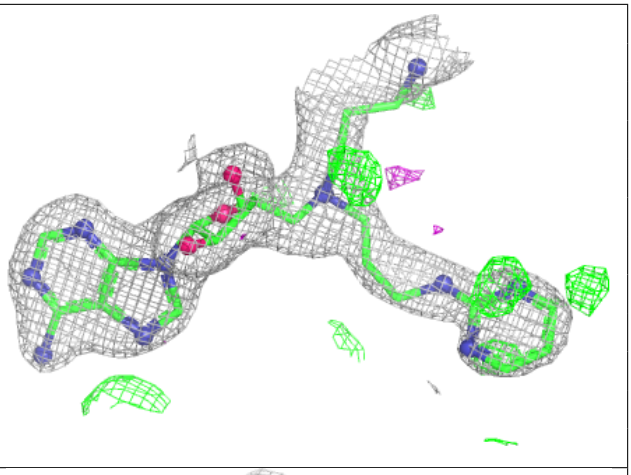


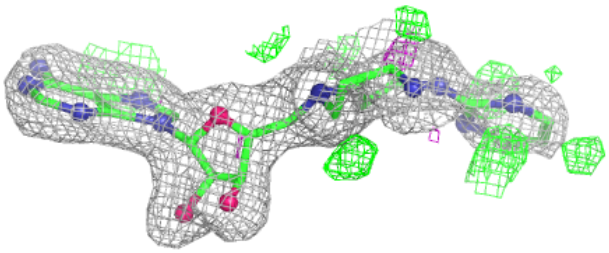


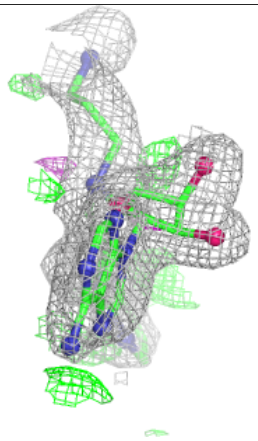


Electron density around KY8 B 501 (B):

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

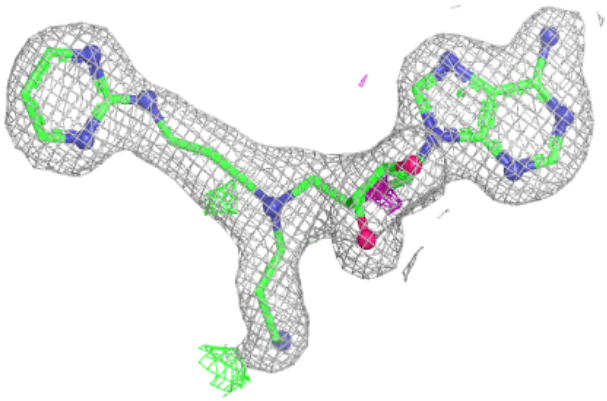


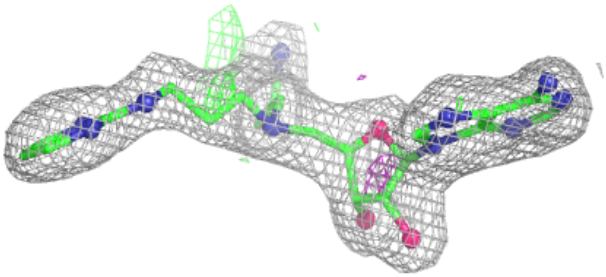


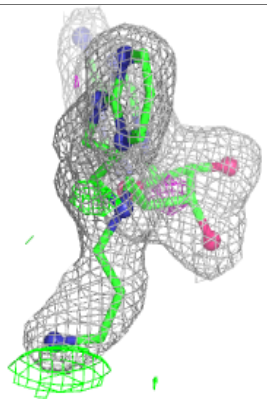


Electron density around KY8 D 501:

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

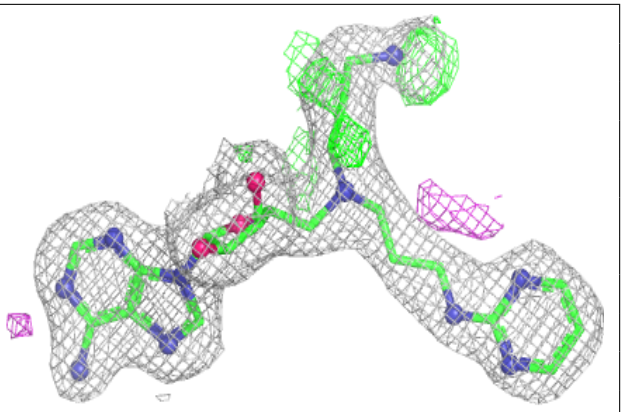


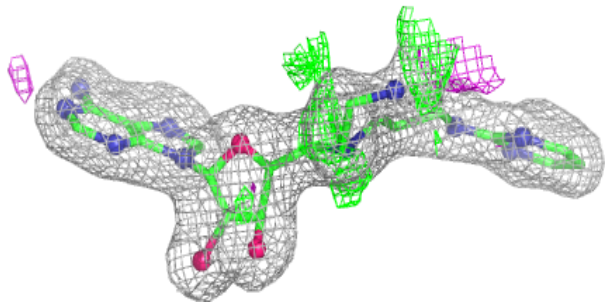


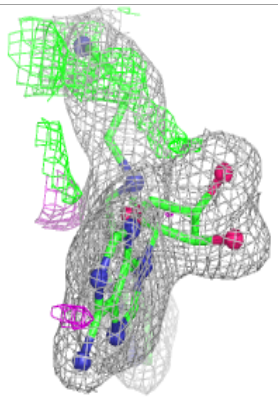


Electron density around KY8 C 501:

$2mF_o$-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.