



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:22 am BST

PDB ID : 6S71
Title : Crystal structure of CARM1 in complex with inhibitor WH5C
Authors : Gunnell, E.A.; Muhsen, U.; Dowden, J.; Dreveny, I.
Deposited on : 2019-07-04
Resolution : 2.06 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

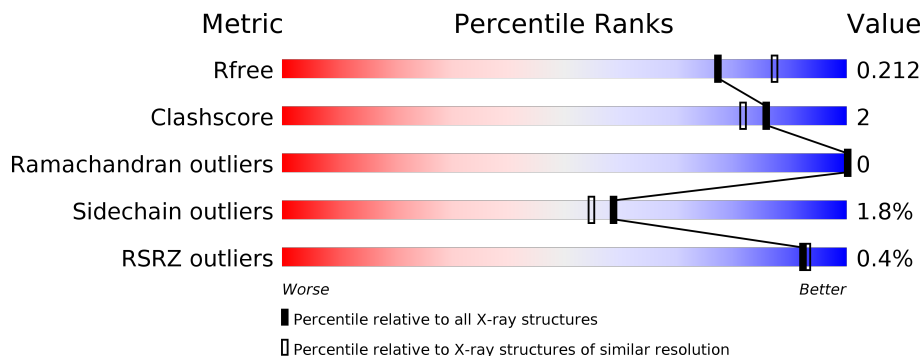
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	351	 92% 5% . . .
1	B	351	 92% . . .
1	C	351	 93% . . .
1	D	351	 89% 7% . . .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11755 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	2757	1781	454	506	16	0	2	0
1	B	342	2754	1778	456	506	14	0	1	0
1	C	342	2781	1795	463	507	16	0	5	0
1	D	342	2747	1774	453	505	15	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

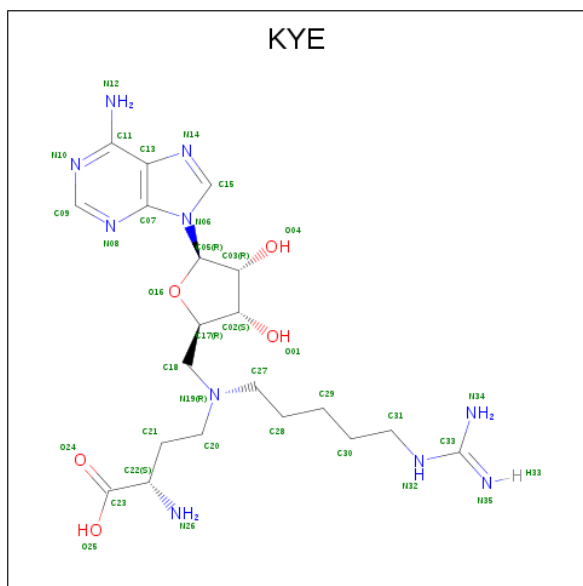
Chain	Residue	Modelled	Actual	Comment	Reference
A	480	HIS	-	expression tag	UNP Q86X55
A	481	HIS	-	expression tag	UNP Q86X55
A	482	HIS	-	expression tag	UNP Q86X55
A	483	HIS	-	expression tag	UNP Q86X55
A	484	HIS	-	expression tag	UNP Q86X55
A	485	HIS	-	expression tag	UNP Q86X55
B	480	HIS	-	expression tag	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 {S})-4-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl-(5-carbamimidamidopentyl)amino]-2-azanyl-butanoic acid (three-letter code: KYE) (formula: C₂₀H₃₄N₁₀O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			35	20	10	5		
2	B	1	Total	C	N	O	0	0
			35	20	10	5		
2	C	1	Total	C	N	O	0	0
			35	20	10	5		
2	D	1	Total	C	N	O	0	0
			35	20	10	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	129	Total O 129 129	0	0
4	B	164	Total O 164 164	0	0
4	C	103	Total O 103 103	0	0
4	D	138	Total O 138 138	0	0

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: Histone-arginine methyltransferase CARM1

Chain A:  92% 5% ..



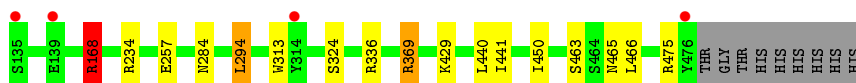
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain B:  92% ..




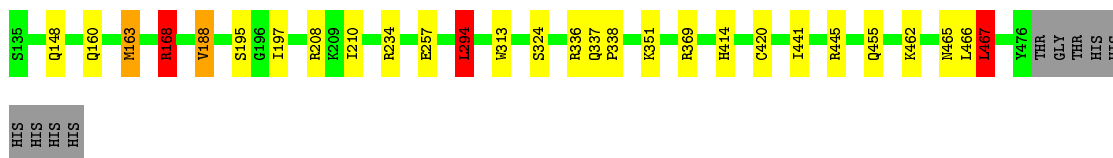
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain C:  % 93% ..



- Molecule 1: Histone-arginine methyltransferase CARM1

Chain D:  89% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 98.63Å 206.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.18 – 2.06 103.18 – 2.06	Depositor EDS
% Data completeness (in resolution range)	96.6 (103.18-2.06) 91.6 (103.18-2.06)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.07Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.210 0.185 , 0.212	Depositor DCC
R_{free} test set	2000 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtrriage
Anisotropy	0.272	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11755	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.43 % 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 1.8456e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: GOL, KYE

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	0.63	1/2830 (0.0%)	0.79	5/3833 (0.1%)
1	B	0.65	0/2825	0.84	5/3828 (0.1%)
1	C	0.60	0/2861	0.79	5/3874 (0.1%)
1	D	0.64	0/2820	0.83	8/3821 (0.2%)
All	All	0.63	1/11336 (0.0%)	0.81	23/15356 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	GLN	CD-OE1	5.23	1.35	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	NE-CZ-NH1	-16.41	112.10	120.30
1	B	168	ARG	NE-CZ-NH2	14.18	127.39	120.30
1	C	234	ARG	NE-CZ-NH2	-12.74	113.93	120.30
1	D	168	ARG	NE-CZ-NH1	11.91	126.25	120.30
1	D	168	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	C	168	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	C	168	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	A	168	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	D	234	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	D	445	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	294	LEU	CA-CB-CG	6.46	130.15	115.30
1	B	369	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	165	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	294	LEU	CA-CB-CG	5.91	128.90	115.30
1	D	294	LEU	CA-CB-CG	5.88	128.82	115.30
1	C	475	ARG	NE-CZ-NH2	-5.75	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	467	LEU	CB-CG-CD2	-5.23	102.10	111.00
1	D	163	MET	CG-SD-CE	5.15	108.44	100.20
1	A	322	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	467	LEU	CA-CB-CG	5.11	127.06	115.30
1	C	369	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	392	ASP	CB-CG-OD1	5.02	122.82	118.30

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	2757	0	2709	12	0
1	B	2754	0	2698	11	0
1	C	2781	0	2737	7	0
1	D	2747	0	2697	20	0
2	A	35	0	0	2	0
2	B	35	0	0	2	0
2	C	35	0	0	0	0
2	D	35	0	0	1	0
3	A	12	0	16	3	0
3	B	12	0	16	1	0
3	C	6	0	8	0	0
3	D	12	0	16	1	0
4	A	129	0	0	2	0
4	B	164	0	0	1	0
4	C	103	0	0	1	0
4	D	138	0	0	1	0
All	All	11755	0	10897	48	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 (48) 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:148:GLN:OE1	3:D:502:GOL:O3	1.96	0.84
1:A:352:SER:HB3	3:A:503:GOL:H12	1.64	0.80
1:C:284:ASN:HB2	4:C:687:HOH:O	1.83	0.79
1:A:197:ILE:HG22	2:A:501:KYE:O25	1.88	0.74
1:D:160:GLN:HA	1:D:163:MET:HE3	1.73	0.70
1:D:420:CYS:SG	1:D:467:LEU:HD22	2.30	0.70
1:C:336:ARG:HG2	1:C:466:LEU:O	1.96	0.64
1:D:420:CYS:SG	1:D:467:LEU:CD2	2.86	0.64
1:D:336:ARG:HG2	1:D:466:LEU:O	2.00	0.62
1:A:352:SER:CB	3:A:503:GOL:H12	2.31	0.61
1:C:168:ARG:HD2	1:C:257:GLU:OE1	2.04	0.57
1:B:313:TRP:CH2	1:D:163:MET:HE1	2.39	0.57
1:D:168:ARG:HD2	1:D:257:GLU:OE1	2.04	0.57
1:B:168:ARG:NH1	2:B:501:KYE:O24	2.36	0.57
1:A:247:LEU:HB3	4:A:609:HOH:O	2.04	0.56
1:B:313:TRP:CH2	1:D:163:MET:CE	2.88	0.56
1:B:159:GLN:NE2	2:B:501:KYE:O25	2.38	0.54
1:B:312:PHE:HE2	1:D:163:MET:HE1	1.73	0.52
1:D:337:GLN:NE2	4:D:606:HOH:O	2.36	0.50
1:D:195:SER:OG	1:D:197:ILE:HG12	2.12	0.48
1:D:188:VAL:HG22	1:D:210:ILE:HG23	1.95	0.48
1:C:440:LEU:HD22	1:C:450:ILE:HG12	1.97	0.47
1:A:352:SER:H	3:A:503:GOL:H12	1.80	0.47
1:A:455:GLN:OE1	1:A:462:LYS:NZ	2.48	0.46
1:B:188:VAL:HG22	1:B:210:ILE:HG23	1.96	0.46
1:B:440:LEU:HD22	1:B:450:ILE:HG12	1.98	0.46
1:A:188:VAL:HG22	1:A:210:ILE:HG23	1.96	0.46
1:A:440:LEU:HD22	1:A:450:ILE:HG12	1.99	0.45
1:A:315:GLN:HG3	4:A:679:HOH:O	2.17	0.44
1:A:264:PHE:CE2	1:A:292:VAL:HG21	2.53	0.44
1:D:369:ARG:HG3	1:D:441:ILE:CD1	2.48	0.44
1:C:294:LEU:HD23	1:C:294:LEU:N	2.32	0.44
1:D:420:CYS:SG	1:D:467:LEU:HD21	2.57	0.44
1:D:338:PRO:HB3	1:D:467:LEU:HD21	1.99	0.43
1:D:455:GLN:HB3	1:D:462:LYS:HG3	2.00	0.43
1:D:294:LEU:HD12	1:D:294:LEU:N	2.33	0.43
1:A:197:ILE:CG2	2:A:501:KYE:O25	2.63	0.43
1:D:351:LYS:HD3	1:D:351:LYS:HA	1.89	0.43
1:C:313:TRP:O	1:C:324:SER:HA	2.19	0.42
1:C:369:ARG:HG3	1:C:441:ILE:CD1	2.50	0.41
1:D:313:TRP:O	1:D:324:SER:HA	2.20	0.41
1:B:264:PHE:CE2	1:B:292:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLN:HA	1:D:163:MET:CE	2.48	0.41
1:B:148:GLN:OE1	3:B:503:GOL:O1	2.30	0.41
1:B:294:LEU:HD12	1:B:294:LEU:N	2.36	0.40
1:B:269:LEU:HB2	4:B:723:HOH:O	2.20	0.40
1:A:349[A]:MET:SD	1:A:384:VAL:HG22	2.62	0.40
2:D:501:KYE:C20	2:D:501:KYE:O24	2.69	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%)	334 (98%)	8 (2%)	0	100	100
1	B	341/351 (97%)	333 (98%)	8 (2%)	0	100	100
1	C	345/351 (98%)	336 (97%)	9 (3%)	0	100	100
1	D	341/351 (97%)	333 (98%)	8 (2%)	0	100	100
All	All	1369/1404 (98%)	1336 (98%)	33 (2%)	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%)	297 (99%)	3 (1%)	76	75
1	B	299/306 (98%)	293 (98%)	6 (2%)	55	51
1	C	303/306 (99%)	298 (98%)	5 (2%)	60	57
1	D	299/306 (98%)	292 (98%)	7 (2%)	50	45
All	All	1201/1224 (98%)	1180 (98%)	21 (2%)	59	57

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

Mol	Chain	Res	Type
1	A	168	ARG
1	A	188	VAL
1	A	294	LEU
1	B	168	ARG
1	B	188	VAL
1	B	208	ARG
1	B	209	LYS
1	B	294	LEU
1	B	424	SER
1	C	168	ARG
1	C	294	LEU
1	C	429	LYS
1	C	463	SER
1	C	465	ASN
1	D	168	ARG
1	D	188	VAL
1	D	208	ARG
1	D	294	LEU
1	D	414	HIS
1	D	465	ASN
1	D	467	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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
3	GOL	C	502	-	5,5,5	0.18	0	5,5,5	0.24	0
2	KYE	D	501	-	30,37,37	3.39	10 (33%)	29,51,51	1.75	5 (17%)
2	KYE	A	501	-	30,37,37	3.49	9 (30%)	29,51,51	1.51	5 (17%)
3	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.25	0
2	KYE	C	501	-	30,37,37	2.88	7 (23%)	29,51,51	1.71	7 (24%)
2	KYE	B	501	-	30,37,37	3.32	7 (23%)	29,51,51	1.71	8 (27%)
3	GOL	B	503	-	5,5,5	0.20	0	5,5,5	0.48	0
3	GOL	B	502	-	5,5,5	0.10	0	5,5,5	0.59	0
3	GOL	D	502	-	5,5,5	0.13	0	5,5,5	0.45	0
3	GOL	D	503	-	5,5,5	0.27	0	5,5,5	0.52	0
3	GOL	A	502	-	5,5,5	0.19	0	5,5,5	0.34	0

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	GOL	C	502	-	-	1/4/4/4	-
2	KYE	D	501	-	-	6/18/42/42	0/3/3/3
2	KYE	A	501	-	-	6/18/42/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	503	-	-	2/4/4/4	-
2	KYE	C	501	-	-	6/18/42/42	0/3/3/3
2	KYE	B	501	-	-	11/18/42/42	0/3/3/3
3	GOL	B	503	-	-	0/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	D	503	-	-	0/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	KYE	O16-C05	-12.18	1.24	1.41
2	D	501	KYE	O16-C05	-10.99	1.25	1.41
2	B	501	KYE	O16-C05	-10.93	1.25	1.41
2	B	501	KYE	C03-C02	-10.51	1.24	1.53
2	A	501	KYE	C03-C02	-10.41	1.24	1.53
2	D	501	KYE	C03-C02	-10.41	1.24	1.53
2	C	501	KYE	C03-C02	-8.93	1.28	1.53
2	C	501	KYE	O16-C05	-8.68	1.29	1.41
2	D	501	KYE	C03-C05	6.93	1.64	1.53
2	C	501	KYE	C03-C05	6.71	1.64	1.53
2	A	501	KYE	C03-C05	6.17	1.63	1.53
2	B	501	KYE	C03-C05	6.00	1.62	1.53
2	A	501	KYE	C18-C17	-4.14	1.38	1.51
2	A	501	KYE	O01-C02	3.42	1.51	1.43
2	B	501	KYE	C18-C17	-3.30	1.41	1.51
2	D	501	KYE	C18-C17	-3.21	1.41	1.51
2	A	501	KYE	C11-N12	3.15	1.45	1.34
2	B	501	KYE	C11-N12	3.05	1.45	1.34
2	C	501	KYE	C11-N12	3.03	1.45	1.34
2	D	501	KYE	C11-N12	3.01	1.45	1.34
2	B	501	KYE	O01-C02	2.95	1.49	1.43
2	C	501	KYE	O01-C02	2.81	1.49	1.43
2	D	501	KYE	C13-C07	-2.80	1.33	1.40
2	C	501	KYE	C18-C17	-2.79	1.43	1.51
2	A	501	KYE	C13-C07	-2.68	1.33	1.40
2	D	501	KYE	O01-C02	2.63	1.49	1.43
2	B	501	KYE	C13-C07	-2.35	1.34	1.40
2	D	501	KYE	O16-C17	2.35	1.50	1.45
2	D	501	KYE	C15-N14	-2.34	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	KYE	C15-N14	-2.08	1.31	1.34
2	C	501	KYE	O16-C17	2.06	1.49	1.45
2	D	501	KYE	C22-N26	-2.01	1.42	1.47
2	A	501	KYE	C13-N14	-2.00	1.32	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	KYE	N08-C09-N10	-4.68	121.36	128.68
2	A	501	KYE	N08-C09-N10	-4.41	121.78	128.68
2	C	501	KYE	O01-C02-C17	-4.37	98.42	111.05
2	C	501	KYE	N08-C09-N10	-4.06	122.33	128.68
2	B	501	KYE	O16-C05-C03	-4.03	101.03	106.93
2	B	501	KYE	N08-C09-N10	-3.96	122.48	128.68
2	D	501	KYE	O16-C17-C18	3.92	115.37	108.90
2	D	501	KYE	C27-N19-C20	-3.34	103.51	111.44
2	A	501	KYE	C07-C13-N14	-2.81	106.47	109.40
2	A	501	KYE	O16-C05-C03	-2.64	103.07	106.93
2	D	501	KYE	O16-C05-C03	-2.46	103.33	106.93
2	B	501	KYE	C27-N19-C20	-2.37	105.81	111.44
2	B	501	KYE	N32-C33-N35	2.33	124.80	120.70
2	B	501	KYE	C07-C13-N14	-2.29	107.02	109.40
2	C	501	KYE	C03-C02-C17	2.27	107.05	102.64
2	A	501	KYE	O01-C02-C17	-2.26	104.51	111.05
2	B	501	KYE	O01-C02-C17	-2.20	104.70	111.05
2	B	501	KYE	O16-C17-C18	2.19	112.51	108.90
2	A	501	KYE	C02-C03-C05	2.15	104.22	100.98
2	C	501	KYE	C07-C13-N14	-2.13	107.17	109.40
2	C	501	KYE	N34-C33-N32	2.12	124.08	119.19
2	D	501	KYE	O01-C02-C17	-2.09	105.00	111.05
2	C	501	KYE	C28-C27-N19	2.08	119.09	113.84
2	B	501	KYE	C03-C02-C17	2.06	106.64	102.64
2	C	501	KYE	O01-C02-C03	2.03	118.40	111.82

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	KYE	C02-C17-C18-N19
2	D	501	KYE	O16-C17-C18-N19
2	A	501	KYE	C02-C17-C18-N19
2	A	501	KYE	O16-C17-C18-N19

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Mol	Chain	Res	Type	Atoms
2	A	501	KYE	N19-C20-C21-C22
2	C	501	KYE	O16-C17-C18-N19
2	C	501	KYE	N19-C20-C21-C22
2	B	501	KYE	C02-C17-C18-N19
2	B	501	KYE	O16-C17-C18-N19
2	B	501	KYE	N19-C20-C21-C22
2	B	501	KYE	C20-C21-C22-C23
2	B	501	KYE	C20-C21-C22-N26
2	B	501	KYE	C28-C27-N19-C18
3	B	502	GOL	C1-C2-C3-O3
3	D	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O1-C1-C2-C3
2	C	501	KYE	C29-C30-C31-N32
2	D	501	KYE	C17-C18-N19-C20
2	A	501	KYE	N19-C27-C28-C29
3	A	502	GOL	O1-C1-C2-O2
2	C	501	KYE	C28-C29-C30-C31
2	B	501	KYE	C28-C29-C30-C31
3	B	502	GOL	O2-C2-C3-O3
3	D	502	GOL	O1-C1-C2-O2
2	B	501	KYE	C27-C28-C29-C30
2	B	501	KYE	C29-C30-C31-N32
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-O2
2	D	501	KYE	C28-C29-C30-C31
2	C	501	KYE	C27-C28-C29-C30
3	C	502	GOL	O2-C2-C3-O3
2	B	501	KYE	C30-C31-N32-C33
2	B	501	KYE	C17-C18-N19-C20
2	C	501	KYE	C02-C17-C18-N19
2	D	501	KYE	N19-C27-C28-C29
2	D	501	KYE	C30-C31-N32-C33
2	A	501	KYE	C27-C28-C29-C30
2	A	501	KYE	C28-C27-N19-C20

There are no ring outliers.

6 monomers are involved in 10 short contacts:

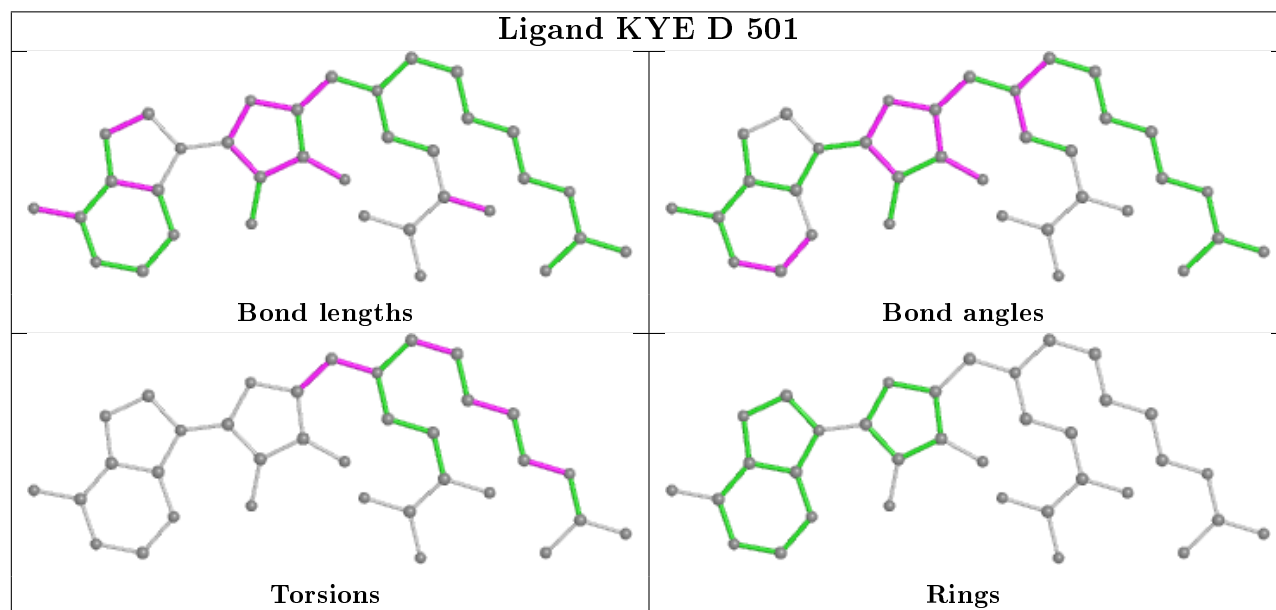
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	KYE	1	0
2	A	501	KYE	2	0
3	A	503	GOL	3	0

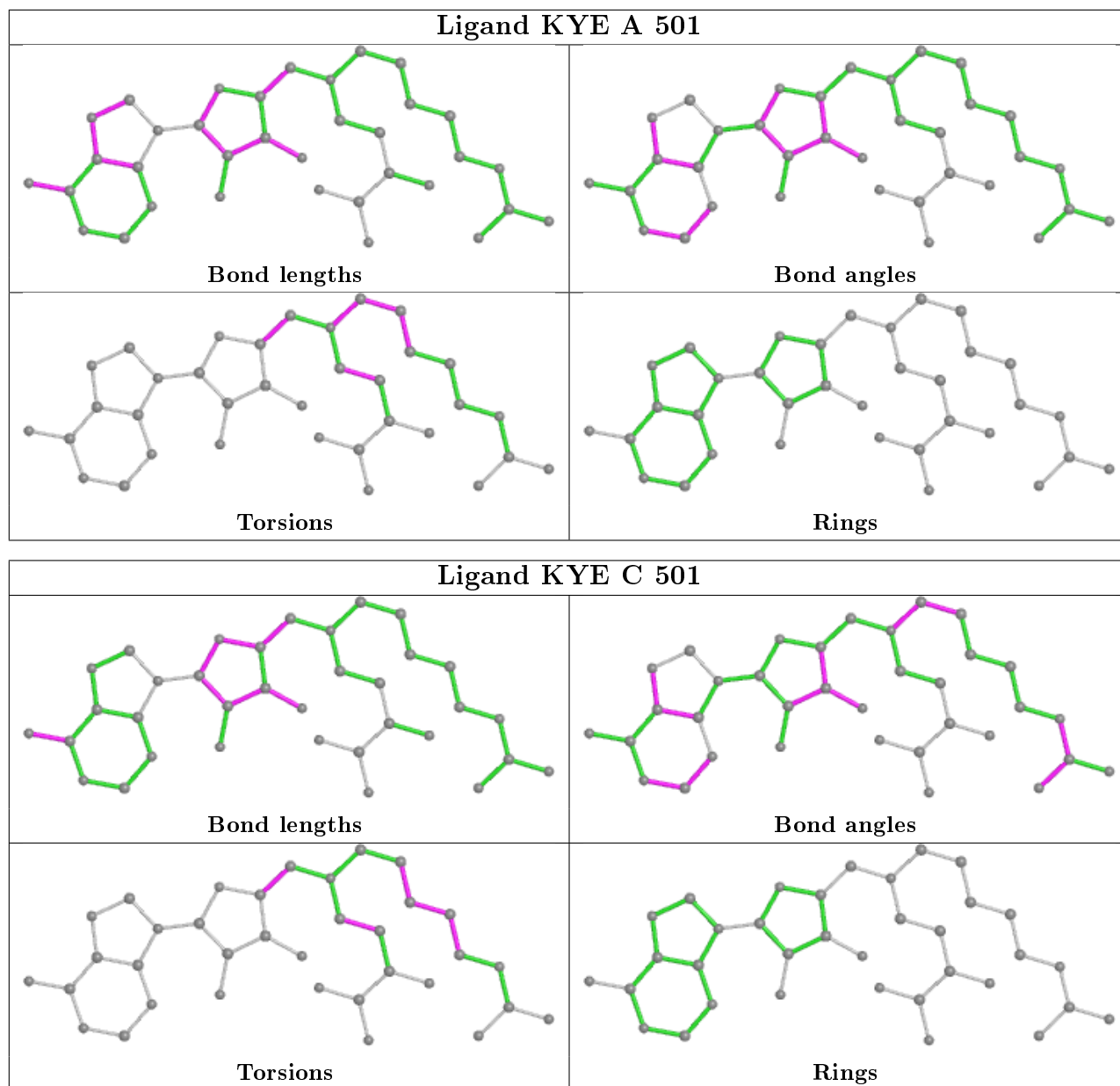
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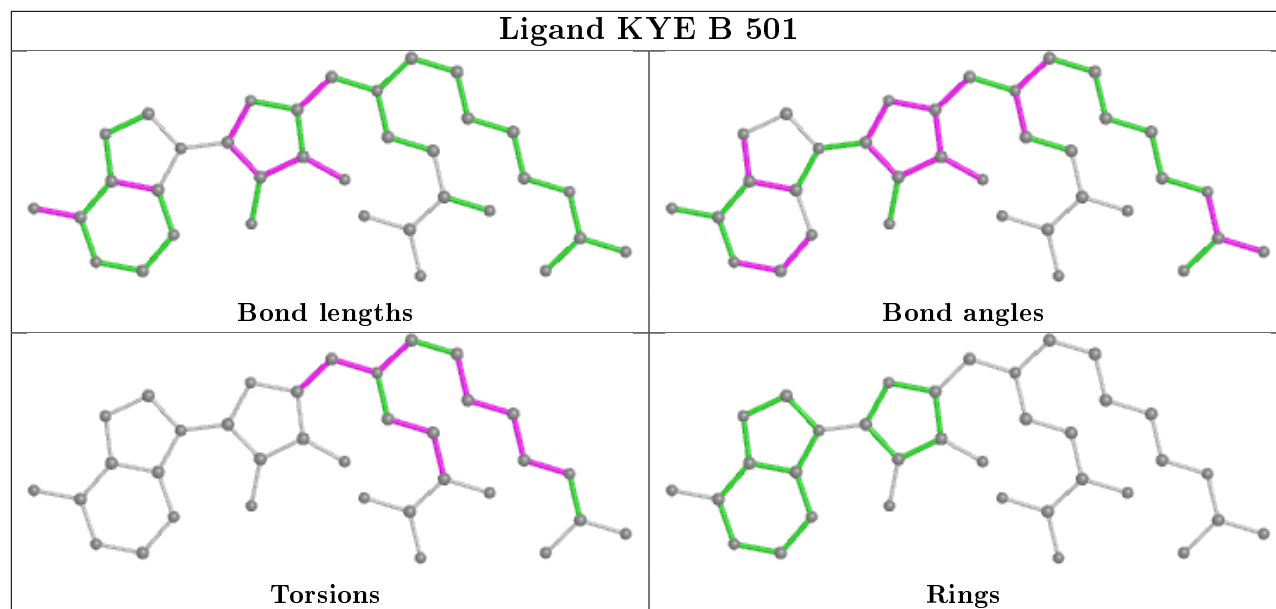
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	KYE	2	0
3	B	503	GOL	1	0
3	D	502	GOL	1	0

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.







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%)	-0.38	1 (0%) 94 94	32, 46, 64, 108	0
1	B	342/351 (97%)	-0.42	1 (0%) 94 94	24, 35, 54, 73	0
1	C	342/351 (97%)	-0.32	4 (1%) 79 80	32, 46, 67, 97	0
1	D	342/351 (97%)	-0.38	0 100 100	25, 40, 61, 80	0
All	All	1368/1404 (97%)	-0.38	6 (0%) 92 93	24, 42, 64, 108	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	TYR	5.9
1	C	135	SER	3.0
1	C	314	TYR	2.9
1	B	476	TYR	2.7
1	C	476	TYR	2.2
1	C	139	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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,

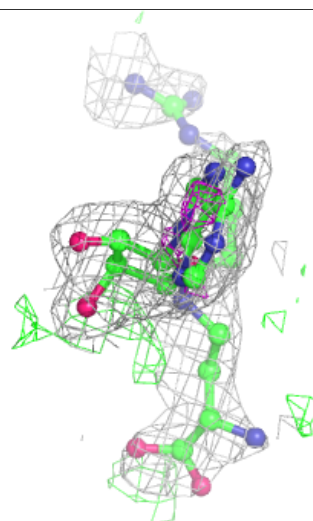
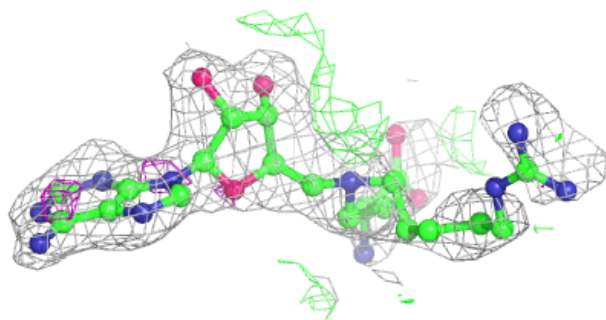
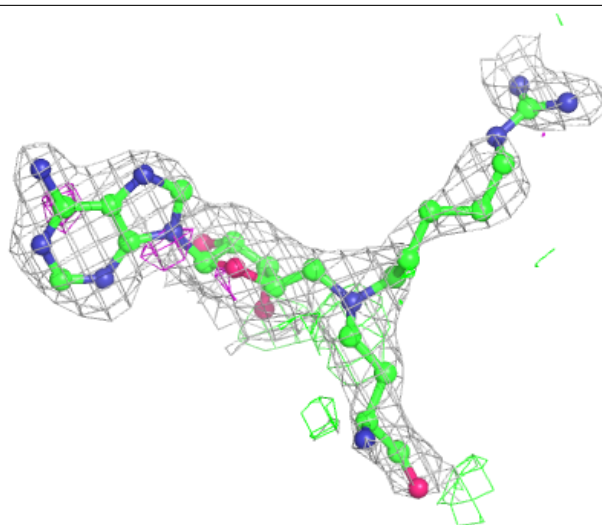
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	D	502	6/6	0.71	0.18	64,66,67,70	0
3	GOL	C	502	6/6	0.79	0.17	77,79,80,80	0
3	GOL	A	503	6/6	0.80	0.29	60,64,66,71	0
3	GOL	B	502	6/6	0.85	0.11	60,63,65,66	0
2	KYE	A	501	35/35	0.86	0.17	45,58,87,92	0
3	GOL	A	502	6/6	0.87	0.12	72,80,82,86	0
3	GOL	D	503	6/6	0.88	0.11	67,68,72,79	0
2	KYE	B	501	35/35	0.88	0.17	42,52,82,86	0
2	KYE	D	501	35/35	0.91	0.11	30,39,59,62	0
3	GOL	B	503	6/6	0.91	0.17	70,72,77,77	0
2	KYE	C	501	35/35	0.94	0.11	38,44,79,83	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.

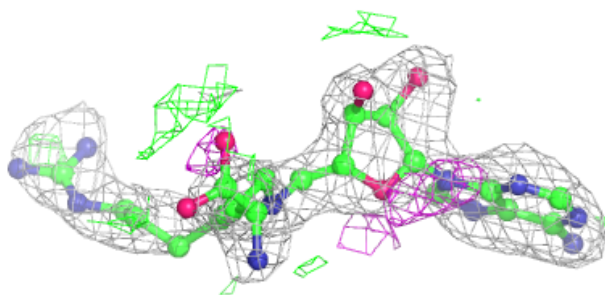
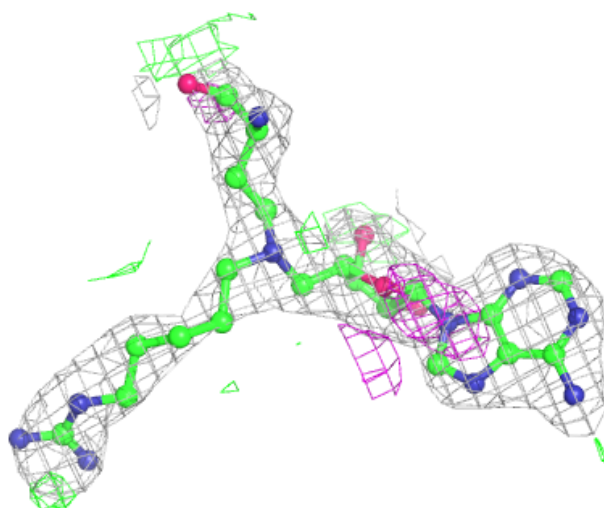
Electron density around KYE A 501:

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



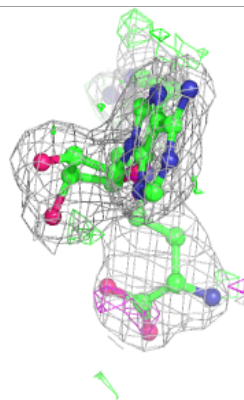
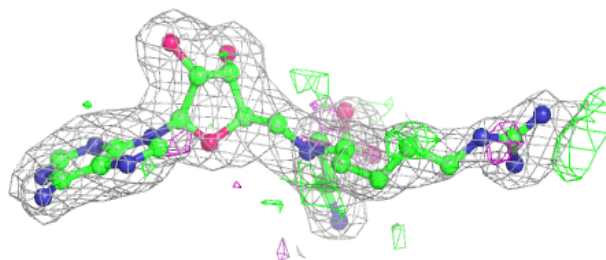
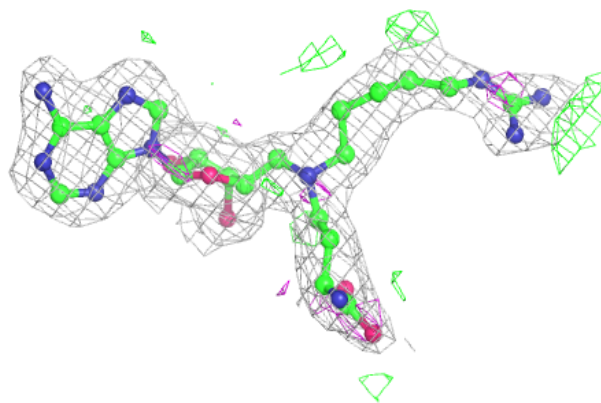
Electron density around KYE B 501:

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

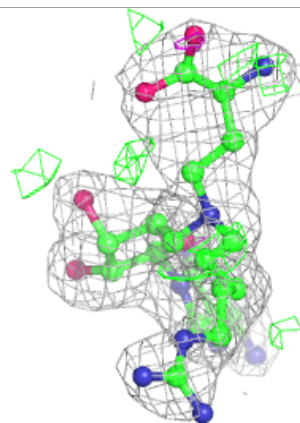
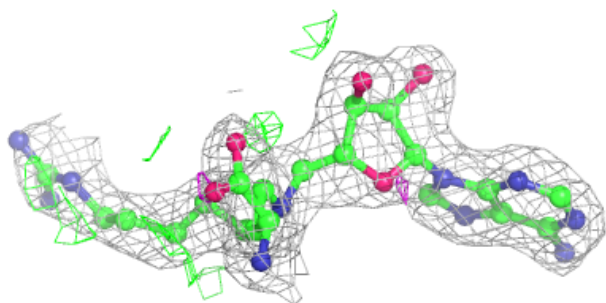
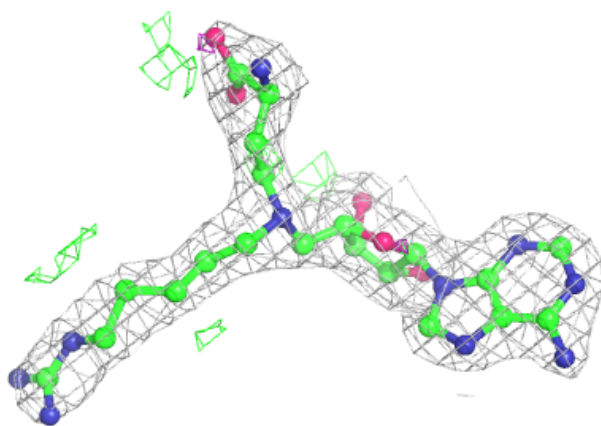


Electron density around KYE D 501:

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

**Electron density around KYE 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

There are no such residues in this entry.