Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 08:09 am BST

PDB ID	:	6S7A
Title	:	Crystal structure of CARM1 in complex with inhibitor AA175
Authors	:	Gunnell, E.A.; Al-Noori, A.; Dowden, J.; Dreveny, I.
Deposited on	:	2019-07-04
Resolution	:	1.86 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:

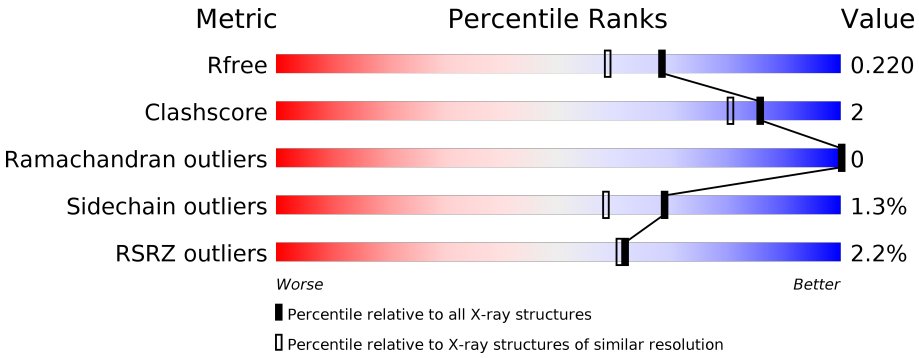
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 <=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	2% 91% 6%
1	B	351	% 89% 8%
1	C	351	3% 93%
1	D	351	2% 91% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11870 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
1	A	342	Total	C	N	O	S	0	0	0
			2744	1772	453	505	14			
1	B	342	Total	C	N	O	S	0	3	0
			2770	1790	456	509	15			
1	C	342	Total	C	N	O	S	0	1	0
			2750	1775	454	506	15			
1	D	342	Total	C	N	O	S	0	1	0
			2750	1775	454	506	15			

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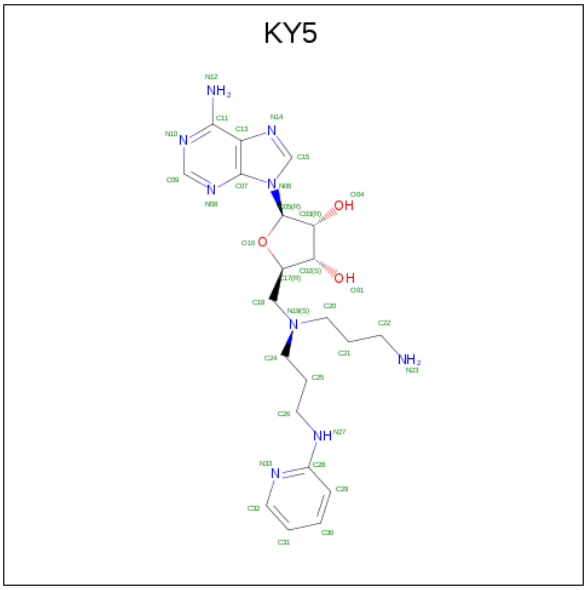
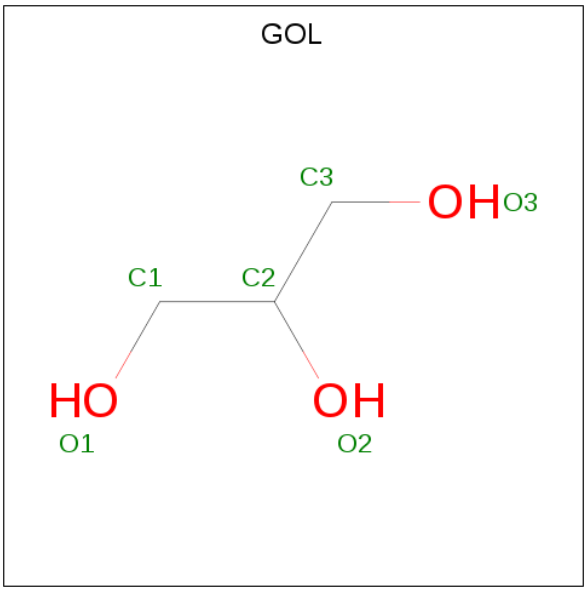
Chain	Residue	Modelled	Actual	Comment	Reference
D	483	HIS	-	expression tag	UNP Q86X55
D	484	HIS	-	expression tag	UNP Q86X55
D	485	HIS	-	expression tag	UNP Q86X55

- Molecule 2 is (2 {R},3 {R},4 {S},5 {R})-2-(6-aminopurin-9-yl)-5-[[3-azanylpropyl-[3-(pyridin-2-ylamino)propyl]amino]methyl]oxolane-3,4-diol (three-letter code: KY5) (formula: $C_{21}H_{31}N_9O_3$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	21	9	3		
2	B	1	Total	C	N	O	0	0
			33	21	9	3		
2	C	1	Total	C	N	O	0	0
			33	21	9	3		
2	D	1	Total	C	N	O	0	0
			33	21	9	3		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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.

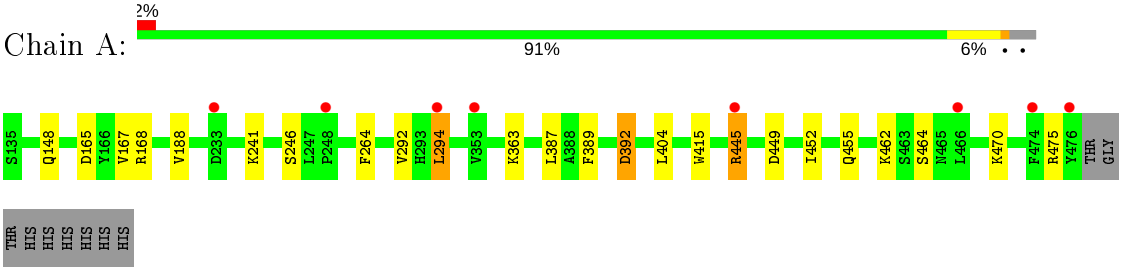
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	119	Total O 119 119	0	0
4	B	261	Total O 261 261	0	0
4	C	101	Total O 101 101	0	0
4	D	207	Total O 207 207	0	0

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.

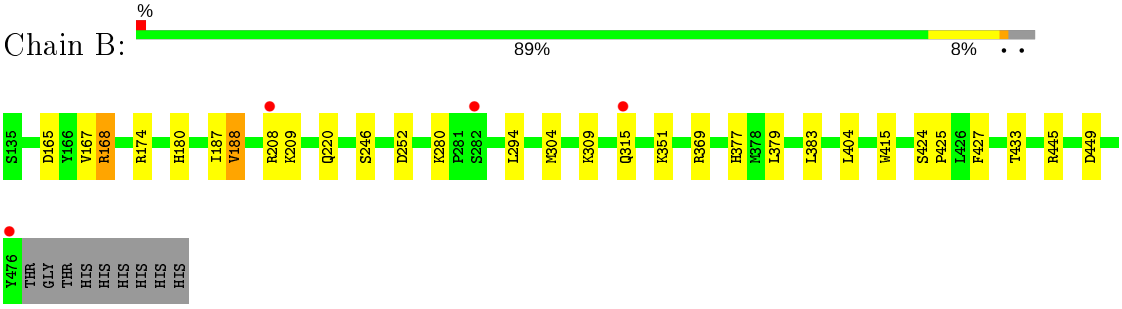
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain A:



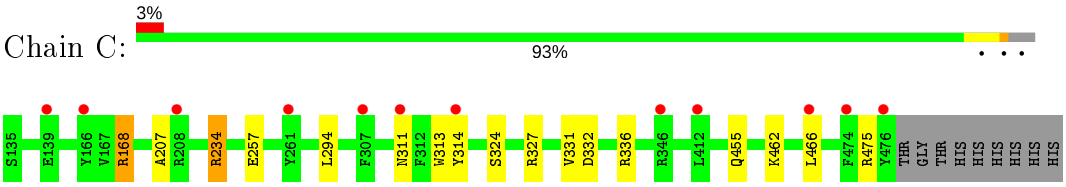
- Molecule 1: Histone-arginine methyltransferase CARM1

Chain B:



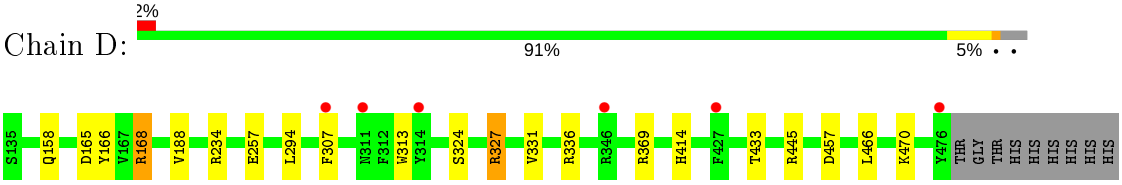
- Molecule 1: Histone-arginine methyltransferase CARM1

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	74.78Å 98.62Å 207.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.42 – 1.86 207.14 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (71.42-1.86) 100.0 (207.14-1.86)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.199 , 0.220 0.200 , 0.220	Depositor DCC
R_{free} test set	6448 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11870	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 43.50 % 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 1.7471e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, KY5

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	0.73	0/2814	0.86	7/3813 (0.2%)
1	B	0.84	0/2841	0.87	10/3849 (0.3%)
1	C	0.72	0/2820	0.86	4/3821 (0.1%)
1	D	0.81	2/2820 (0.1%)	0.95	8/3821 (0.2%)
All	All	0.78	2/11295 (0.0%)	0.89	29/15304 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	ARG	CZ-NH1	-5.84	1.25	1.33
1	D	166	TYR	CG-CD1	5.12	1.45	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	168	ARG	NE-CZ-NH1	-17.73	111.43	120.30
1	C	234	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	D	168	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	A	294	LEU	CA-CB-CG	8.49	134.83	115.30
1	D	234	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	392	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	B	449	ASP	CB-CG-OD1	6.63	124.26	118.30
1	D	188	VAL	CG1-CB-CG2	6.56	121.40	110.90
1	A	449	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	165	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	445	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	D	168	ARG	CB-CG-CD	-6.18	95.53	111.60
1	A	475	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	168	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	168	ARG	CB-CG-CD	-5.81	96.49	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	174	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	165	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	309	LYS	CD-CE-NZ	-5.58	98.87	111.70
1	B	445	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	392	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	445	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	445	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	D	369	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	188	VAL	CG1-CB-CG2	5.35	119.46	110.90
1	B	369	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	475	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	304[A]	MET	CB-CG-SD	5.04	127.54	112.40
1	B	304[B]	MET	CB-CG-SD	5.04	127.54	112.40
1	D	165	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 (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	2744	0	2692	17	0
1	B	2770	0	2714	13	0
1	C	2750	0	2696	12	0
1	D	2750	0	2696	11	0
2	A	33	0	0	1	0
2	B	33	0	0	0	0
2	C	33	0	0	0	0
2	D	33	0	0	1	0
3	A	6	0	8	0	0
3	B	12	0	16	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
4	A	119	0	0	1	0
4	B	261	0	0	3	1
4	C	101	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	207	0	0	1	1
All	All	11870	0	10846	49	1

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 (49) 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:C:207:ALA:O	1:C:234:ARG:NH2	1.90	1.04
1:C:314:TYR:OH	1:D:327:ARG:NH1	2.08	0.85
1:C:327:ARG:CZ	1:C:331:VAL:HG21	2.11	0.80
1:A:445:ARG:HH12	1:A:470:LYS:HB3	1.47	0.79
1:B:315:GLN:NE2	4:B:601:HOH:O	2.20	0.75
1:B:383:LEU:HG	1:B:427[B]:PHE:CE1	2.29	0.68
1:A:294:LEU:HD23	1:A:387:LEU:HD13	1.77	0.65
1:B:220:GLN:HG3	4:B:726:HOH:O	2.03	0.58
1:B:383:LEU:HD22	1:B:425:PRO:HB2	1.84	0.58
1:A:294:LEU:HG	1:A:389:PHE:CE2	2.39	0.58
1:B:180:HIS:ND1	4:B:603:HOH:O	2.32	0.58
1:A:445:ARG:NH1	1:A:470:LYS:HB3	2.19	0.57
1:D:336:ARG:HG2	1:D:466:LEU:O	2.06	0.56
1:C:336:ARG:HG2	1:C:466:LEU:O	2.08	0.54
1:C:327:ARG:NH1	1:C:331:VAL:HG21	2.22	0.54
1:A:294:LEU:HD11	1:A:389:PHE:CE2	2.44	0.53
1:A:445:ARG:NH1	1:A:470:LYS:CB	2.75	0.50
1:A:167:VAL:HG12	1:A:404:LEU:CD1	2.43	0.49
1:D:433:THR:HG22	1:D:457:ASP:OD2	2.13	0.48
1:A:455:GLN:HB3	1:A:462:LYS:HG2	1.95	0.48
1:B:377:HIS:ND1	1:B:433[B]:THR:HG22	2.30	0.47
1:A:294:LEU:CD1	1:A:389:PHE:CE2	2.98	0.47
1:C:314:TYR:OH	1:D:327:ARG:CZ	2.64	0.46
1:A:167:VAL:HG12	1:A:404:LEU:HD11	1.98	0.45
1:C:313:TRP:O	1:C:324:SER:HA	2.17	0.45
1:C:455:GLN:HB3	1:C:462:LYS:HG2	1.98	0.45
1:D:168:ARG:NH1	2:D:501:KY5:N33	2.64	0.44
1:D:313:TRP:O	1:D:324:SER:HA	2.18	0.44
1:D:168:ARG:NE	1:D:257:GLU:OE1	2.46	0.44
1:A:452:ILE:O	1:A:464:SER:HA	2.17	0.44
1:B:252:ASP:OD1	1:B:280:LYS:HE3	2.18	0.43
1:C:168:ARG:NE	1:C:257:GLU:OE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:THR:CG2	1:D:457:ASP:OD2	2.67	0.43
1:A:168:ARG:HD2	1:A:415:TRP:CZ3	2.54	0.43
1:A:294:LEU:CG	1:A:389:PHE:CE2	3.02	0.42
1:A:363:LYS:HA	1:A:363:LYS:HD2	1.94	0.42
1:B:167:VAL:HG12	1:B:404:LEU:CD1	2.49	0.42
1:B:187:ILE:HD11	1:B:208:ARG:NH1	2.35	0.42
1:C:311:ASN:ND2	1:D:307:PHE:CE2	2.87	0.42
1:B:168:ARG:HD2	1:B:415:TRP:CZ3	2.55	0.41
1:C:332:ASP:HB3	1:C:336:ARG:NH1	2.36	0.41
1:C:311:ASN:HD21	1:D:307:PHE:HE2	1.67	0.41
1:B:351:LYS:HE2	1:B:379:LEU:HD11	2.03	0.41
1:D:158:GLN:OE1	4:D:601:HOH:O	2.22	0.41
1:B:167:VAL:HG12	1:B:404:LEU:HD11	2.03	0.41
1:B:252:ASP:OD1	1:B:280:LYS:CE	2.69	0.41
1:A:241:LYS:HA	2:A:501:KY5:N10	2.36	0.41
1:A:264:PHE:CE2	1:A:292:VAL:HG21	2.57	0.40
1:A:392:ASP:OD2	4:A:601:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:767:HOH:O	4:D:760:HOH:O[4_555]	2.17	0.03

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	340/351 (97%)	332 (98%)	8 (2%)	0	100	100
1	B	343/351 (98%)	334 (97%)	9 (3%)	0	100	100
1	C	341/351 (97%)	332 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	341/351 (97%)	331 (97%)	10 (3%)	0	100	100
All	All	1365/1404 (97%)	1329 (97%)	36 (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	298/306 (97%)	295 (99%)	3 (1%)	76	69
1	B	301/306 (98%)	295 (98%)	6 (2%)	55	40
1	C	299/306 (98%)	298 (100%)	1 (0%)	92	91
1	D	299/306 (98%)	294 (98%)	5 (2%)	60	47
All	All	1197/1224 (98%)	1182 (99%)	15 (1%)	69	58

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	188	VAL
1	A	246	SER
1	B	168	ARG
1	B	188	VAL
1	B	209	LYS
1	B	246	SER
1	B	294	LEU
1	B	424	SER
1	C	294	LEU
1	D	294	LEU
1	D	327	ARG
1	D	331	VAL
1	D	414	HIS
1	D	470	LYS

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

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

10 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	B	502	-	5,5,5	0.24	0	5,5,5	0.28	0
3	GOL	D	502	-	5,5,5	0.30	0	5,5,5	0.30	0
2	KY5	D	501	-	33,36,36	3.92	17 (51%)	35,49,49	2.16	8 (22%)
2	KY5	A	501	-	33,36,36	4.52	21 (63%)	35,49,49	1.82	10 (28%)
2	KY5	C	501	-	33,36,36	4.30	19 (57%)	35,49,49	1.68	6 (17%)
2	KY5	B	501	-	33,36,36	4.05	17 (51%)	35,49,49	1.70	4 (11%)
3	GOL	A	502	-	5,5,5	0.10	0	5,5,5	0.56	0
3	GOL	C	502	-	5,5,5	0.23	0	5,5,5	0.42	0
3	GOL	B	503	-	5,5,5	0.33	0	5,5,5	0.36	0
3	GOL	D	503	-	5,5,5	0.16	0	5,5,5	0.52	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	B	502	-	-	1/4/4/4	-
3	GOL	D	502	-	-	4/4/4/4	-
2	KY5	D	501	-	-	2/15/35/35	0/4/4/4
2	KY5	A	501	-	-	8/15/35/35	0/4/4/4
2	KY5	C	501	-	-	6/15/35/35	0/4/4/4
2	KY5	B	501	-	-	0/15/35/35	0/4/4/4
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	B	503	-	-	4/4/4/4	-
3	GOL	D	503	-	-	0/4/4/4	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	KY5	O16-C05	-12.16	1.24	1.41
2	A	501	KY5	C02-C17	-11.11	1.24	1.53
2	C	501	KY5	O16-C05	-10.91	1.25	1.41
2	C	501	KY5	C02-C17	-10.62	1.25	1.53
2	B	501	KY5	O16-C05	-10.13	1.26	1.41
2	B	501	KY5	C02-C17	-9.68	1.28	1.53
2	D	501	KY5	C02-C17	-9.51	1.28	1.53
2	A	501	KY5	C28-N33	9.31	1.52	1.34
2	D	501	KY5	O16-C05	-9.28	1.28	1.41
2	D	501	KY5	C28-N33	8.96	1.51	1.34
2	B	501	KY5	C28-N33	8.40	1.50	1.34
2	C	501	KY5	C28-N33	8.11	1.49	1.34
2	D	501	KY5	C32-N33	6.90	1.49	1.34
2	B	501	KY5	C29-C28	6.52	1.54	1.39
2	C	501	KY5	C32-N33	6.43	1.48	1.34
2	C	501	KY5	C28-N27	-6.29	1.27	1.36
2	B	501	KY5	C32-N33	6.24	1.47	1.34
2	A	501	KY5	C32-N33	6.16	1.47	1.34
2	C	501	KY5	C29-C28	6.12	1.53	1.39
2	A	501	KY5	C29-C28	5.56	1.52	1.39
2	A	501	KY5	C30-C29	5.35	1.50	1.38
2	A	501	KY5	C28-N27	-5.27	1.28	1.36
2	B	501	KY5	C28-N27	-5.20	1.28	1.36
2	B	501	KY5	C30-C29	5.20	1.49	1.38
2	C	501	KY5	C30-C29	5.18	1.49	1.38
2	A	501	KY5	C31-C32	5.08	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	KY5	C31-C32	4.99	1.52	1.37
2	A	501	KY5	O04-C03	-4.96	1.31	1.43
2	D	501	KY5	C18-N19	4.92	1.56	1.47
2	C	501	KY5	O04-C03	-4.79	1.31	1.43
2	C	501	KY5	C31-C32	4.79	1.51	1.37
2	B	501	KY5	C31-C30	4.75	1.50	1.38
2	C	501	KY5	C31-C30	4.58	1.50	1.38
2	A	501	KY5	C31-C30	4.57	1.50	1.38
2	D	501	KY5	C31-C32	4.47	1.50	1.37
2	D	501	KY5	C30-C29	4.18	1.47	1.38
2	D	501	KY5	O16-C17	4.17	1.54	1.45
2	C	501	KY5	C03-C05	-4.07	1.47	1.53
2	C	501	KY5	C18-N19	4.07	1.54	1.47
2	D	501	KY5	C31-C30	4.01	1.48	1.38
2	D	501	KY5	C28-N27	-3.98	1.30	1.36
2	B	501	KY5	O04-C03	-3.94	1.33	1.43
2	A	501	KY5	C03-C02	-3.91	1.42	1.53
2	D	501	KY5	C29-C28	3.91	1.48	1.39
2	D	501	KY5	O04-C03	-3.90	1.33	1.43
2	A	501	KY5	C03-C05	-3.85	1.47	1.53
2	A	501	KY5	C11-N12	3.66	1.47	1.34
2	A	501	KY5	O01-C02	3.62	1.51	1.43
2	C	501	KY5	C03-C02	-3.46	1.43	1.53
2	D	501	KY5	C11-N12	3.33	1.46	1.34
2	B	501	KY5	C18-N19	3.32	1.53	1.47
2	C	501	KY5	C11-N12	3.26	1.45	1.34
2	D	501	KY5	C03-C05	-3.21	1.48	1.53
2	B	501	KY5	C03-C05	-3.17	1.49	1.53
2	B	501	KY5	C11-N12	3.14	1.45	1.34
2	A	501	KY5	O16-C17	3.10	1.51	1.45
2	A	501	KY5	C18-N19	3.03	1.52	1.47
2	C	501	KY5	O16-C17	2.96	1.51	1.45
2	B	501	KY5	C03-C02	-2.93	1.45	1.53
2	C	501	KY5	O01-C02	2.77	1.49	1.43
2	A	501	KY5	C07-N08	2.71	1.39	1.35
2	B	501	KY5	C24-N19	2.70	1.53	1.47
2	A	501	KY5	C20-N19	2.69	1.53	1.47
2	A	501	KY5	C18-C17	-2.59	1.43	1.51
2	D	501	KY5	C03-C02	-2.57	1.46	1.53
2	A	501	KY5	C24-N19	2.33	1.52	1.47
2	B	501	KY5	O01-C02	2.27	1.48	1.43
2	C	501	KY5	C07-N08	2.25	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	KY5	C18-C17	-2.22	1.44	1.51
2	D	501	KY5	C09-N08	2.15	1.35	1.32
2	D	501	KY5	C20-N19	2.13	1.52	1.47
2	A	501	KY5	C26-N27	2.12	1.50	1.45
2	B	501	KY5	C18-C17	-2.09	1.45	1.51
2	C	501	KY5	C24-N19	2.09	1.52	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	KY5	N27-C28-N33	6.27	126.41	116.95
2	D	501	KY5	N08-C09-N10	-5.30	120.40	128.68
2	A	501	KY5	N08-C09-N10	-4.80	121.18	128.68
2	D	501	KY5	C29-C28-N33	-4.54	115.47	122.57
2	B	501	KY5	N08-C09-N10	-4.52	121.61	128.68
2	A	501	KY5	C25-C26-N27	-4.36	99.77	111.49
2	B	501	KY5	O16-C17-C18	-4.32	101.75	108.90
2	C	501	KY5	N08-C09-N10	-4.19	122.12	128.68
2	B	501	KY5	C03-C02-C17	4.07	110.56	102.64
2	D	501	KY5	C30-C29-C28	3.97	124.04	117.73
2	C	501	KY5	C25-C26-N27	-3.88	101.06	111.49
2	C	501	KY5	O16-C17-C18	-3.48	103.13	108.90
2	D	501	KY5	C32-N33-C28	3.23	121.81	117.22
2	D	501	KY5	C03-C02-C17	3.02	108.52	102.64
2	B	501	KY5	C25-C26-N27	-3.00	103.42	111.49
2	D	501	KY5	O16-C17-C18	-2.94	104.04	108.90
2	C	501	KY5	C03-C02-C17	2.87	108.21	102.64
2	A	501	KY5	N27-C28-N33	2.78	121.14	116.95
2	A	501	KY5	C21-C20-N19	2.67	120.57	113.84
2	A	501	KY5	C09-N10-C11	2.47	122.97	118.75
2	A	501	KY5	O16-C17-C18	-2.46	104.83	108.90
2	C	501	KY5	C25-C24-N19	-2.43	107.72	113.84
2	A	501	KY5	O16-C05-C03	-2.30	103.57	106.93
2	A	501	KY5	C31-C32-N33	-2.29	119.69	123.43
2	C	501	KY5	C29-C28-N27	2.11	125.59	121.04
2	D	501	KY5	C09-N10-C11	2.06	122.28	118.75
2	A	501	KY5	C32-N33-C28	2.05	120.13	117.22
2	A	501	KY5	N12-C11-N10	2.01	122.74	118.57

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	GOL	O1-C1-C2-C3
3	D	502	GOL	C1-C2-C3-O3
2	A	501	KY5	C02-C17-C18-N19
2	A	501	KY5	O16-C17-C18-N19
3	B	503	GOL	O1-C1-C2-C3
3	B	503	GOL	C1-C2-C3-O3
2	A	501	KY5	C21-C20-N19-C18
2	A	501	KY5	N19-C20-C21-C22
2	A	501	KY5	N19-C24-C25-C26
2	A	501	KY5	C17-C18-N19-C24
2	C	501	KY5	C24-C25-C26-N27
3	D	502	GOL	O1-C1-C2-O2
2	C	501	KY5	C25-C24-N19-C18
2	A	501	KY5	C24-C25-C26-N27
3	D	502	GOL	O2-C2-C3-O3
3	B	503	GOL	O2-C2-C3-O3
2	C	501	KY5	C25-C24-N19-C20
3	B	503	GOL	O1-C1-C2-O2
2	C	501	KY5	O16-C17-C18-N19
2	D	501	KY5	C17-C18-N19-C20
2	D	501	KY5	C25-C26-N27-C28
2	A	501	KY5	C20-C21-C22-N23
3	B	502	GOL	O2-C2-C3-O3
2	C	501	KY5	C02-C17-C18-N19
2	C	501	KY5	C25-C26-N27-C28

There are no ring outliers.

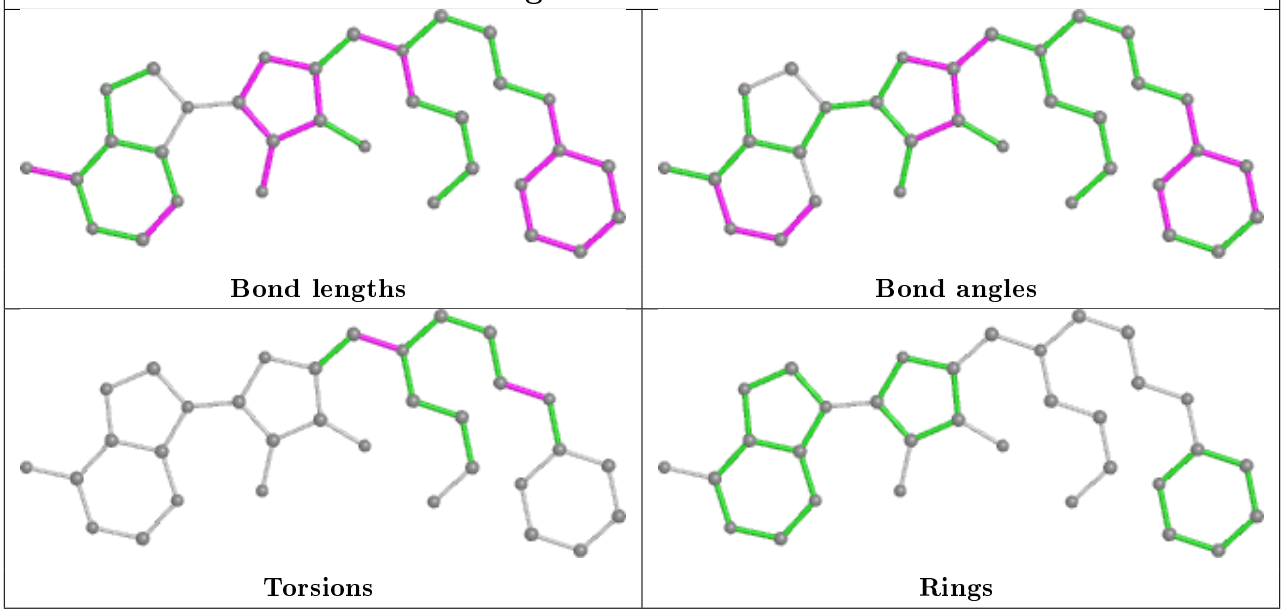
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	KY5	1	0
2	A	501	KY5	1	0

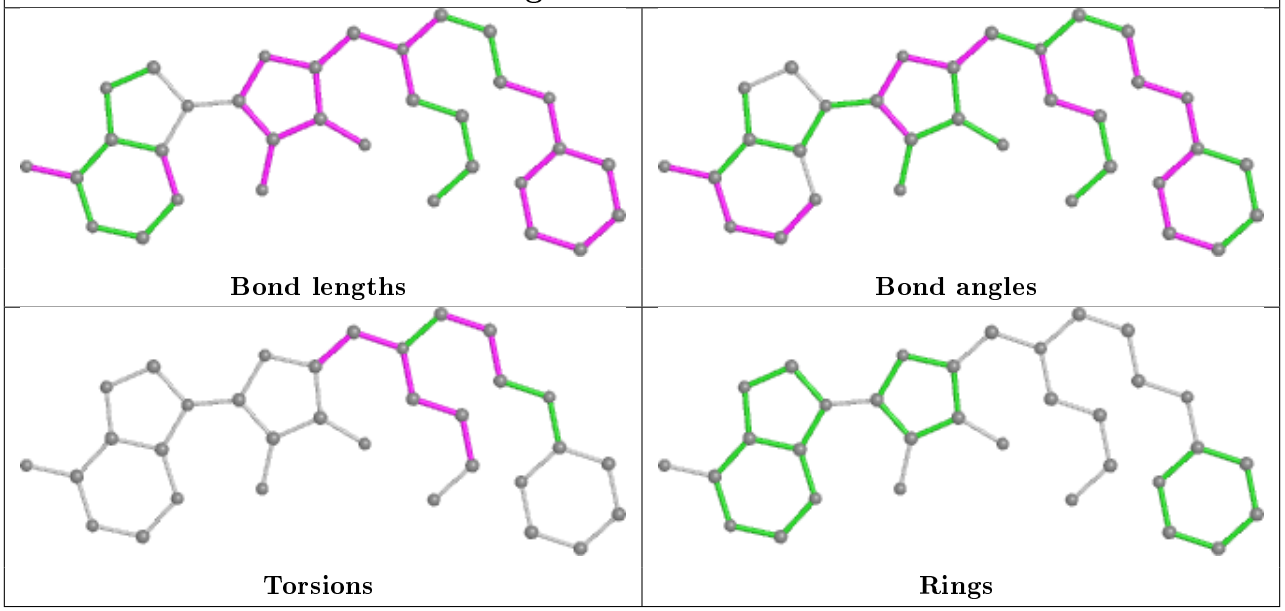
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

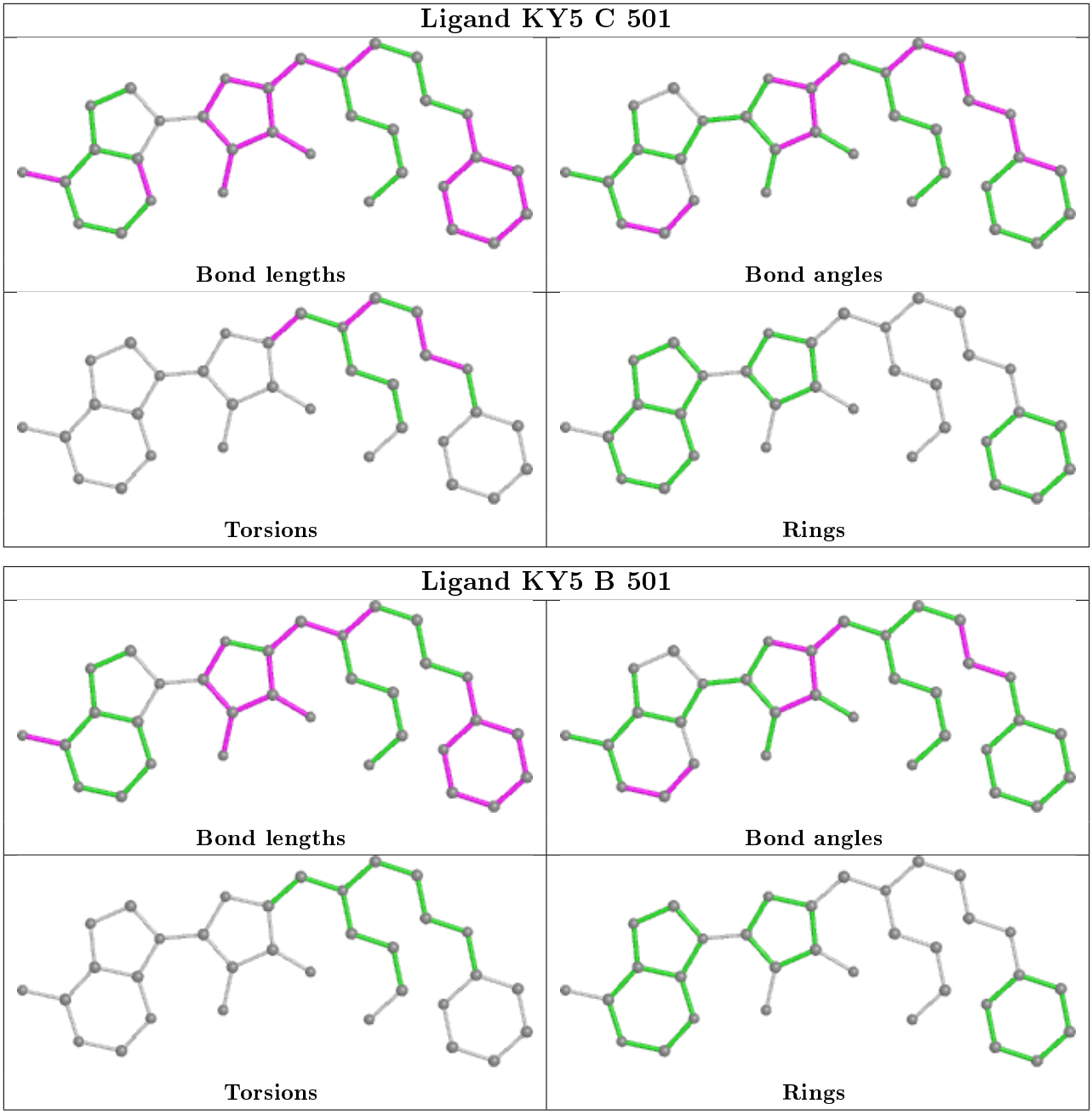
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand KY5 D 501



Ligand KY5 A 501





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.23	8 (2%) 60 59	34, 52, 73, 94	0
1	B	342/351 (97%)	-0.04	4 (1%) 79 79	20, 32, 47, 57	0
1	C	342/351 (97%)	0.19	12 (3%) 44 41	38, 51, 65, 85	0
1	D	342/351 (97%)	0.03	6 (1%) 68 68	22, 36, 54, 69	0
All	All	1368/1404 (97%)	0.10	30 (2%) 62 61	20, 45, 64, 94	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	TYR	6.0
1	A	476	TYR	4.0
1	C	476	TYR	4.0
1	B	476	TYR	3.5
1	C	166	TYR	3.1
1	A	294	LEU	3.0
1	C	412	LEU	2.8
1	C	346	ARG	2.7
1	C	314	TYR	2.7
1	C	474	PHE	2.7
1	D	311	ASN	2.7
1	C	208	ARG	2.6
1	C	466	LEU	2.6
1	B	282	SER	2.5
1	A	233	ASP	2.5
1	A	466	LEU	2.4
1	C	311	ASN	2.4
1	D	307	PHE	2.3
1	C	307	PHE	2.3
1	A	248	PRO	2.3
1	D	476	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	315	GLN	2.2
1	D	346	ARG	2.2
1	A	474	PHE	2.1
1	A	445	ARG	2.1
1	B	208	ARG	2.1
1	C	261	TYR	2.1
1	C	139	GLU	2.1
1	A	353	VAL	2.1
1	D	427	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)

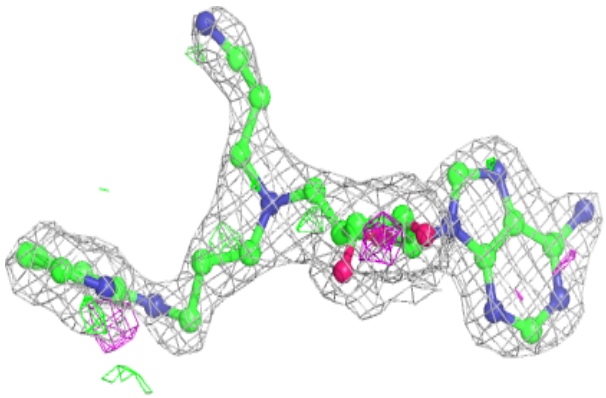
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

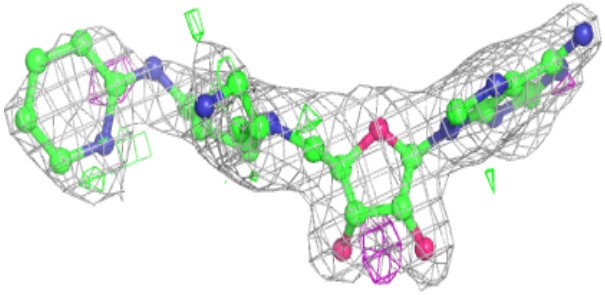
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	503	6/6	0.80	0.16	64,68,71,76	0
3	GOL	D	502	6/6	0.81	0.17	61,63,66,68	0
3	GOL	C	502	6/6	0.84	0.16	77,78,80,85	0
2	KY5	A	501	33/33	0.88	0.18	42,48,66,68	0
3	GOL	A	502	6/6	0.88	0.26	71,74,77,78	0
3	GOL	B	502	6/6	0.89	0.12	64,64,66,71	0
2	KY5	C	501	33/33	0.92	0.14	39,44,72,72	5
3	GOL	D	503	6/6	0.92	0.14	63,65,70,70	0
2	KY5	D	501	33/33	0.93	0.11	26,31,52,54	0
2	KY5	B	501	33/33	0.95	0.11	27,31,49,51	0

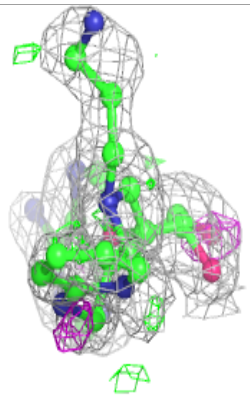
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KY5 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)

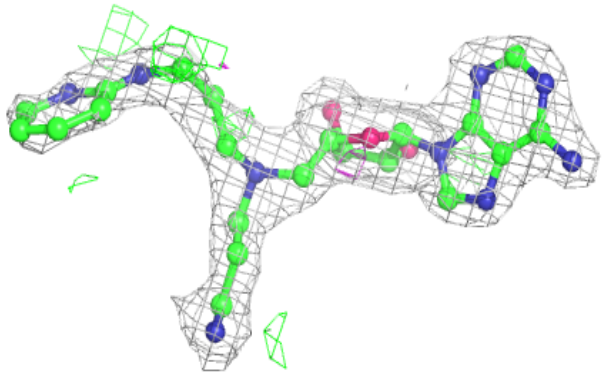


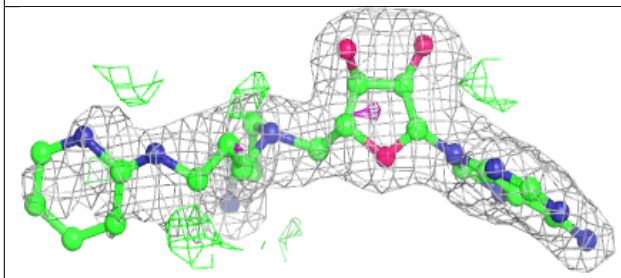


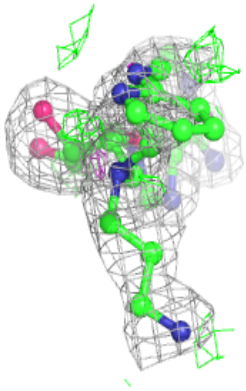


Electron density around KY5 C 501:

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

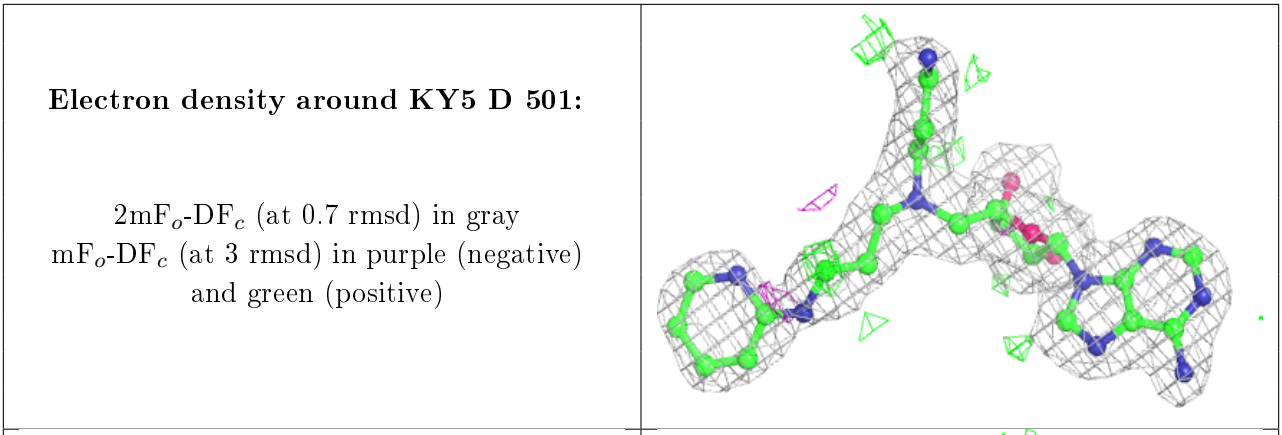


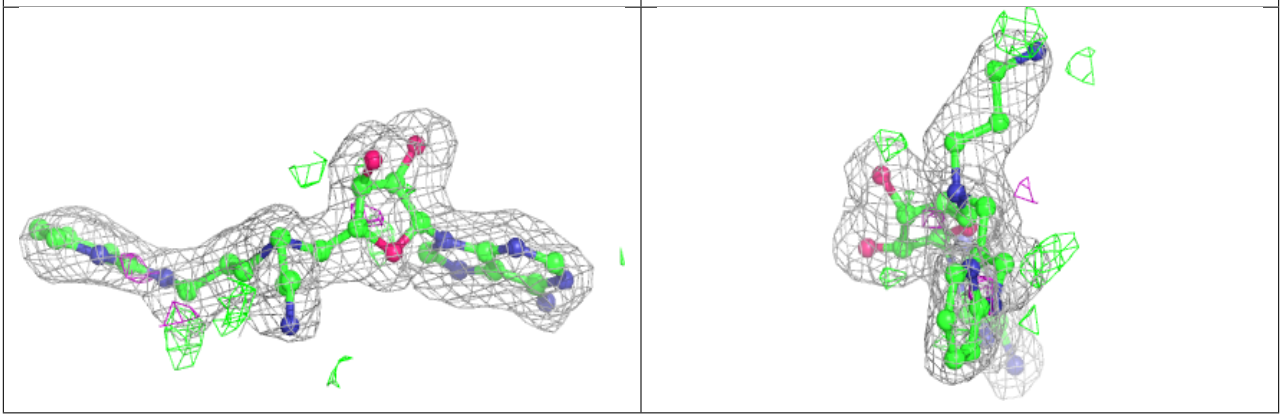




Electron density around KY5 D 501:

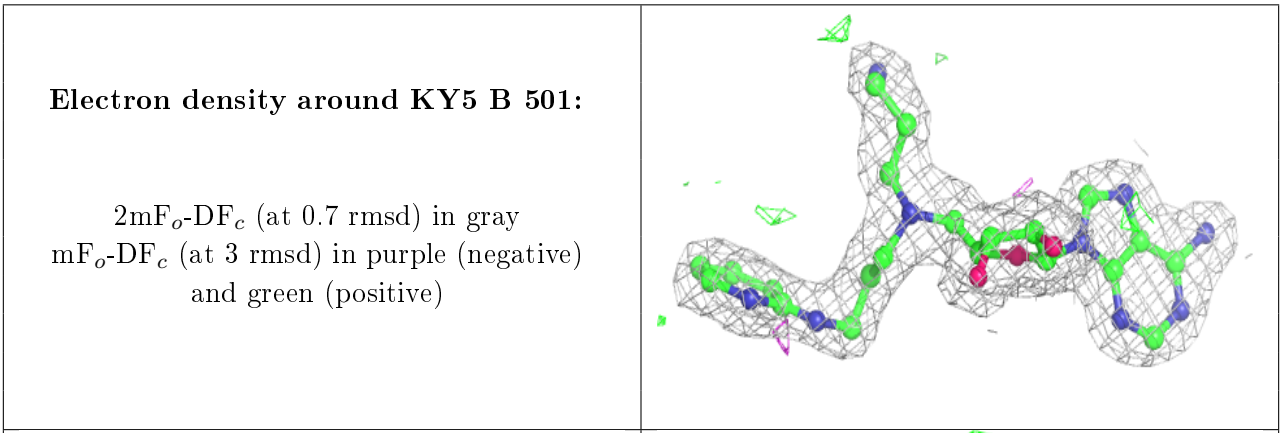
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

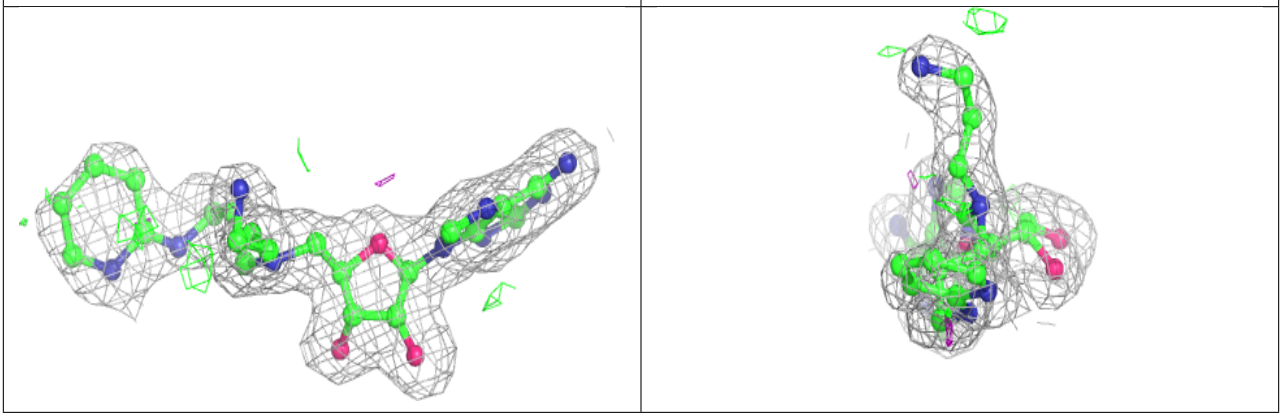




Electron density around KY5 B 501:

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





6.5 Other polymers (i)

There are no such residues in this entry.