



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:51 PM UTC

PDB ID : 6YU1 / pdb_00006yu1
Title : CLK3 bound with beta-carboline KH-CARB13 (Cpd 3)
Authors : Schroeder, M.; Chaikuad, A.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2020-04-25
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

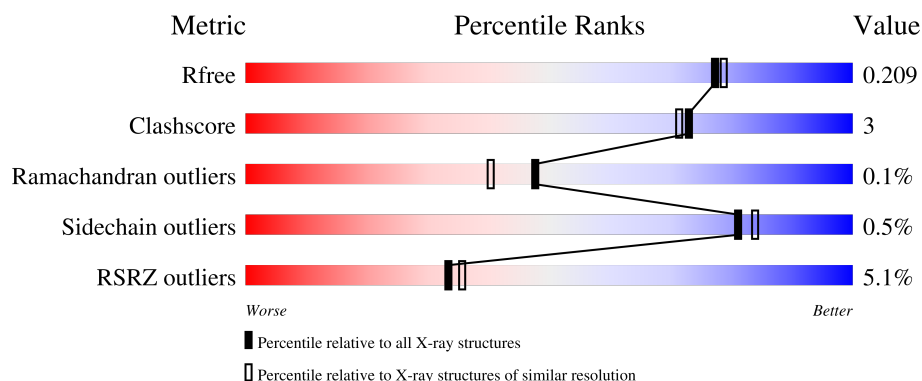
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

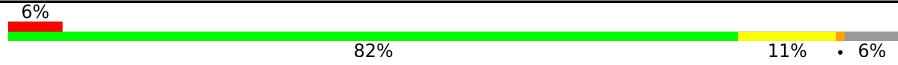
The reported resolution of this entry is 1.90 Å.

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	360	
1	c	360	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6334 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.

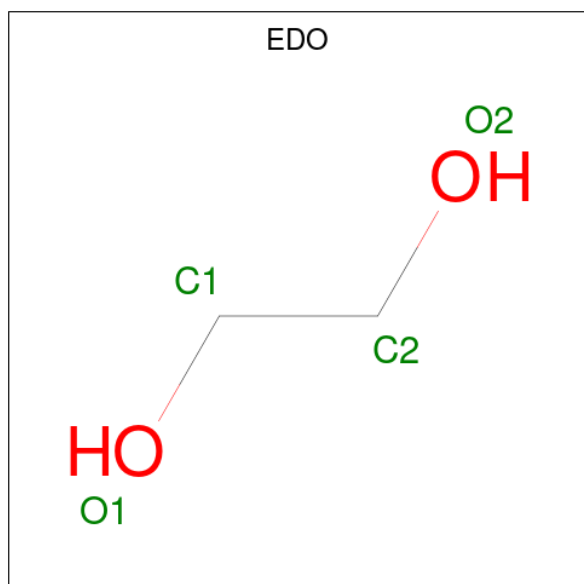
- Molecule 1 is a protein called Dual specificity protein kinase CLK3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	a	340	Total	C	N	O	S	0	3	0
			2787	1783	489	498	17			
1	c	350	Total	C	N	O	S	0	8	0
			2920	1859	520	522	19			

There are 4 discrepancies between the modelled and reference sequences:

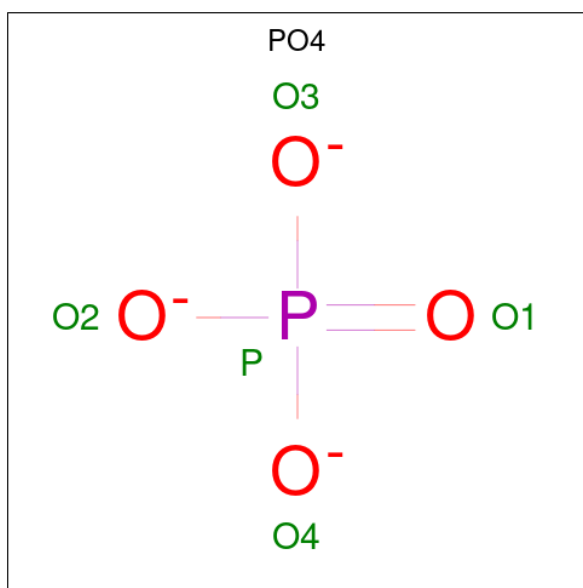
Chain	Residue	Modelled	Actual	Comment	Reference
a	125	SER	-	expression tag	UNP P49761
a	126	MET	-	expression tag	UNP P49761
c	125	SER	-	expression tag	UNP P49761
c	126	MET	-	expression tag	UNP P49761

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



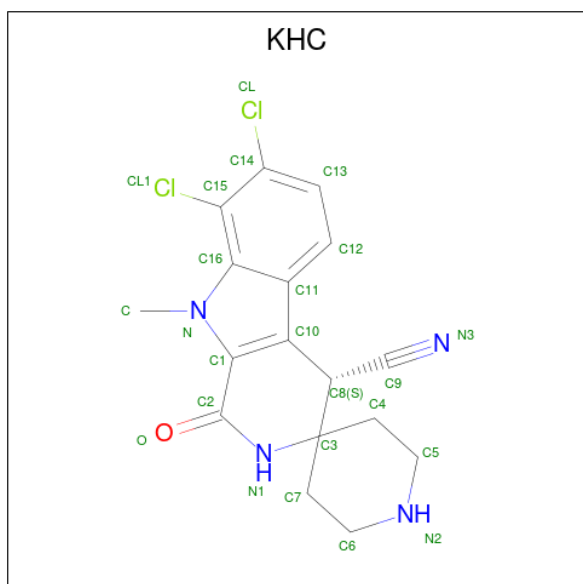
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	a	1	Total C O 4 2 2	0	0
2	a	1	Total C O 4 2 2	0	0
2	a	1	Total C O 4 2 2	0	0
2	a	1	Total C O 4 2 2	0	0
2	a	1	Total C O 4 2 2	0	0
2	a	1	Total C O 4 2 2	0	0
2	a	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0
2	c	1	Total C O 4 2 2	0	0

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



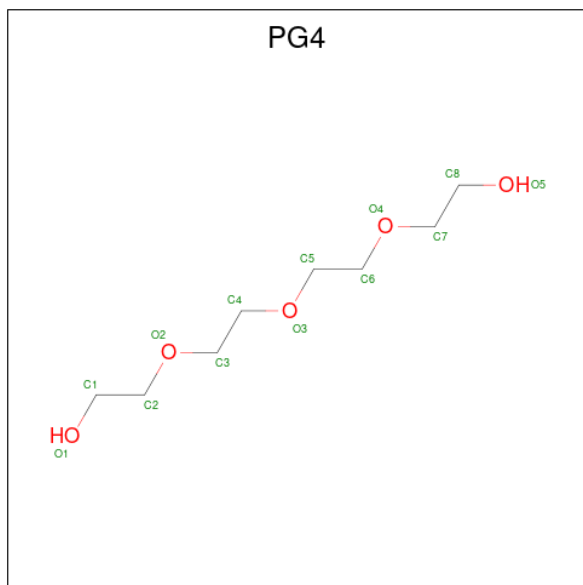
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	a	1	Total	O	P	0	0
			5	4	1		
3	a	1	Total	O	P	0	0
			5	4	1		
3	c	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is (4 {S})-7,8-bis(chloranyl)-9-methyl-1-oxidanylidene-spiro[2,4-dihydropyrido[3,4-b]indole-3,4'-piperidine]-4-carbonitrile (CCD ID: KHC) (formula: $C_{17}H_{16}Cl_2N_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	a	1	Total	C	Cl	N	O	
			24	17	2	4	1	
4	c	1	Total	C	Cl	N	O	
			24	17	2	4	1	

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

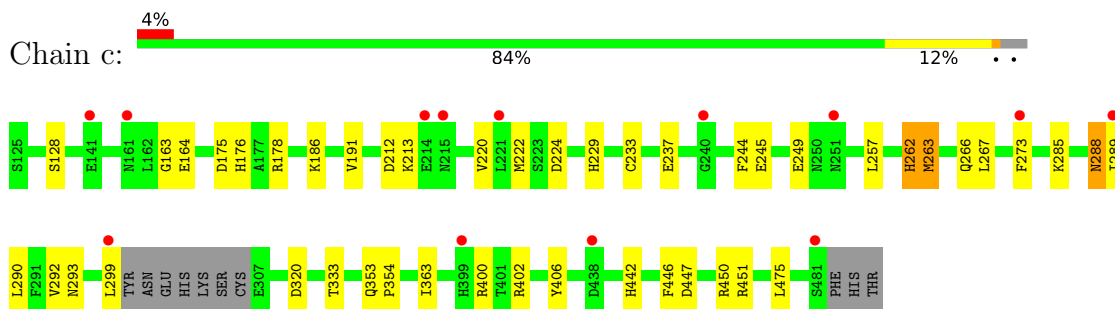


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	c	1	Total	C	O		
			13	8	5		
5	c	1	Total	C	O		
			13	8	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	a	193	Total	O		
			193	193		
6	c	257	Total	O		
			257	257		

- Molecule 1: Dual specificity protein kinase CLK3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.27Å 131.03Å 83.62Å 90.00° 107.71° 90.00°	Depositor
Resolution (Å)	75.13 – 1.90 75.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (75.13-1.90) 98.5 (75.13-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.176 , 0.203 (Not available) , 0.209	Depositor DCC
R_{free} test set	3937 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6334	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KHC, EDO, PO4, PG4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	a	1.42	27/2859 (0.9%)	1.39	13/3866 (0.3%)
1	c	1.35	13/2994 (0.4%)	1.37	22/4041 (0.5%)
All	All	1.38	40/5853 (0.7%)	1.38	35/7907 (0.4%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	288[A]	ASN	CA-C	12.38	1.69	1.52
1	c	288[B]	ASN	CA-C	12.38	1.69	1.52
1	a	439	SER	N-CA	12.29	1.62	1.45
1	a	147	ARG	C-O	10.59	1.36	1.23
1	a	295	GLU	C-O	10.56	1.36	1.24
1	a	157	GLU	C-O	-10.34	1.11	1.24
1	c	263[A]	MET	C-O	9.86	1.36	1.24
1	c	263[B]	MET	C-O	9.86	1.36	1.24
1	c	292	VAL	C-O	7.24	1.32	1.24
1	a	311	VAL	C-O	7.16	1.32	1.24
1	a	291	PHE	C-O	7.06	1.32	1.24
1	a	438	ASP	N-CA	6.82	1.54	1.46
1	a	292	VAL	C-O	6.61	1.32	1.24
1	a	439	SER	CA-C	6.52	1.61	1.53
1	c	442	HIS	CE1-NE2	6.49	1.39	1.32
1	a	245	GLU	CD-OE1	6.47	1.37	1.25
1	c	229	HIS	CE1-NE2	6.11	1.38	1.32
1	c	176	HIS	CE1-NE2	6.04	1.38	1.32
1	a	415	ASP	N-CA	6.03	1.54	1.46
1	a	281	HIS	CE1-NE2	5.93	1.38	1.32
1	a	152	LEU	C-O	5.92	1.31	1.23
1	a	147	ARG	CA-C	5.59	1.59	1.52
1	a	416	GLU	N-CA	5.54	1.53	1.46
1	a	174	LEU	CA-C	5.51	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	291	PHE	CA-C	5.48	1.59	1.52
1	a	339	HIS	CE1-NE2	5.42	1.38	1.32
1	a	449	MET	C-O	5.42	1.30	1.24
1	a	415	ASP	C-O	5.34	1.30	1.23
1	a	158	ILE	N-CA	5.29	1.52	1.46
1	a	250	ASN	CA-C	5.24	1.60	1.52
1	c	262	HIS	CE1-NE2	5.24	1.37	1.32
1	c	363	ILE	C-O	5.20	1.30	1.24
1	a	361	GLY	C-O	5.12	1.29	1.23
1	a	479	GLU	CG-CD	5.10	1.64	1.52
1	c	450	ARG	C-O	5.10	1.30	1.24
1	c	220	VAL	C-O	5.07	1.30	1.23
1	a	262	HIS	CE1-NE2	5.04	1.37	1.32
1	a	155	ARG	C-O	5.03	1.30	1.24
1	c	299	LEU	C-O	5.03	1.33	1.23
1	a	294	SER	N-CA	5.01	1.51	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	447	ASP	CA-CB-CG	-11.88	100.72	112.60
1	c	222	MET	N-CA-CB	-8.32	97.50	110.06
1	c	447	ASP	CA-CB-CG	-7.60	105.00	112.60
1	a	292	VAL	O-C-N	7.45	129.39	121.87
1	c	288[A]	ASN	O-C-N	6.90	130.75	122.26
1	c	288[B]	ASN	O-C-N	6.90	130.75	122.26
1	c	191	VAL	CA-C-N	6.70	127.56	119.99
1	c	191	VAL	C-N-CA	6.70	127.56	119.99
1	c	288[A]	ASN	N-CA-C	-6.65	104.47	112.59
1	c	288[B]	ASN	N-CA-C	-6.65	104.47	112.59
1	c	475	LEU	CA-C-O	-6.57	113.96	121.19
1	a	446	PHE	CA-CB-CG	-6.11	107.69	113.80
1	c	451[A]	ARG	N-CA-C	-6.01	104.81	111.36
1	c	451[B]	ARG	N-CA-C	-6.01	104.81	111.36
1	c	446	PHE	CA-CB-CG	-5.88	107.92	113.80
1	a	290	LEU	CA-C-O	-5.60	114.78	120.71
1	a	174	LEU	CB-CA-C	5.60	118.99	109.53
1	a	272	ARG	CG-CD-NE	-5.59	99.70	112.00
1	c	293	ASN	CB-CA-C	5.58	118.73	110.14
1	a	293	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	c	164	GLU	CB-CG-CD	5.51	121.98	112.60
1	c	333	THR	CA-CB-OG1	-5.47	101.39	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	174	LEU	N-CA-C	-5.42	101.64	110.20
1	c	262	HIS	CA-CB-CG	-5.34	108.46	113.80
1	c	213	LYS	CA-C-N	5.32	127.85	120.29
1	c	213	LYS	C-N-CA	5.32	127.85	120.29
1	c	400	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	a	438	ASP	CA-CB-CG	5.17	117.78	112.60
1	a	224	ASP	CA-CB-CG	5.12	117.72	112.60
1	a	213	LYS	CA-C-N	5.11	128.78	120.60
1	a	213	LYS	C-N-CA	5.11	128.78	120.60
1	c	163	GLY	CA-C-O	-5.07	114.84	122.54
1	c	237	GLU	CB-CA-C	5.04	117.75	109.90
1	c	224	ASP	CA-CB-CG	5.01	117.61	112.60
1	a	152	LEU	O-C-N	5.00	129.39	123.24

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	2787	0	2679	17	0
1	c	2920	0	2819	13	0
2	a	28	0	42	6	0
2	c	60	0	90	3	0
3	a	10	0	0	0	0
3	c	5	0	0	0	0
4	a	24	0	0	1	0
4	c	24	0	0	0	0
5	c	26	0	36	5	0
6	a	193	0	0	4	0
6	c	257	0	0	2	0
All	All	6334	0	5666	37	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 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:269:HIS:ND1	6:a:601:HOH:O	2.20	0.75
1:a:378:GLU:HG2	6:a:670:HOH:O	1.97	0.65
1:a:262:HIS:CD2	1:a:479:GLU:HG2	2.34	0.63
1:a:151:TRP:HA	1:a:156:TYR:O	2.00	0.61
2:c:512:EDO:O1	2:c:513:EDO:H11	2.01	0.60
1:a:395:SER:H	2:a:505:EDO:H12	1.68	0.59
1:a:262:HIS:CG	1:a:479:GLU:HG2	2.39	0.58
1:c:175:ASP:OD2	1:c:178:ARG:NH1	2.35	0.57
1:a:402:ARG:HH12	2:a:508:EDO:H12	1.69	0.56
1:a:137:GLU:OE1	2:a:506:EDO:H22	2.05	0.56
2:c:512:EDO:O1	2:c:513:EDO:C1	2.54	0.56
1:c:245:GLU:O	1:c:249:GLU:HG2	2.06	0.55
2:a:508:EDO:H21	6:c:712:HOH:O	2.06	0.55
1:c:257:LEU:C	1:c:257:LEU:HD13	2.33	0.54
1:a:137:GLU:CD	2:a:506:EDO:H22	2.35	0.52
1:a:450:ARG:HD3	6:a:698:HOH:O	2.10	0.51
5:c:505:PG4:H41	5:c:505:PG4:O4	2.12	0.49
1:c:406:TYR:OH	5:c:503:PG4:H22	2.12	0.49
1:a:262:HIS:CE1	1:a:479:GLU:HG2	2.48	0.48
1:a:214:GLU:OE1	1:a:214:GLU:N	2.37	0.48
1:a:441:GLU:HG3	6:a:671:HOH:O	2.14	0.48
1:c:212:ASP:HB2	1:c:273:PHE:CZ	2.48	0.48
1:c:186:LYS:O	1:c:233:CYS:HA	2.15	0.47
5:c:505:PG4:O4	5:c:505:PG4:C4	2.64	0.46
1:c:402:ARG:HH22	5:c:503:PG4:H42	1.80	0.46
1:a:387:GLU:OE1	2:a:502:EDO:O2	2.31	0.45
4:a:510:KHC:CL1	4:a:510:KHC:C	3.02	0.45
5:c:505:PG4:H61	6:c:703:HOH:O	2.16	0.44
1:c:289[A]:ILE:C	1:c:290:LEU:HD12	2.42	0.43
1:c:262:HIS:CE1	1:c:266:GLN:NE2	2.85	0.43
1:c:244:PHE:CD1	2:c:512:EDO:H11	2.54	0.43
1:a:242:ASN:ND2	1:a:245:GLU:HG3	2.35	0.41
1:a:144:LEU:O	1:a:169:LYS:NZ	2.51	0.41
1:c:263[A]:MET:O	1:c:267:LEU:HG	2.21	0.41
1:c:353:GLN:N	1:c:354:PRO:CD	2.84	0.41
1:a:353:GLN:N	1:a:354:PRO:CD	2.84	0.40
1:c:285:LYS:HE2	1:c:288[B]:ASN:ND2	2.37	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	339/360 (94%)	327 (96%)	12 (4%)	0	100	100
1	c	354/360 (98%)	340 (96%)	13 (4%)	1 (0%)	36	29
All	All	693/720 (96%)	667 (96%)	25 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	320	ASP

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	296/326 (91%)	294 (99%)	2 (1%)	76	78
1	c	314/326 (96%)	313 (100%)	1 (0%)	86	88
All	All	610/652 (94%)	607 (100%)	3 (0%)	81	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	311	VAL
1	a	378	GLU
1	c	128	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	a	253	GLN
1	a	437	GLN
1	c	143	HIS
1	c	161	ASN
1	c	253	GLN
1	c	277	ASN
1	c	377	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

29 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	EDO	c	510	-	3,3,3	0.09	0	2,2,2	0.06	0
2	EDO	c	514	-	3,3,3	0.10	0	2,2,2	0.13	0
2	EDO	a	509	-	3,3,3	0.13	0	2,2,2	0.10	0
3	PO4	c	504	-	4,4,4	0.78	0	6,6,6	0.39	0
5	PG4	c	505	-	12,12,12	0.27	0	11,11,11	0.23	0
2	EDO	c	508	-	3,3,3	0.23	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	a	504	-	4,4,4	0.87	0	6,6,6	0.43	0
2	EDO	c	507	-	3,3,3	0.21	0	2,2,2	0.12	0
2	EDO	a	505	-	3,3,3	0.10	0	2,2,2	0.11	0
4	KHC	a	510	-	25,27,27	0.31	0	24,42,42	0.98	3 (12%)
2	EDO	c	517	-	3,3,3	0.23	0	2,2,2	0.64	0
2	EDO	c	512	-	3,3,3	0.23	0	2,2,2	0.12	0
2	EDO	a	506	-	3,3,3	0.28	0	2,2,2	0.28	0
2	EDO	a	508	-	3,3,3	0.26	0	2,2,2	0.38	0
2	EDO	c	509	-	3,3,3	0.50	0	2,2,2	0.08	0
2	EDO	c	501	-	3,3,3	0.29	0	2,2,2	0.33	0
2	EDO	c	515	-	3,3,3	0.33	0	2,2,2	0.54	0
2	EDO	c	518	-	3,3,3	0.78	0	2,2,2	0.97	0
2	EDO	c	502	-	3,3,3	0.06	0	2,2,2	0.11	0
4	KHC	c	519	-	25,27,27	0.31	0	24,42,42	1.11	3 (12%)
2	EDO	a	507	-	3,3,3	0.15	0	2,2,2	0.06	0
2	EDO	c	513	-	3,3,3	0.15	0	2,2,2	0.15	0
2	EDO	a	501	-	3,3,3	0.29	0	2,2,2	0.53	0
2	EDO	a	502	-	3,3,3	0.05	0	2,2,2	0.03	0
2	EDO	c	516	-	3,3,3	0.28	0	2,2,2	0.28	0
2	EDO	c	506	-	3,3,3	0.37	0	2,2,2	0.19	0
2	EDO	c	511	-	3,3,3	0.12	0	2,2,2	0.23	0
5	PG4	c	503	-	12,12,12	0.21	0	11,11,11	0.22	0
3	PO4	a	503	-	4,4,4	0.47	0	6,6,6	0.54	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
2	EDO	c	510	-	-	0/1/1/1	-
2	EDO	c	514	-	-	1/1/1/1	-
2	EDO	a	509	-	-	0/1/1/1	-
5	PG4	c	505	-	-	6/10/10/10	-
2	EDO	c	508	-	-	0/1/1/1	-
2	EDO	c	507	-	-	0/1/1/1	-
2	EDO	a	505	-	-	1/1/1/1	-
4	KHC	a	510	-	-	0/0/31/31	0/4/4/4
2	EDO	c	517	-	-	0/1/1/1	-
2	EDO	c	512	-	-	1/1/1/1	-
2	EDO	a	506	-	-	1/1/1/1	-
2	EDO	a	508	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	c	509	-	-	0/1/1/1	-
2	EDO	c	501	-	-	0/1/1/1	-
2	EDO	c	515	-	-	1/1/1/1	-
2	EDO	c	518	-	-	1/1/1/1	-
2	EDO	c	502	-	-	1/1/1/1	-
4	KHC	c	519	-	-	0/0/31/31	0/4/4/4
2	EDO	a	507	-	-	0/1/1/1	-
2	EDO	c	513	-	-	0/1/1/1	-
2	EDO	a	501	-	-	0/1/1/1	-
2	EDO	a	502	-	-	0/1/1/1	-
2	EDO	c	516	-	-	1/1/1/1	-
2	EDO	c	506	-	-	0/1/1/1	-
2	EDO	c	511	-	-	1/1/1/1	-
5	PG4	c	503	-	-	5/10/10/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	519	KHC	C8-C9-N3	-3.77	170.81	177.65
4	a	510	KHC	C2-C1-N	-2.88	127.35	131.92
4	a	510	KHC	C8-C9-N3	-2.29	173.49	177.65
4	c	519	KHC	O-C2-C1	-2.20	122.22	127.62
4	c	519	KHC	C2-C1-N	-2.13	128.55	131.92
4	a	510	KHC	O-C2-C1	-2.10	122.45	127.62

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	c	503	PG4	O3-C5-C6-O4
2	a	506	EDO	O1-C1-C2-O2
2	c	502	EDO	O1-C1-C2-O2
2	c	514	EDO	O1-C1-C2-O2
2	c	516	EDO	O1-C1-C2-O2
5	c	505	PG4	O4-C7-C8-O5
5	c	503	PG4	C8-C7-O4-C6
5	c	505	PG4	C3-C4-O3-C5
5	c	503	PG4	C4-C3-O2-C2
5	c	503	PG4	O4-C7-C8-O5
2	a	508	EDO	O1-C1-C2-O2

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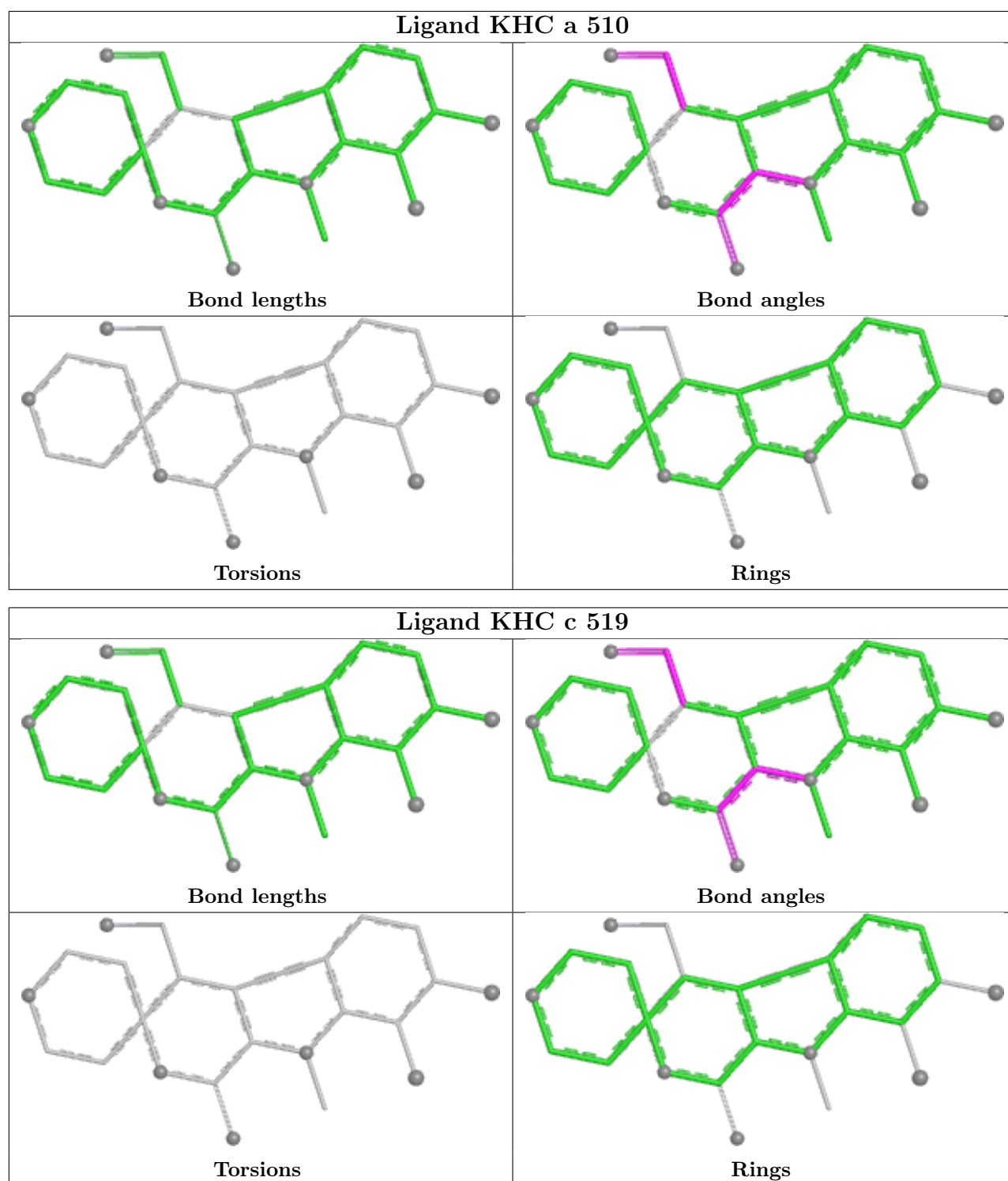
Mol	Chain	Res	Type	Atoms
5	c	505	PG4	C5-C6-O4-C7
2	a	505	EDO	O1-C1-C2-O2
2	c	511	EDO	O1-C1-C2-O2
2	c	515	EDO	O1-C1-C2-O2
2	c	518	EDO	O1-C1-C2-O2
5	c	505	PG4	C8-C7-O4-C6
2	c	512	EDO	O1-C1-C2-O2
5	c	505	PG4	C4-C3-O2-C2
5	c	505	PG4	C6-C5-O3-C4
5	c	503	PG4	C5-C6-O4-C7

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	c	505	PG4	3	0
2	a	505	EDO	1	0
4	a	510	KHC	1	0
2	c	512	EDO	3	0
2	a	506	EDO	2	0
2	a	508	EDO	2	0
2	c	513	EDO	2	0
2	a	502	EDO	1	0
5	c	503	PG4	2	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	340/360 (94%)	0.42	22 (6%) 25 26	11, 30, 56, 72	3 (0%)
1	c	350/360 (97%)	0.09	13 (3%) 45 48	10, 24, 46, 67	8 (2%)
All	All	690/720 (95%)	0.25	35 (5%) 33 36	10, 27, 50, 72	11 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	300	TYR	4.4
1	a	438	ASP	4.1
1	c	481	SER	4.0
1	c	215	ASN	3.8
1	a	156	TYR	3.6
1	c	299	LEU	3.5
1	c	214	GLU	3.3
1	a	135	SER	3.3
1	a	291	PHE	3.3
1	a	149	GLY	3.3
1	a	148	ILE	3.1
1	a	481	SER	3.0
1	c	221	LEU	2.8
1	c	399[A]	HIS	2.8
1	a	292	VAL	2.7
1	a	423	TYR	2.7
1	c	438[A]	ASP	2.7
1	a	178	ARG	2.6
1	c	273	PHE	2.5
1	c	251	ASN	2.4
1	a	179	GLY	2.4
1	a	174	LEU	2.3
1	c	289[A]	ILE	2.3
1	a	311	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	a	151	TRP	2.3
1	a	215	ASN	2.3
1	c	161	ASN	2.3
1	c	240	GLY	2.2
1	a	415	ASP	2.2
1	a	177	ALA	2.2
1	c	141	GLU	2.2
1	a	293	ASN	2.1
1	a	439	SER	2.1
1	a	437	GLN	2.0
1	a	147	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	KHC	a	510	24/24	0.68	0.21	47,65,67,77	0
4	KHC	c	519	24/24	0.69	0.19	40,52,67,78	0
5	PG4	c	505	13/13	0.74	0.23	48,55,69,70	0
5	PG4	c	503	13/13	0.77	0.22	41,52,58,60	0
2	EDO	c	514	4/4	0.81	0.20	54,56,57,58	0
2	EDO	a	509	4/4	0.82	0.17	53,54,57,57	0
2	EDO	c	518	4/4	0.83	0.19	34,38,40,41	0
3	PO4	a	503	5/5	0.83	0.14	47,51,56,56	0
2	EDO	c	507	4/4	0.83	0.21	45,51,51,53	0
2	EDO	a	505	4/4	0.84	0.16	49,54,54,60	0
2	EDO	c	516	4/4	0.84	0.19	44,48,50,52	0
2	EDO	c	510	4/4	0.86	0.13	34,35,37,40	0

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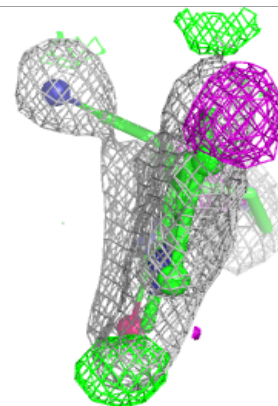
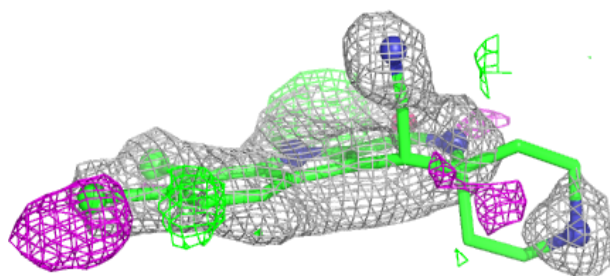
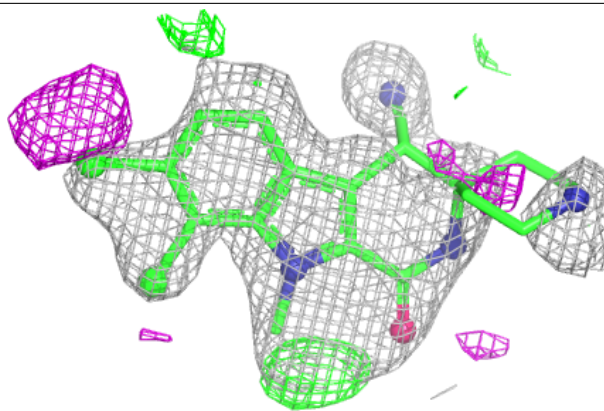
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	a	508	4/4	0.88	0.20	35,36,39,39	0
2	EDO	c	508	4/4	0.89	0.14	24,26,28,33	0
2	EDO	c	502	4/4	0.89	0.17	56,56,56,61	0
2	EDO	a	502	4/4	0.90	0.13	41,43,44,45	0
2	EDO	a	506	4/4	0.90	0.14	37,40,40,41	0
2	EDO	c	513	4/4	0.92	0.12	38,44,44,47	0
2	EDO	c	517	4/4	0.92	0.13	25,32,33,36	0
2	EDO	c	511	4/4	0.92	0.11	48,48,49,50	0
2	EDO	c	515	4/4	0.92	0.12	31,37,38,45	0
2	EDO	c	509	4/4	0.93	0.11	29,33,37,46	0
2	EDO	c	501	4/4	0.93	0.12	26,26,30,30	4
2	EDO	a	507	4/4	0.94	0.10	38,40,41,41	0
2	EDO	c	506	4/4	0.94	0.09	29,31,32,33	0
2	EDO	c	512	4/4	0.95	0.08	28,36,37,43	0
2	EDO	a	501	4/4	0.96	0.13	25,33,36,38	0
3	PO4	c	504	5/5	0.98	0.06	30,33,33,34	5
3	PO4	a	504	5/5	0.99	0.07	24,25,27,28	5

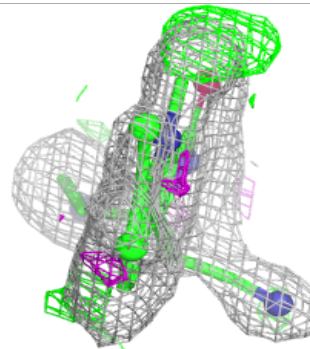
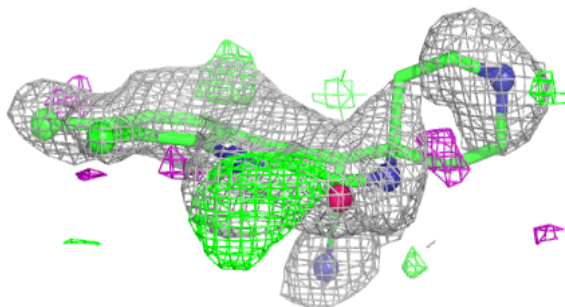
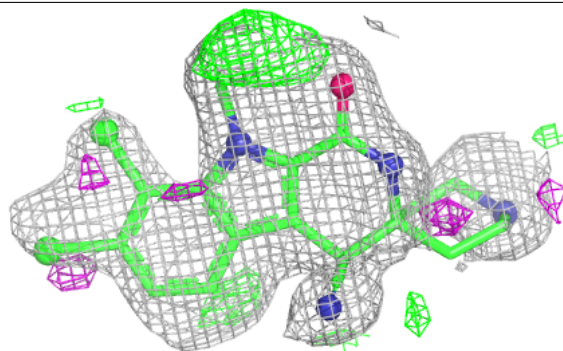
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KHC a 510:

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

**Electron density around KHC c 519:**

$2mF_o-DF_c$ (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.