



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:40 AM UTC

PDB ID : 8FUX / pdb_00008fux
Title : KpsC D160C ternary complex
Authors : Kimber, M.S.; Doyle, L.; Whitfield, C.
Deposited on : 2023-01-18
Resolution : 1.20 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

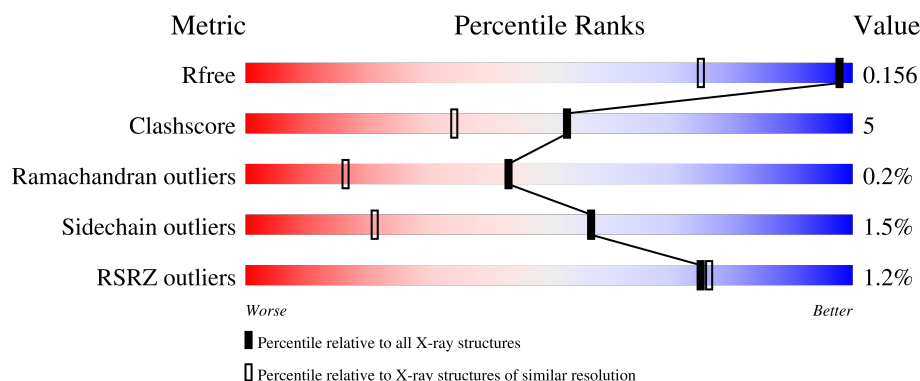
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1216 (1.20-1.20)
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	329	% 90% 8% .
1	B	329	% 85% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	B	406	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12393 atoms, of which 5810 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.

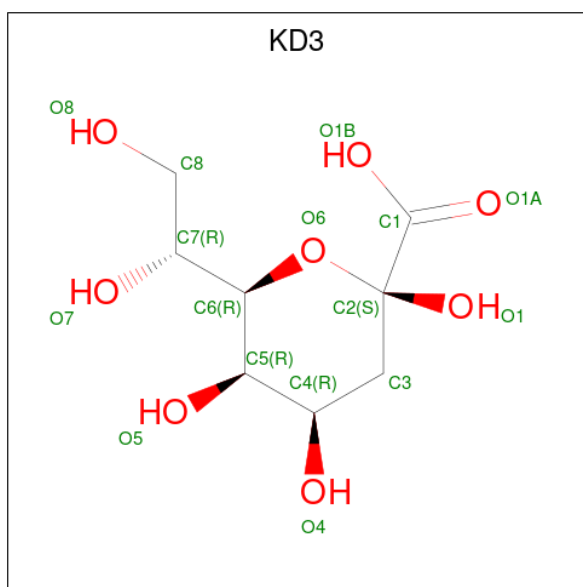
- Molecule 1 is a protein called Capsule polysaccharide export protein KpsC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	H	N	O	S	0	39	0
			5513	1757	2803	460	478	15			
1	B	318	Total	C	H	N	O	S	0	54	0
			5653	1788	2877	490	484	14			

There are 16 discrepancies between the modelled and reference sequences:

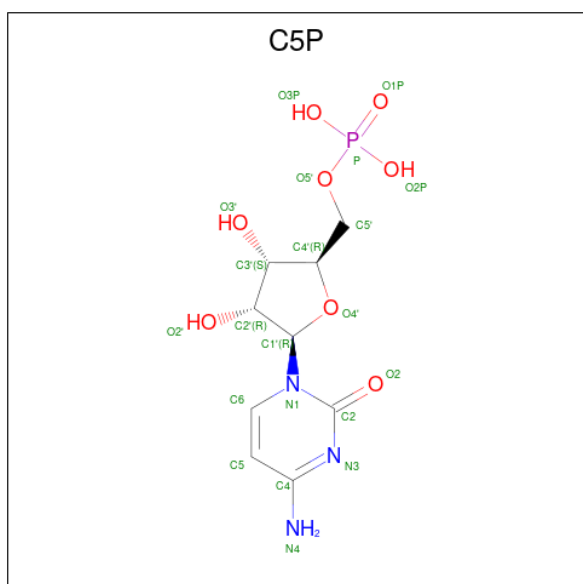
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A0H2Z2W8
A	1	GLY	-	expression tag	UNP A0A0H2Z2W8
A	160	CYS	ASP	engineered mutation	UNP A0A0H2Z2W8
A	324	HIS	-	expression tag	UNP A0A0H2Z2W8
A	325	HIS	-	expression tag	UNP A0A0H2Z2W8
A	326	HIS	-	expression tag	UNP A0A0H2Z2W8
A	327	HIS	-	expression tag	UNP A0A0H2Z2W8
A	328	HIS	-	expression tag	UNP A0A0H2Z2W8
B	0	MET	-	initiating methionine	UNP A0A0H2Z2W8
B	1	GLY	-	expression tag	UNP A0A0H2Z2W8
B	160	CYS	ASP	engineered mutation	UNP A0A0H2Z2W8
B	324	HIS	-	expression tag	UNP A0A0H2Z2W8
B	325	HIS	-	expression tag	UNP A0A0H2Z2W8
B	326	HIS	-	expression tag	UNP A0A0H2Z2W8
B	327	HIS	-	expression tag	UNP A0A0H2Z2W8
B	328	HIS	-	expression tag	UNP A0A0H2Z2W8

- Molecule 2 is 3-deoxy-beta-D-manno-oct-2-ulopyranosonic acid (CCD ID: KD3) (formula: $C_8H_{14}O_8$) (labeled as "Ligand of Interest" by depositor).



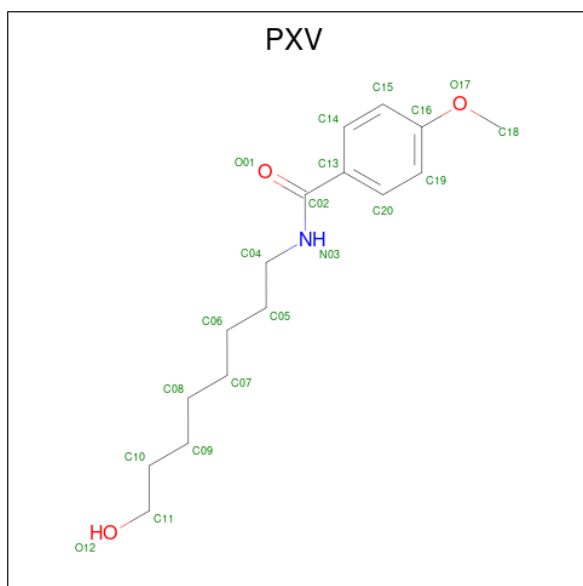
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			26	8	11	7		
2	A	1	Total	C	H	O	0	0
			27	8	12	7		
2	B	1	Total	C	H	O	0	0
			27	8	11	8		
2	B	1	Total	C	H	O	0	0
			27	8	12	7		

- Molecule 3 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: $C_9H_{14}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



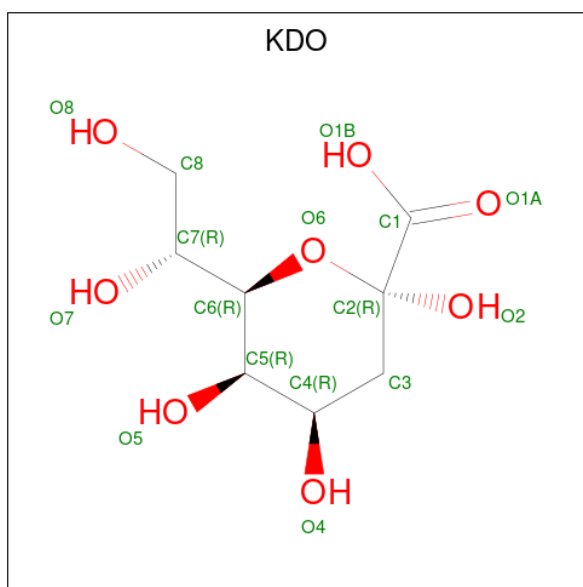
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	
			33	9	12	3	8	1	
								0	0

- Molecule 4 is N-(8-hydroxyoctyl)-4-methoxybenzamide (CCD ID: PXV) (formula: $C_{16}H_{25}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O		
			44	16	24	1	3	0	0
4	B	1	Total	C	H	N	O		
			43	16	24	1	2	0	0

- Molecule 5 is 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid (CCD ID: KDO) (formula: $C_8H_{14}O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			27	8	12	7		
5	B	1	Total	C	H	O	0	0
			27	8	12	7		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		

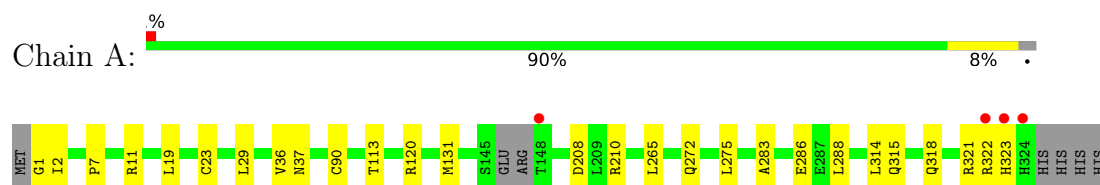
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	488	Total	O	0	0
			488	488		
8	B	449	Total	O	0	2
			451	451		

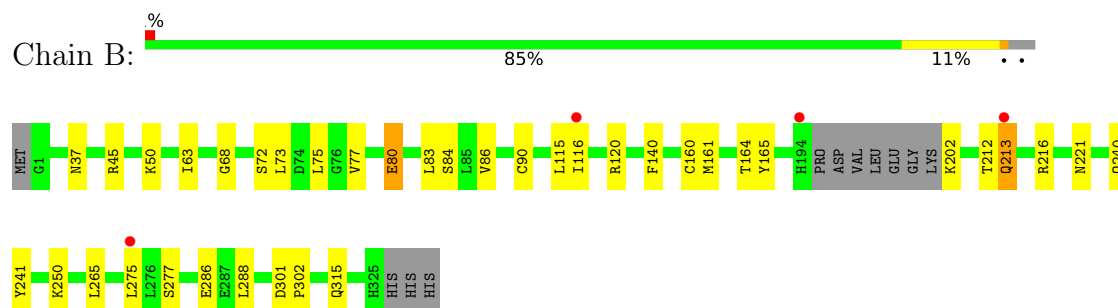
3 Residue-property plots

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: Capsule polysaccharide export protein KpsC



- Molecule 1: Capsule polysaccharide export protein KpsC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.54Å 80.30Å 65.98Å 90.00° 103.04° 90.00°	Depositor
Resolution (Å)	48.43 – 1.20 48.43 – 1.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.43-1.20) 99.7 (48.43-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.20Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.124 , 0.157 0.123 , 0.156	Depositor DCC
R_{free} test set	13274 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12393	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PO4, KD3, C5P, PXV, KDO

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	0.85	2/2893 (0.1%)	0.86	0/3935
1	B	0.89	4/3005 (0.1%)	0.80	0/4085
All	All	0.87	6/5898 (0.1%)	0.83	0/8020

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	CYS	CA-CB	7.28	1.66	1.53
1	B	50	LYS	CG-CD	-6.27	1.33	1.52
1	B	90	CYS	CB-SG	-5.47	1.63	1.81
1	A	90[A]	CYS	C-N	-5.42	1.25	1.33
1	A	90[B]	CYS	C-N	-5.42	1.25	1.33
1	B	250	LYS	CE-NZ	-5.37	1.33	1.49

There are no bond angle outliers.

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	2710	2803	2807	24	0
1	B	2776	2877	2820	32	2
2	A	30	23	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	23	0	0	0
3	A	21	12	12	1	0
4	A	20	24	0	0	0
4	B	19	24	0	0	0
5	A	15	12	12	0	0
5	B	15	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	5	0	0	2	0
8	A	488	0	0	13	2
8	B	451	0	0	13	0
All	All	6583	5810	5663	57	2

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 5.

All (57) 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:37[B]:ASN:OD1	8:A:601:HOH:O	1.96	0.82
1:A:11[B]:ARG:NH1	8:A:604:HOH:O	2.15	0.80
1:A:208:ASP:OD1	8:A:602:HOH:O	2.00	0.78
1:A:2[B]:ILE:HD13	1:A:19[B]:LEU:HD22	1.68	0.76
1:A:7[B]:PRO:HG3	8:B:508:HOH:O	1.86	0.76
1:A:272[A]:GLN:NE2	8:A:606:HOH:O	2.19	0.76
1:A:113[B]:THR:HG23	8:A:964:HOH:O	1.85	0.75
1:B:77:VAL:HG13	8:B:517:HOH:O	1.84	0.75
1:B:116[A]:ILE:CG2	1:B:286[A]:GLU:OE1	2.33	0.75
1:B:37[B]:ASN:OD1	8:B:501:HOH:O	2.04	0.73
1:B:240:GLN:N	7:B:406:PO4:O1	2.19	0.73
1:B:37[A]:ASN:OD1	8:B:502:HOH:O	2.12	0.68
1:B:315[B]:GLN:OE1	8:B:503:HOH:O	2.12	0.67
1:A:286:GLU:OE2	8:A:603:HOH:O	2.13	0.66
1:B:116[A]:ILE:HG23	1:B:286[A]:GLU:OE1	1.95	0.65
1:A:1[B]:GLY:HA2	8:A:624:HOH:O	2.01	0.61
1:A:315[B]:GLN:OE1	8:A:605:HOH:O	2.18	0.56
1:B:116[A]:ILE:HG23	1:B:286[A]:GLU:CD	2.30	0.56
1:A:1[A]:GLY:O	1:A:37[A]:ASN:OD1	2.23	0.56
1:A:275[A]:LEU:HD13	8:A:607:HOH:O	2.06	0.56
1:B:116[B]:ILE:HB	8:B:514:HOH:O	2.06	0.55
1:A:1[B]:GLY:HA3	8:A:616:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2[B]:ILE:CD1	1:A:19[B]:LEU:HD22	2.34	0.55
1:B:75:LEU:HD12	1:B:75:LEU:N	2.23	0.53
1:B:277[B]:SER:OG	8:B:504:HOH:O	2.18	0.53
1:A:210[A]:ARG:NH2	8:A:608:HOH:O	2.28	0.53
1:B:221[A]:ASN:ND2	8:B:511:HOH:O	2.37	0.52
1:A:283:ALA:HB3	1:A:288[B]:LEU:CD1	2.41	0.51
1:B:265:LEU:HD12	1:B:288[B]:LEU:HD12	1.92	0.51
1:B:73:LEU:HB3	1:B:80:GLU:OE2	2.12	0.50
1:A:1[B]:GLY:O	1:A:36:VAL:HA	2.11	0.50
1:B:315[B]:GLN:HG3	8:B:503:HOH:O	2.12	0.49
1:B:116[A]:ILE:HG21	1:B:286[A]:GLU:OE1	2.12	0.48
1:B:116[B]:ILE:N	8:B:514:HOH:O	2.47	0.48
1:A:19[A]:LEU:HD22	1:A:23[A]:CYS:SG	2.54	0.48
1:B:72:SER:HB2	1:B:80:GLU:HG2	1.96	0.48
1:B:240:GLN:H	7:B:406:PO4:P	2.32	0.48
1:A:265:LEU:HD12	1:A:288[A]:LEU:HD12	1.97	0.47
1:B:45:ARG:NH1	1:B:161[B]:MET:HE3	2.30	0.46
1:A:321:ARG:O	1:A:322:ARG:C	2.59	0.46
1:B:68:GLY:HA3	1:B:84[B]:SER:OG	2.17	0.45
1:B:75:LEU:HD12	1:B:75:LEU:H	1.82	0.44
1:A:318:GLN:O	1:A:322:ARG:HG3	2.17	0.44
1:B:63[B]:ILE:HD11	8:B:936:HOH:O	2.18	0.43
1:B:115[B]:LEU:O	1:B:116[B]:ILE:C	2.62	0.43
1:A:275[A]:LEU:HD22	8:A:607:HOH:O	2.19	0.43
3:A:403:C5P:H6	3:A:403:C5P:O5'	2.19	0.43
1:B:116[A]:ILE:CG2	1:B:286[A]:GLU:CD	2.90	0.43
1:B:164[A]:THR:HG23	1:B:165:TYR:N	2.33	0.42
1:A:131[B]:MET:SD	1:A:314:LEU:HD22	2.59	0.42
1:B:212[A]:THR:O	1:B:213[A]:GLN:C	2.63	0.42
1:B:216[B]:ARG:HD2	8:B:838:HOH:O	2.19	0.41
1:B:315[B]:GLN:CD	8:B:503:HOH:O	2.60	0.41
1:B:83:LEU:HD13	1:B:302:PRO:HG3	2.03	0.41
1:A:120:ARG:HD3	8:A:971:HOH:O	2.20	0.40
1:B:301:ASP:HA	1:B:302:PRO:HD3	1.83	0.40

All (2) 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)
1:B:286[B]:GLU:OE2	8:A:930:HOH:O[1_454]	1.91	0.29
1:B:120[B]:ARG:HH12	8:A:603:HOH:O[1_454]	1.53	0.07

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	356/329 (108%)	350 (98%)	5 (1%)	1 (0%)	36	14
1	B	367/329 (112%)	359 (98%)	8 (2%)	0	100	100
All	All	723/658 (110%)	709 (98%)	13 (2%)	1 (0%)	43	17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	HIS

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	302/271 (111%)	300 (99%)	2 (1%)	76	47
1	B	313/271 (116%)	304 (97%)	9 (3%)	37	6
All	All	615/542 (114%)	604 (98%)	11 (2%)	57	16

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

Mol	Chain	Res	Type
1	A	29[A]	LEU
1	A	29[B]	LEU
1	B	80	GLU
1	B	86	VAL
1	B	160	CYS

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Mol	Chain	Res	Type
1	B	202	LYS
1	B	213[A]	GLN
1	B	213[B]	GLN
1	B	241[A]	TYR
1	B	241[B]	TYR
1	B	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	159	ASN
1	A	186	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KD3	A	402	2	15,15,16	1.33	1 (6%)	17,21,24	1.57	4 (23%)
5	KDO	A	405	-	15,15,16	2.18	3 (20%)	17,21,24	1.77	5 (29%)
7	PO4	B	406	-	4,4,4	1.94	1 (25%)	6,6,6	1.91	2 (33%)
5	KDO	B	404	-	15,15,16	1.17	2 (13%)	17,21,24	1.51	5 (29%)
2	KD3	B	402	2	15,15,16	1.10	1 (6%)	17,21,24	1.03	0
2	KD3	A	401	2,4	15,15,16	1.30	2 (13%)	17,21,24	1.33	1 (5%)
3	C5P	A	403	-	22,22,22	1.60	5 (22%)	32,33,33	1.34	3 (9%)
4	PXV	A	404	2	20,20,20	1.73	3 (15%)	23,23,23	1.52	5 (21%)
4	PXV	B	403	2	19,19,20	0.94	1 (5%)	22,22,23	0.93	2 (9%)
2	KD3	B	401	2,4	16,16,16	1.42	3 (18%)	17,24,24	1.33	2 (11%)

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	KD3	A	402	2	-	0/10/26/30	0/1/1/1
5	KDO	A	405	-	-	1/10/26/30	0/1/1/1
5	KDO	B	404	-	-	2/10/26/30	0/1/1/1
2	KD3	B	402	2	-	0/10/26/30	0/1/1/1
2	KD3	A	401	2,4	-	0/10/26/30	0/1/1/1
3	C5P	A	403	-	-	1/10/26/26	0/2/2/2
4	PXV	A	404	2	-	5/16/16/16	0/1/1/1
4	PXV	B	403	2	-	0/15/15/16	0/1/1/1
2	KD3	B	401	2,4	-	3/12/30/30	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	KDO	C2-C1	6.91	1.60	1.52
4	A	404	PXV	C02-N03	5.53	1.46	1.33
2	A	402	KD3	O1A-C1	4.07	1.34	1.22
3	A	403	C5P	C2'-C3'	-3.82	1.43	1.53
7	B	406	PO4	P-O1	-3.48	1.42	1.50
2	A	401	KD3	C2-C1	3.43	1.56	1.52
4	A	404	PXV	C19-C20	-3.22	1.33	1.38
5	A	405	KDO	C3-C2	3.18	1.57	1.52
2	B	401	KD3	C3-C2	-2.91	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	KDO	C2-C1	2.79	1.55	1.52
2	B	402	KD3	O1A-C1	2.77	1.30	1.22
3	A	403	C5P	O4'-C1'	-2.74	1.35	1.42
2	B	401	KD3	C2-C1	2.65	1.57	1.53
4	B	403	PXV	C14-C15	-2.51	1.34	1.38
5	A	405	KDO	O6-C2	2.40	1.48	1.43
3	A	403	C5P	C4-N4	2.36	1.39	1.33
5	B	404	KDO	C3-C2	2.33	1.56	1.52
4	A	404	PXV	O17-C16	2.30	1.42	1.37
3	A	403	C5P	O4'-C4'	2.29	1.50	1.45
2	A	401	KD3	C7-C6	2.20	1.57	1.52
3	A	403	C5P	C5'-C4'	-2.14	1.45	1.51
2	B	401	KD3	O1A-C1	2.13	1.28	1.22

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	405	KDO	O6-C6-C5	4.35	114.09	107.94
2	A	402	KD3	O1B-C1-O1A	-3.19	116.85	124.08
3	A	403	C5P	O4'-C4'-C3'	-3.18	98.84	105.15
4	A	404	PXV	C14-C13-C20	3.15	122.58	118.57
4	A	404	PXV	C20-C19-C16	3.13	123.30	119.73
5	B	404	KDO	O1B-C1-C2	3.09	120.73	112.71
4	A	404	PXV	C19-C20-C13	-3.06	117.53	120.80
5	A	405	KDO	O1B-C1-C2	3.01	120.53	112.71
7	B	406	PO4	O4-P-O3	-2.96	98.71	107.91
2	B	401	KD3	O1A-C1-C2	-2.90	119.02	123.85
2	A	402	KD3	O6-C6-C5	2.84	111.96	107.94
2	A	402	KD3	C8-C7-C6	2.81	117.64	112.05
2	A	401	KD3	O1B-C1-C2	2.80	120.00	112.71
5	B	404	KDO	O6-C2-C3	-2.67	106.96	110.56
2	A	402	KD3	O1B-C1-C2	2.56	119.37	112.71
5	B	404	KDO	O1B-C1-O1A	-2.55	118.30	124.08
4	B	403	PXV	C20-C19-C16	-2.44	116.94	119.73
4	A	404	PXV	C15-C14-C13	-2.43	118.20	120.80
7	B	406	PO4	O4-P-O1	2.42	119.50	110.95
5	A	405	KDO	O1A-C1-C2	-2.41	117.65	122.85
5	A	405	KDO	O8-C8-C7	-2.29	106.34	111.16
2	B	401	KD3	O4-C4-C5	2.26	114.84	110.15
5	B	404	KDO	O4-C4-C5	-2.22	105.55	110.15
3	A	403	C5P	O4'-C1'-N1	2.21	113.38	108.36
5	B	404	KDO	O6-C2-C1	-2.21	103.54	107.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	PXV	C14-C15-C16	2.20	122.25	119.73
5	A	405	KDO	O6-C2-C1	-2.16	103.64	107.72
3	A	403	C5P	C5-C4-N3	2.10	124.85	121.32
4	A	404	PXV	C13-C02-N03	-2.01	112.94	117.12

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	C5P	C5'-O5'-P-O3P
5	B	404	KDO	C6-C7-C8-O8
5	B	404	KDO	O7-C7-C8-O8
2	B	401	KD3	O1A-C1-C2-O6
5	A	405	KDO	O1A-C1-C2-O6
4	A	404	PXV	O01-C02-C13-C14
4	A	404	PXV	O01-C02-C13-C20
4	A	404	PXV	N03-C02-C13-C14
4	A	404	PXV	N03-C02-C13-C20
2	B	401	KD3	O1B-C1-C2-O6
4	A	404	PXV	C07-C08-C09-C10
2	B	401	KD3	O1B-C1-C2-C3

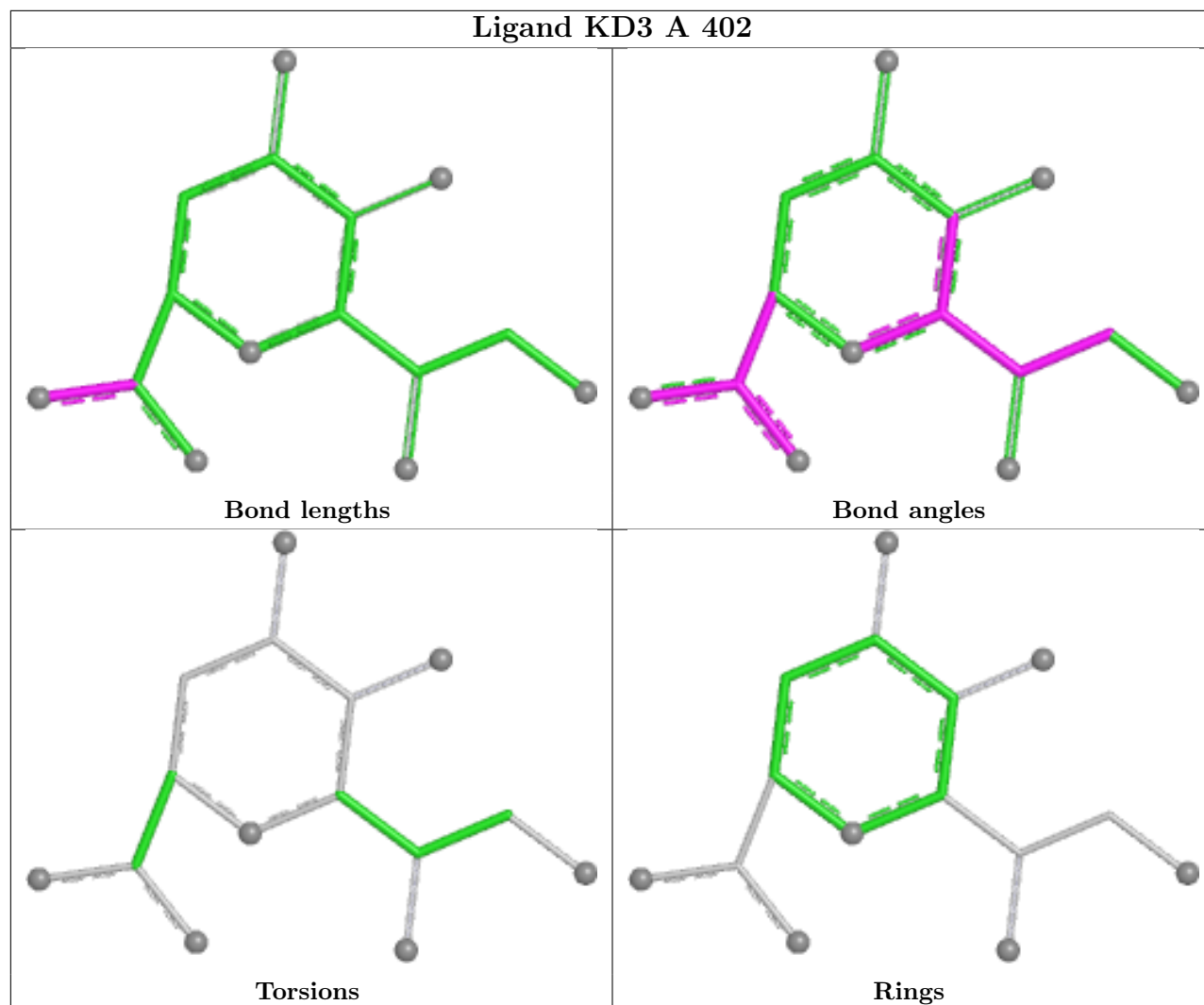
There are no ring outliers.

2 monomers are involved in 3 short contacts:

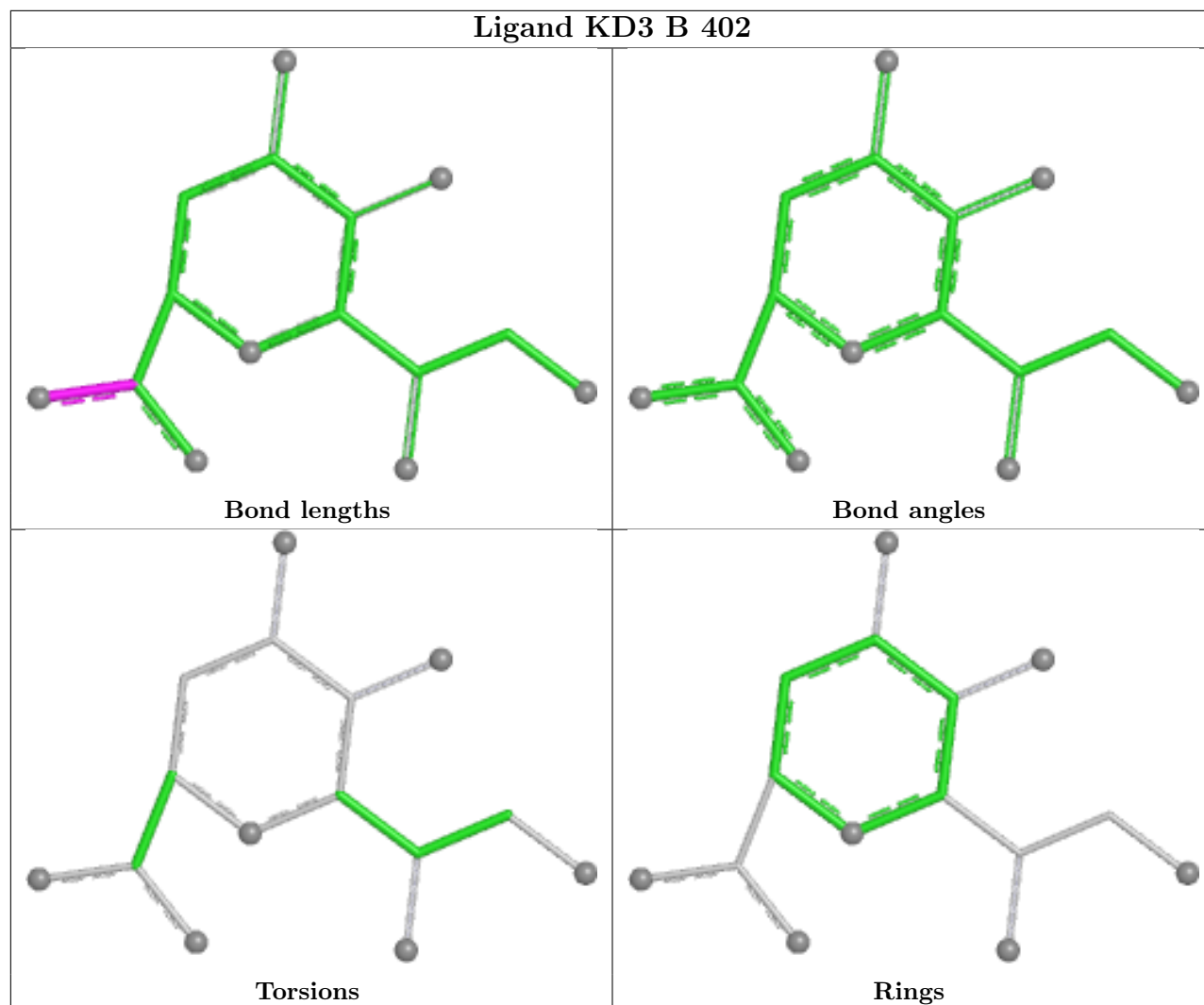
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	406	PO4	2	0
3	A	403	C5P	1	0

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

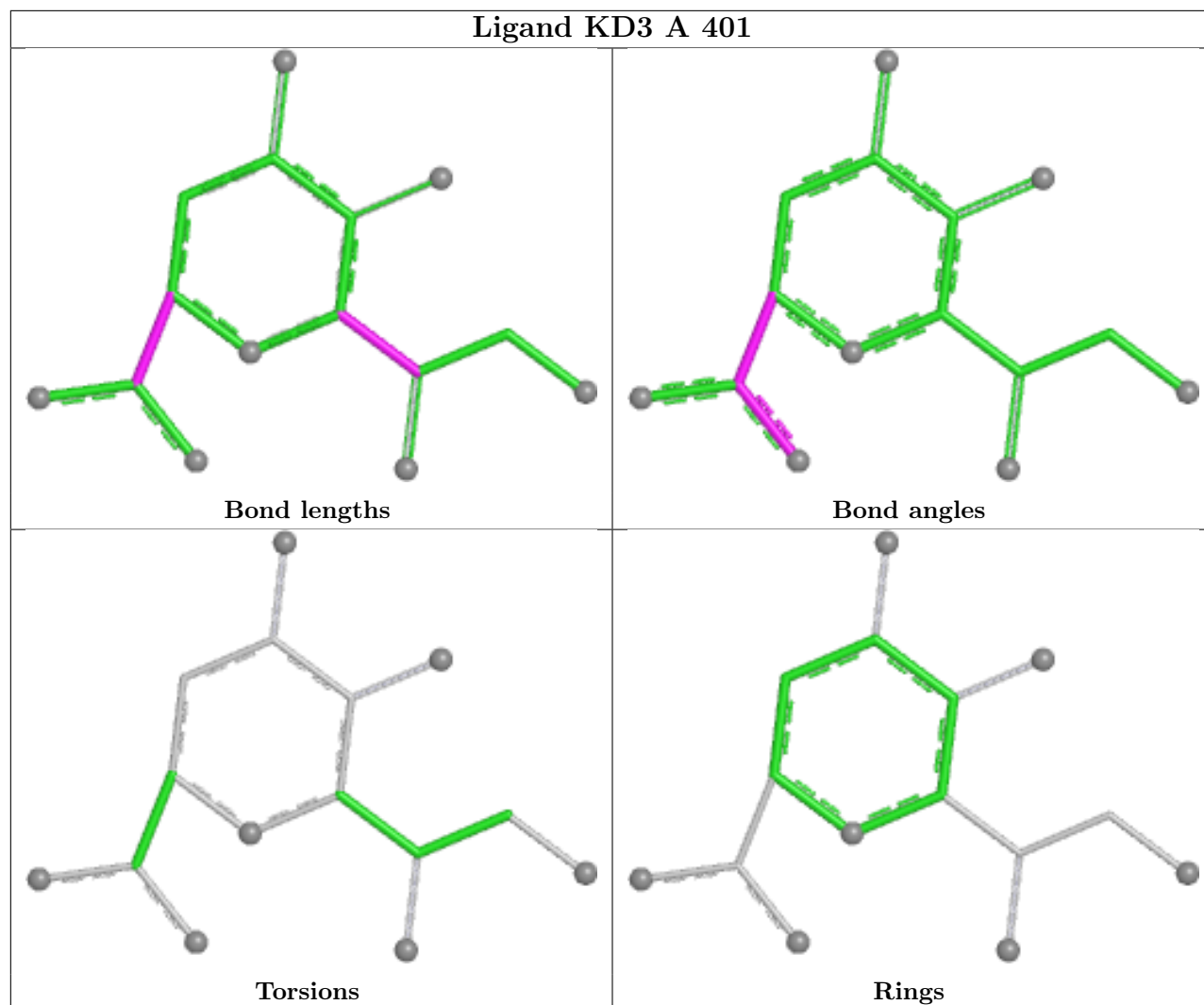
Ligand KD3 A 402



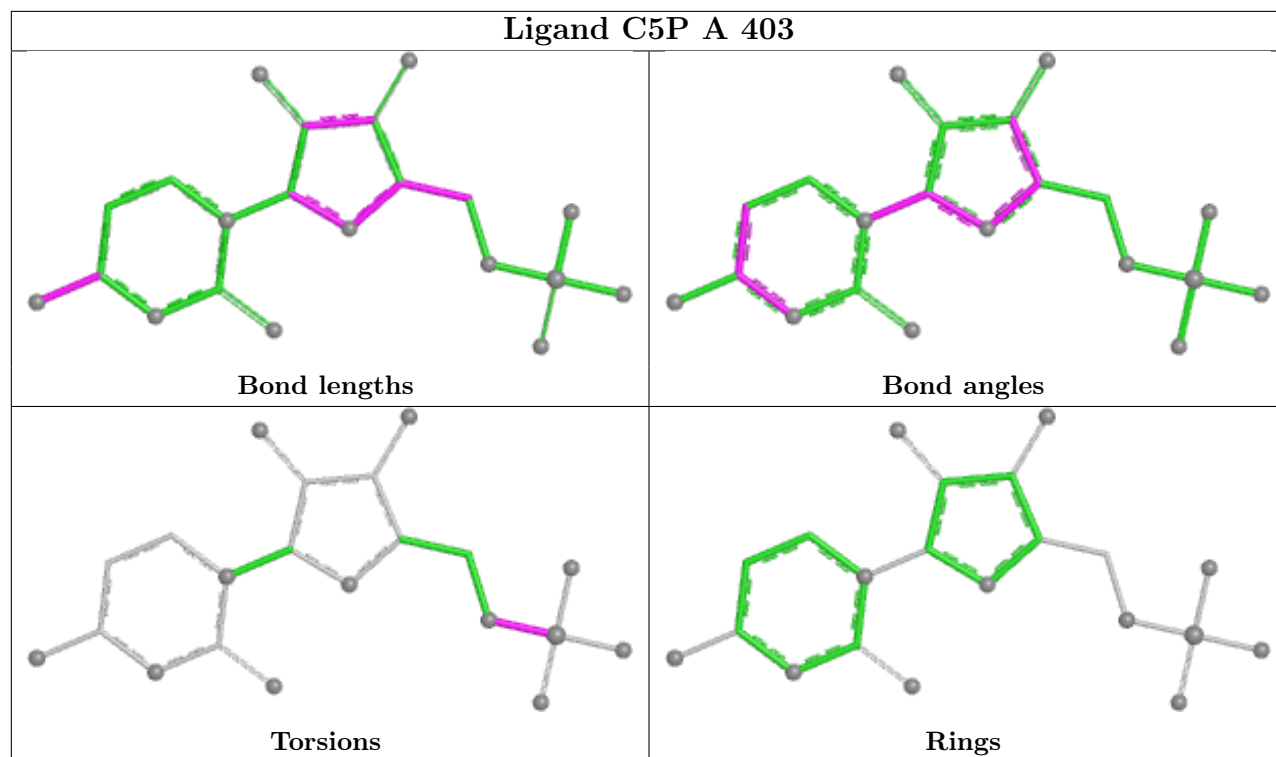
Ligand KD3 B 402



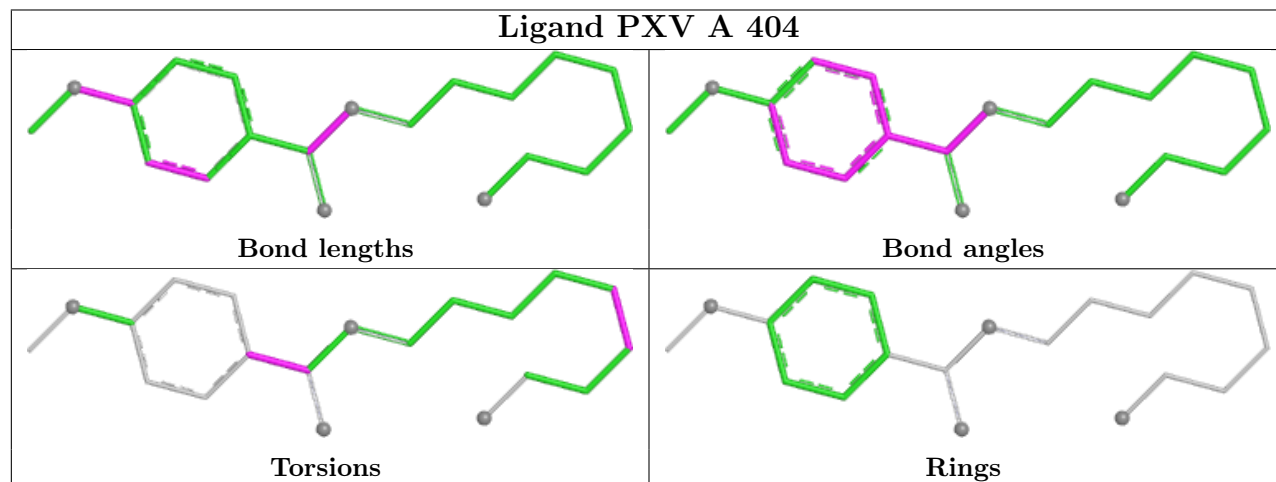
Ligand KD3 A 401



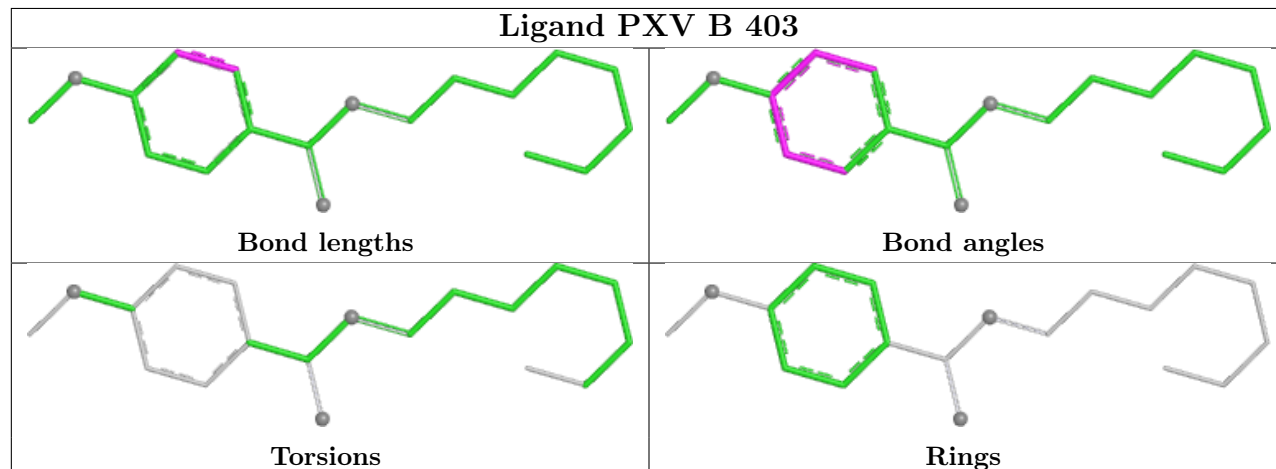
Ligand C5P A 403

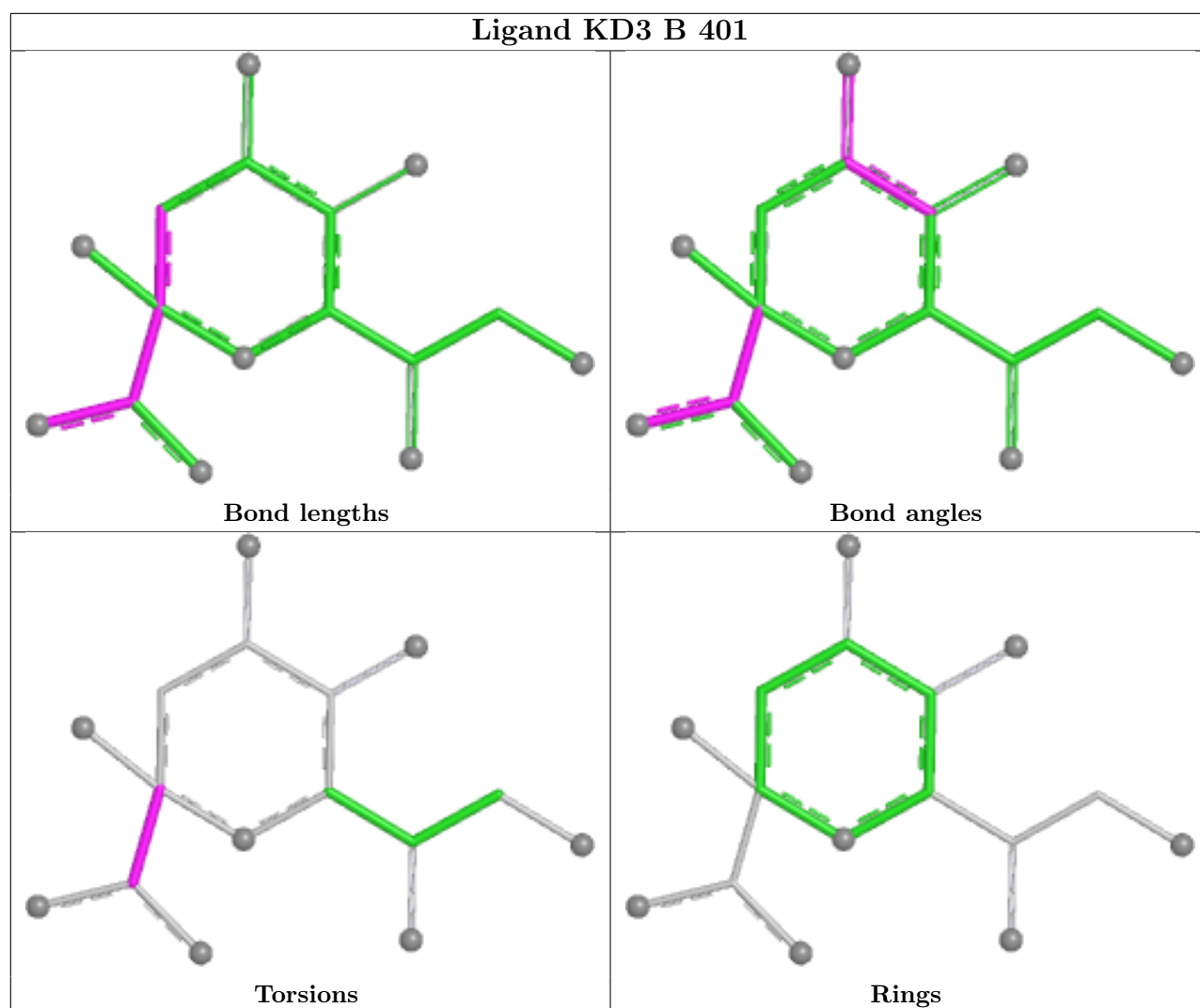


Ligand PXV A 404



Ligand PXV B 403





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	322/329 (97%)	-0.56	4 (1%) 76 78	7, 15, 26, 59	39 (12%)
1	B	318/329 (96%)	-0.51	4 (1%) 75 76	5, 15, 28, 49	47 (14%)
All	All	640/658 (97%)	-0.53	8 (1%) 75 76	5, 15, 27, 59	86 (13%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116[A]	ILE	5.6
1	A	148	THR	4.7
1	B	194	HIS	3.1
1	A	324	HIS	3.1
1	B	213[A]	GLN	2.7
1	A	322	ARG	2.2
1	A	323	HIS	2.2
1	B	275	LEU	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 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,

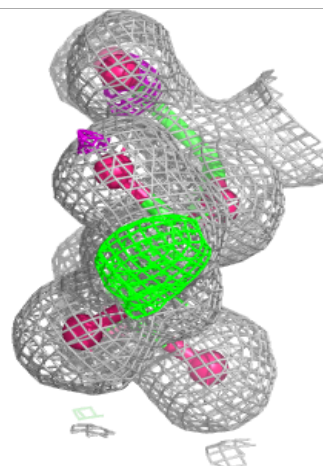
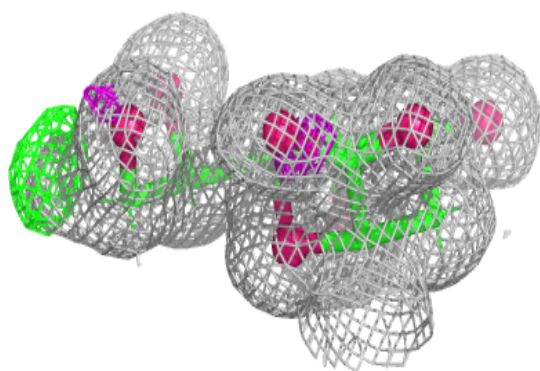
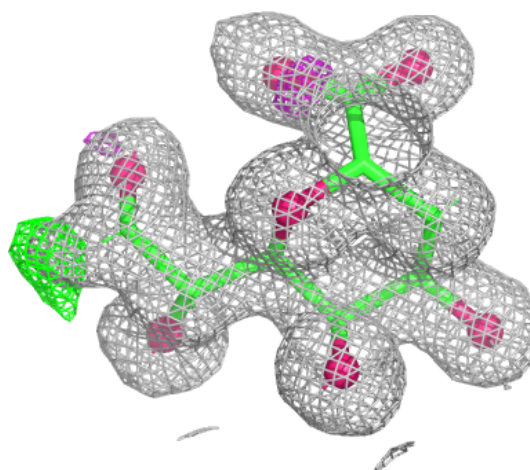
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	KDO	B	404	15/16	0.89	0.11	22,36,43,45	27
7	PO4	B	406	5/5	0.93	0.10	30,33,35,35	5
2	KD3	B	402	15/16	0.97	0.06	12,15,21,25	0
4	PXV	B	403	19/20	0.98	0.04	14,18,21,21	0
2	KD3	A	402	15/16	0.98	0.05	11,14,19,22	0
4	PXV	A	404	20/20	0.98	0.05	14,20,24,25	0
2	KD3	A	401	15/16	0.99	0.03	12,14,16,17	0
5	KDO	A	405	15/16	0.99	0.04	11,13,15,15	0
3	C5P	A	403	21/21	0.99	0.03	9,11,16,18	0
6	CL	B	405	1/1	0.99	0.06	23,23,23,23	1
2	KD3	B	401	16/16	0.99	0.04	12,14,18,19	0
6	CL	A	406	1/1	1.00	0.07	18,18,18,18	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.

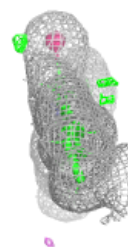
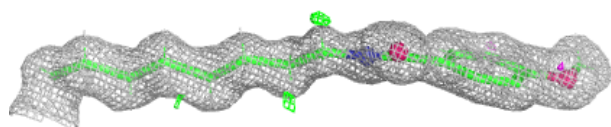
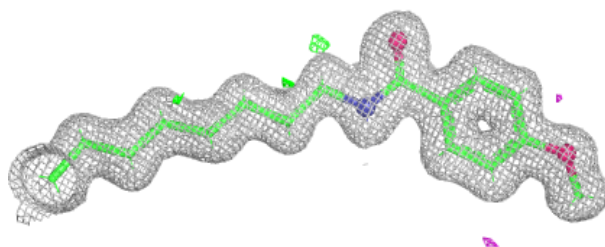
Electron density around KD3 B 402:

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



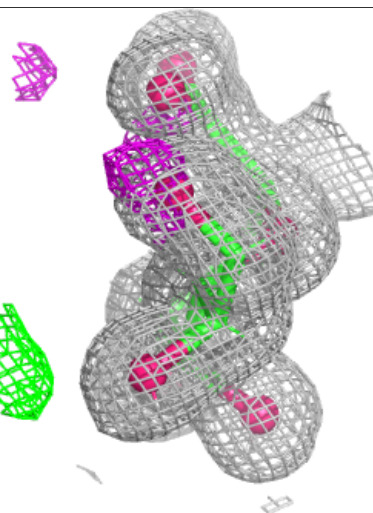
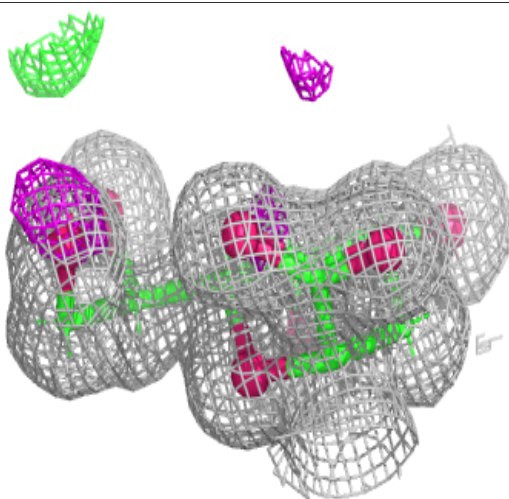
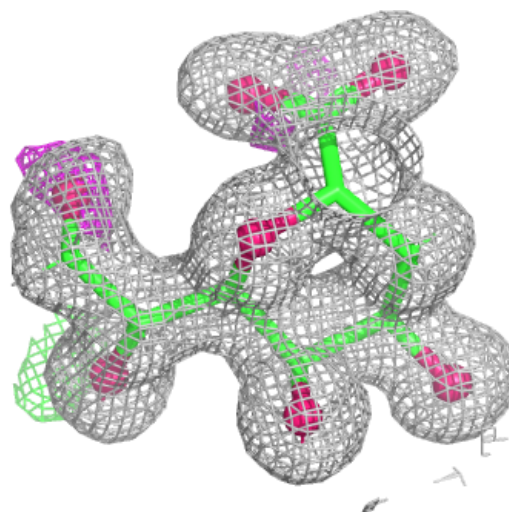
Electron density around PXV B 403:

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



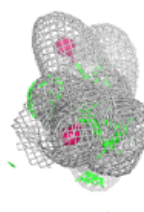
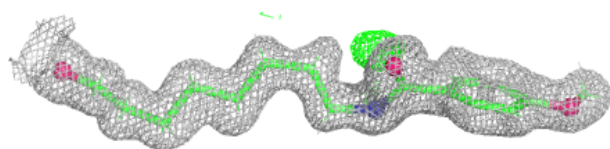
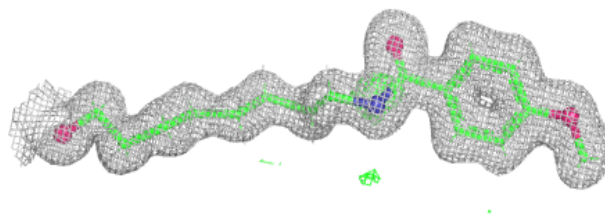
Electron density around KD3 A 402:

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



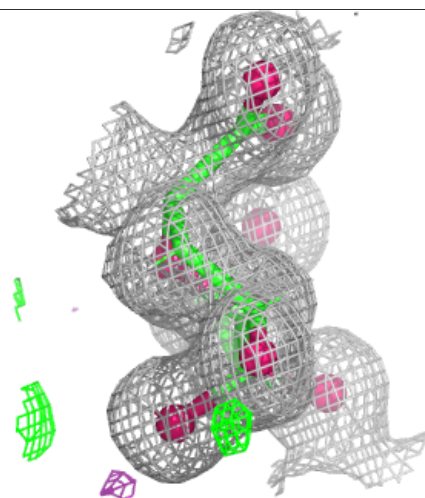
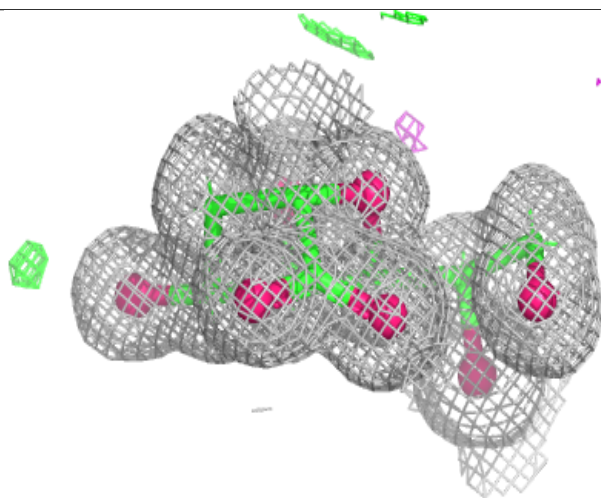
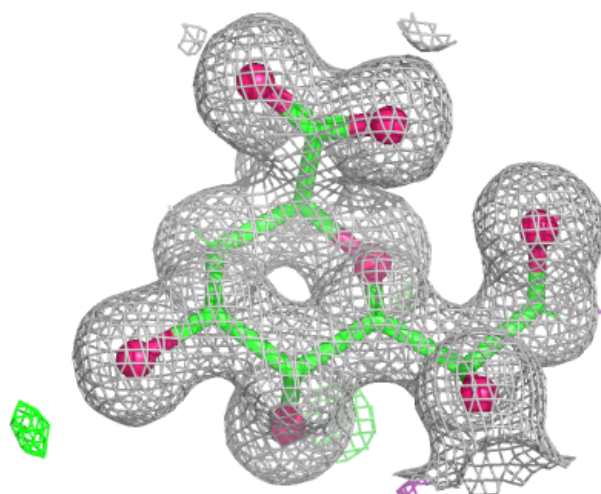
Electron density around PXV A 404:

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



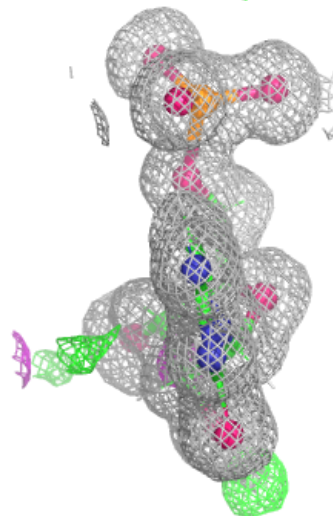
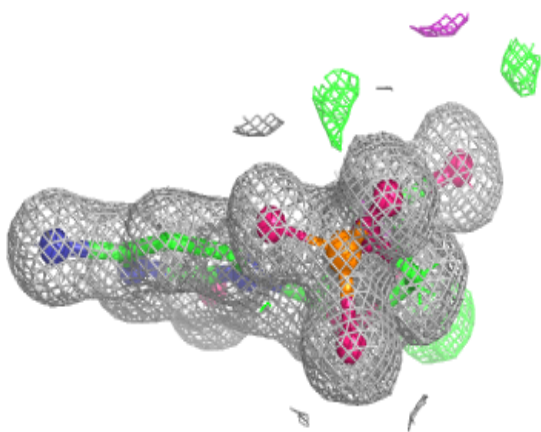
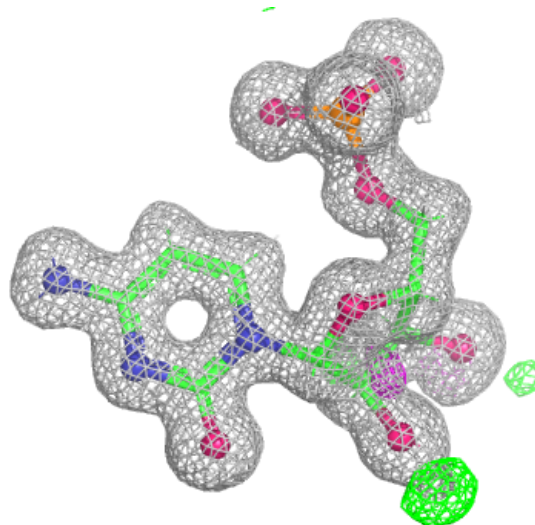
Electron density around KD3 A 401:

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



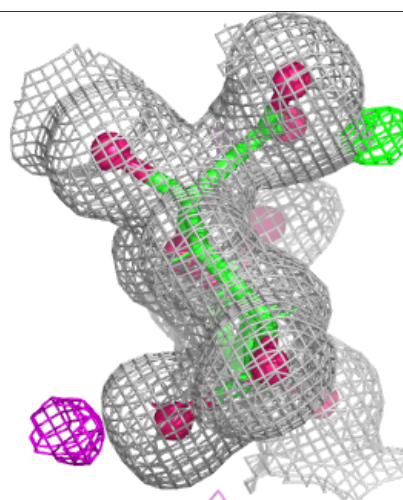
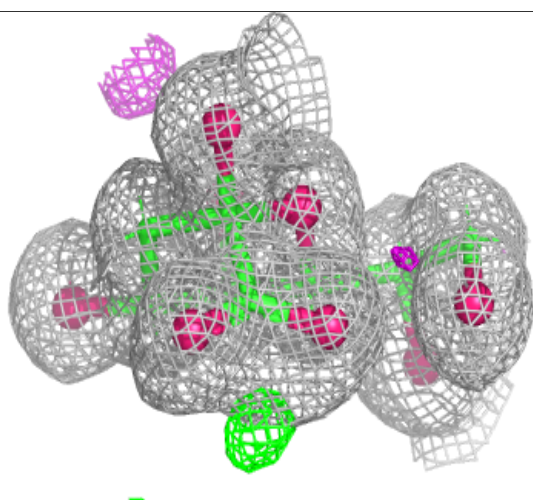
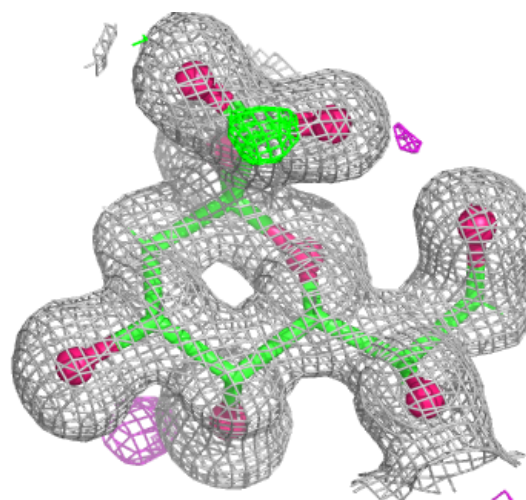
Electron density around C5P A 403:

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



Electron density around KD3 B 401:

$2mF_o-DF_c$ (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.