



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:26 am BST

PDB ID : 6U7A
Title : Rv3722c in complex with kynurenine
Authors : Mandyoli, L.; Sacchettini, J.
Deposited on : 2019-09-01
Resolution : 2.22 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

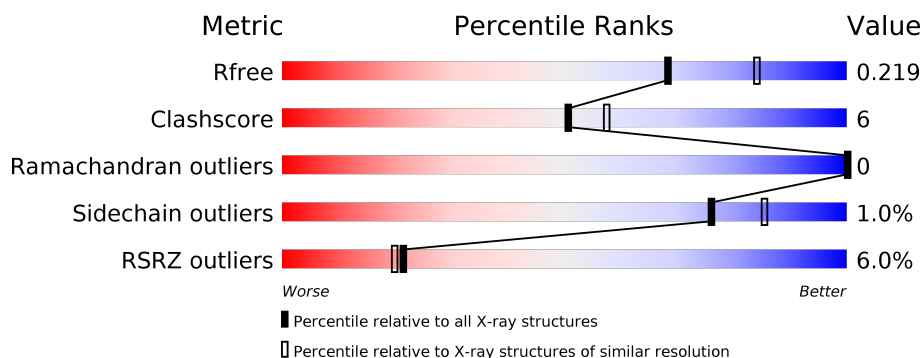
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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	435	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	B	435	<div> <div>5%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	C	435	<div> <div>7%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
1	D	435	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>••</div> </div>
1	E	435	<div> <div>7%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
1	F	435	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	435	
1	H	435	

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
4	GOL	B	503	-	-	X	-
6	KYA	B	501	-	-	X	-
6	KYA	C	501	-	-	X	-
6	KYA	D	501	-	-	X	-
6	KYA	G	501	-	-	X	-
7	PMP	B	502	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27421 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.

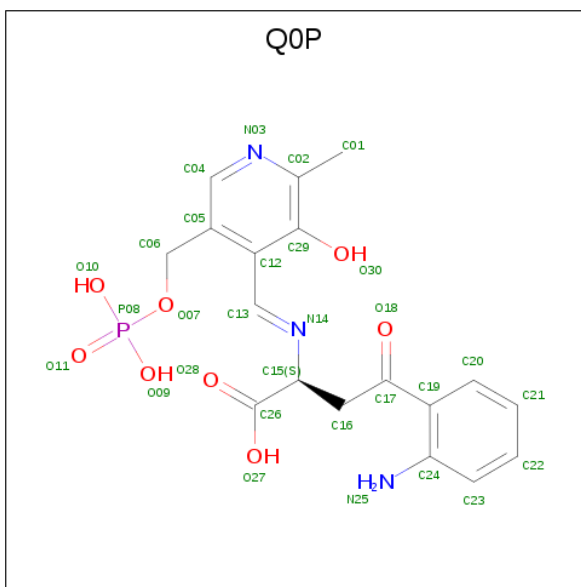
- Molecule 1 is a protein called Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3255	2078	562	604	11			
1	B	423	Total	C	N	O	S	0	0	0
			3255	2078	562	604	11			
1	C	423	Total	C	N	O	S	0	0	0
			3255	2078	562	604	11			
1	D	429	Total	C	N	O	S	0	0	0
			3293	2100	569	613	11			
1	E	423	Total	C	N	O	S	0	0	0
			3255	2078	562	604	11			
1	F	422	Total	C	N	O	S	0	0	0
			3249	2075	561	602	11			
1	G	423	Total	C	N	O	S	0	0	0
			3255	2078	562	604	11			
1	H	416	Total	C	N	O	S	0	0	0
			3202	2046	554	591	11			

There are 8 discrepancies between the modelled and reference sequences:

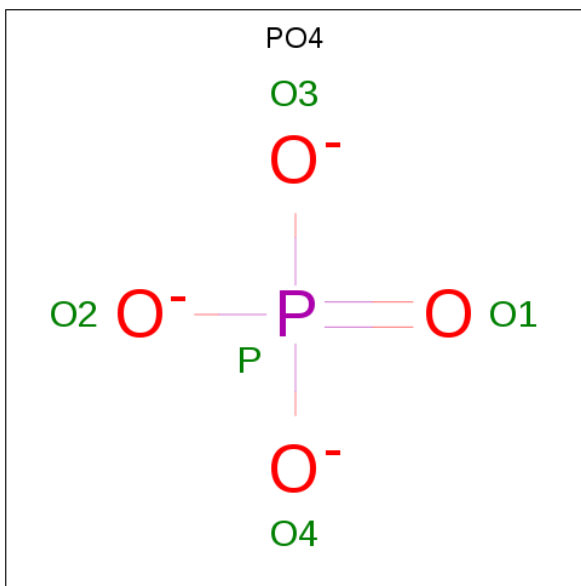
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP A0A0E8TWE4
B	1	VAL	-	expression tag	UNP A0A0E8TWE4
C	1	VAL	-	expression tag	UNP A0A0E8TWE4
D	1	VAL	-	expression tag	UNP A0A0E8TWE4
E	1	VAL	-	expression tag	UNP A0A0E8TWE4
F	1	VAL	-	expression tag	UNP A0A0E8TWE4
G	1	VAL	-	expression tag	UNP A0A0E8TWE4
H	1	VAL	-	expression tag	UNP A0A0E8TWE4

- Molecule 2 is (2S)-4-(2-aminophenyl)-2-[(E)-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene)amino]-4-oxobutanoic acid (three-letter code: Q0P) (formula: C₁₈H₂₀N₃O₈P) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	18	3	8	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



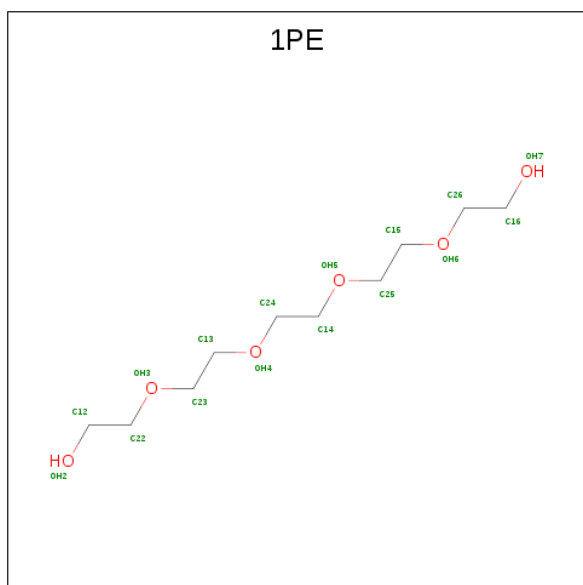
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

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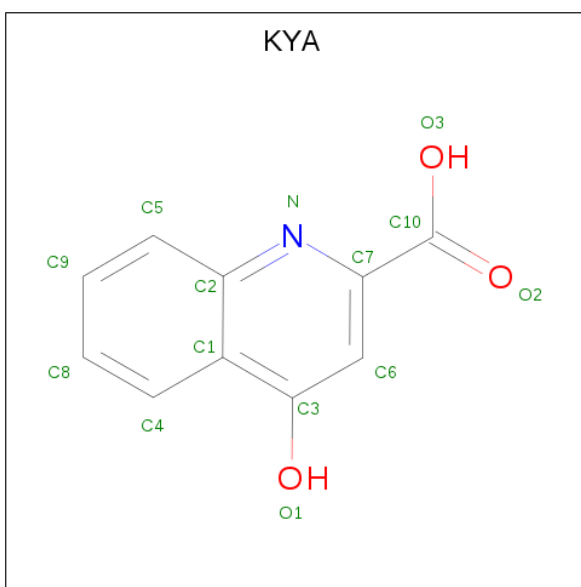
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



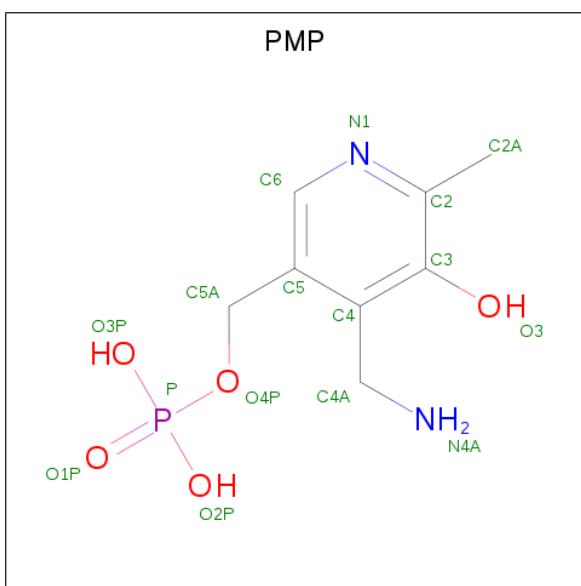
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			16	10	6		
5	D	1	Total	C	O	0	0
			16	10	6		
5	E	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 4-hydroxyquinoline-2-carboxylic acid (three-letter code: KYA) (formula: C₁₀H₇NO₃) (labeled as "Ligand of Interest" by author).



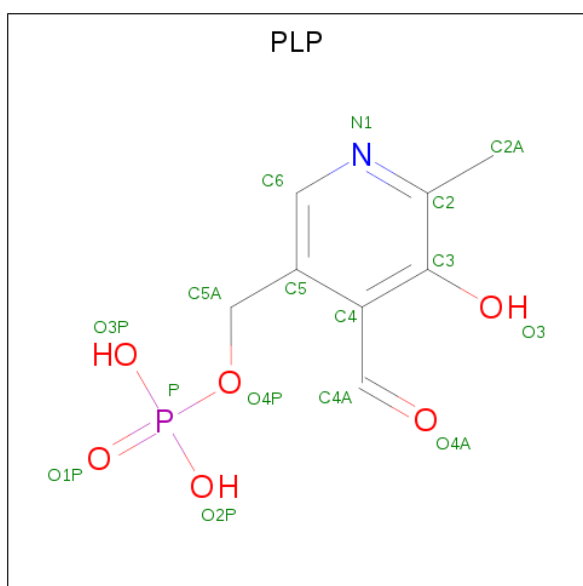
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	10	1	3		
6	C	1	Total	C	N	O	0	0
			14	10	1	3		
6	D	1	Total	C	N	O	0	0
			14	10	1	3		
6	G	1	Total	C	N	O	0	0
			14	10	1	3		

- Molecule 7 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
7	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
7	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
7	G	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 8 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
8	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
8	H	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	145	Total	O	0	0
			145	145		
9	B	122	Total	O	0	0
			122	122		
9	C	136	Total	O	0	0
			136	136		

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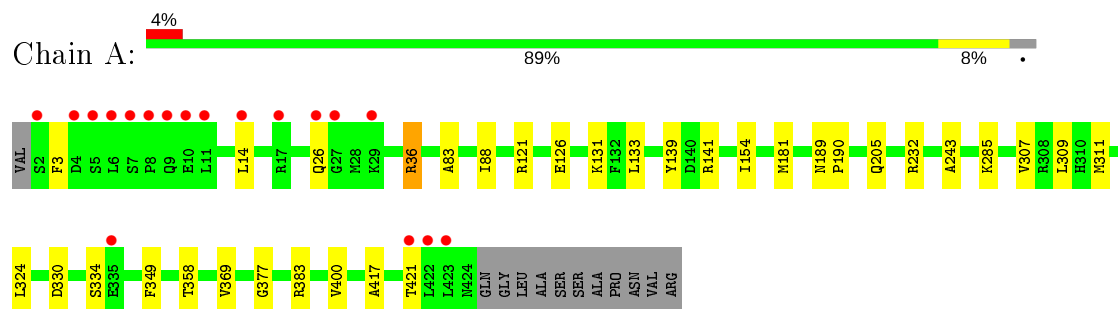
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	144	Total 144	O 144	0	0
9	E	118	Total 118	O 118	0	0
9	F	145	Total 145	O 145	0	0
9	G	122	Total 122	O 122	0	0
9	H	113	Total 113	O 113	0	0

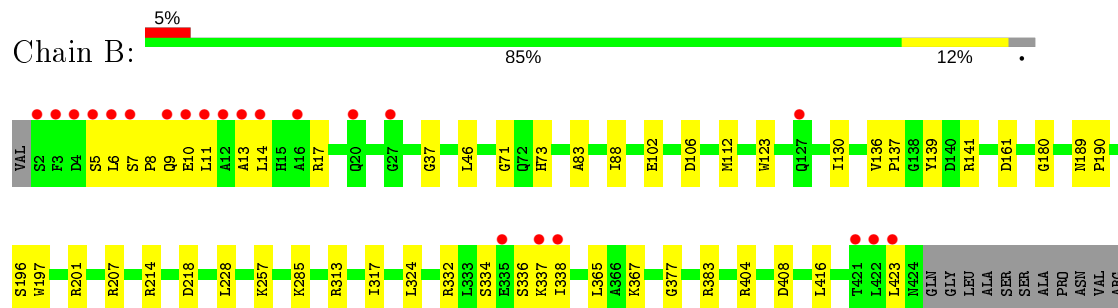
3 Residue-property plots

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.

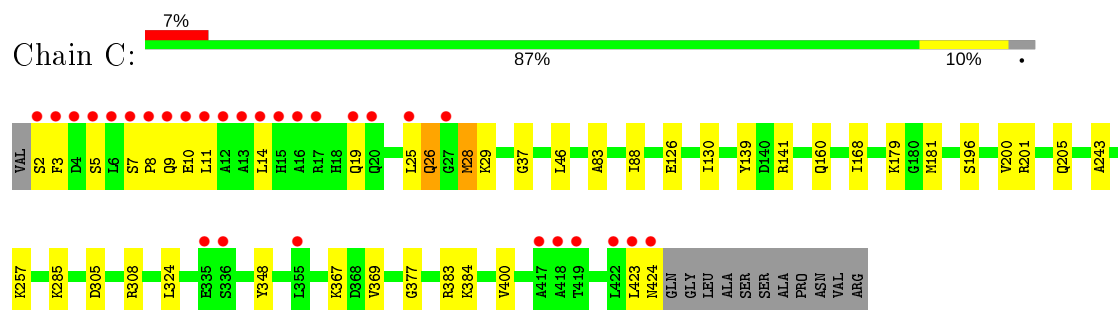
• Molecule 1: Aminotransferase



• Molecule 1: Aminotransferase

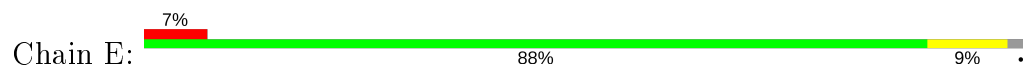


• Molecule 1: Aminotransferase

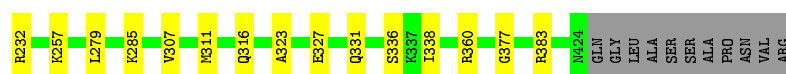
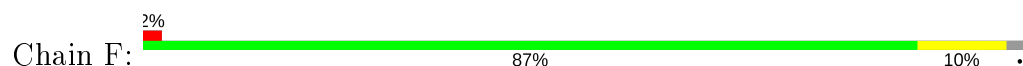




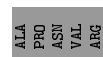
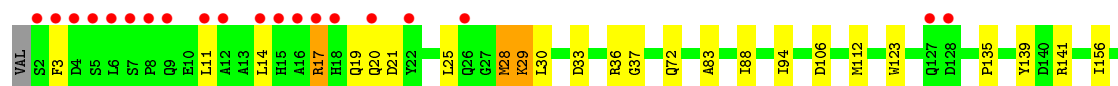
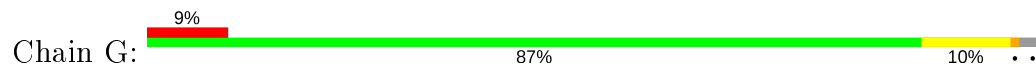
- Molecule 1: Aminotransferase



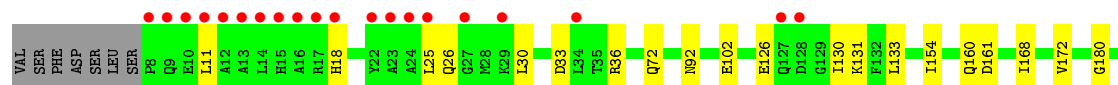
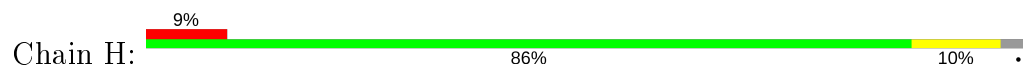
- Molecule 1: Aminotransferase



- Molecule 1: Aminotransferase



- Molecule 1: Aminotransferase



Sequence logo for the 5' region of the 16S rRNA gene. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows nucleotide positions from -10 to 1. The sequence logo shows a strong consensus for the sequence 5'-A417A418T419E420T421L422L423-3'. The nucleotides are color-coded: Adenine (A) in green, Thymine (T) in red, Guanine (G) in blue, and Cytosine (C) in orange. The background is a light gray grid.

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	108.40Å 108.40Å 321.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.46 – 2.22 48.36 – 2.22	Depositor EDS
% Data completeness (in resolution range)	85.2 (32.46-2.22) 85.3 (48.36-2.22)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.178 , 0.219 0.179 , 0.219	Depositor DCC
R_{free} test set	8912 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l 0.027 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27421	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: GOL, PMP, PLP, PO4, 1PE, Q0P, KYA

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	0.52	0/3335	0.74	0/4540
1	B	0.50	0/3335	0.74	0/4540
1	C	0.51	0/3335	0.72	0/4540
1	D	0.47	0/3373	0.73	0/4591
1	E	0.46	0/3335	0.74	0/4540
1	F	0.46	0/3329	0.70	0/4532
1	G	0.46	0/3335	0.73	0/4540
1	H	0.46	0/3281	0.73	0/4466
All	All	0.48	0/26658	0.73	0/36289

There are no bond length outliers.

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	3255	0	3228	24	0
1	B	3255	0	3228	50	0
1	C	3255	0	3228	37	0
1	D	3293	0	3265	38	0
1	E	3255	0	3228	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3249	0	3223	26	0
1	G	3255	0	3228	45	0
1	H	3202	0	3184	26	0
2	A	30	0	0	2	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	G	10	0	0	0	0
3	H	5	0	0	0	0
4	A	12	0	16	1	0
4	B	12	0	16	5	0
4	C	6	0	8	2	0
4	D	6	0	8	2	0
4	G	24	0	31	0	0
5	A	10	0	12	2	0
5	B	16	0	22	5	0
5	D	16	0	22	4	0
5	E	20	0	24	4	0
5	H	7	0	8	2	0
6	B	14	0	6	16	0
6	C	14	0	5	10	0
6	D	14	0	5	11	0
6	G	14	0	6	15	0
7	B	16	0	10	6	0
7	C	16	0	11	3	0
7	D	16	0	11	3	0
7	G	16	0	11	3	0
8	E	16	0	8	1	0
8	F	16	0	8	1	0
8	H	16	0	8	0	0
9	A	145	0	0	2	0
9	B	122	0	0	2	0
9	C	136	0	0	0	0
9	D	144	0	0	0	0
9	E	118	0	0	0	0
9	F	145	0	0	2	0
9	G	122	0	0	1	0
9	H	113	0	0	0	0
All	All	27421	0	26068	300	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 6.

All (300) 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:37:GLY:O	6:C:501:KYA:H5	1.61	0.97
1:D:141:ARG:HH21	6:D:501:KYA:H6	1.25	0.97
1:B:37:GLY:O	6:B:501:KYA:H5	1.65	0.96
1:B:257:LYS:NZ	6:B:501:KYA:H9	1.83	0.92
1:G:28:MET:HE2	1:G:30:LEU:HD21	1.57	0.85
1:G:37:GLY:C	6:G:501:KYA:H5	1.97	0.85
1:B:37:GLY:C	6:B:501:KYA:H5	1.97	0.84
1:C:285:LYS:HE3	1:H:102:GLU:HG3	1.57	0.84
1:C:141:ARG:HH21	6:C:501:KYA:H6	1.44	0.82
1:B:37:GLY:O	6:B:501:KYA:C5	2.30	0.79
1:A:358:THR:HG22	1:A:421:THR:HG21	1.64	0.79
1:B:257:LYS:HZ3	6:B:501:KYA:H9	1.47	0.78
1:G:141:ARG:HH21	6:G:501:KYA:H6	1.49	0.78
1:B:141:ARG:HH21	6:B:501:KYA:H6	1.50	0.76
1:D:285:LYS:HE3	1:E:102:GLU:HG3	1.67	0.75
6:B:501:KYA:C4	7:B:502:PMP:H4A1	2.16	0.75
6:D:501:KYA:C8	7:D:502:PMP:H4A1	2.18	0.74
1:D:384:LYS:HZ3	5:D:505:1PE:H241	1.53	0.74
1:E:190:PRO:HB3	1:E:349:PHE:CB	2.18	0.73
1:C:384:LYS:HD2	4:C:504:GOL:H31	1.69	0.72
1:G:112:MET:CE	1:G:123:TRP:HB2	2.20	0.71
1:D:141:ARG:NH2	6:D:501:KYA:H6	2.05	0.71
1:C:3:PHE:CE2	1:C:14:LEU:HD21	2.26	0.70
1:E:7:SER:OG	1:E:10:GLU:N	2.20	0.70
1:B:257:LYS:HZ1	6:B:501:KYA:H9	1.54	0.69
1:E:166:ASP:O	1:E:170:GLU:HG3	1.93	0.69
1:B:257:LYS:NZ	6:B:501:KYA:C9	2.56	0.69
1:E:313:ARG:HH12	5:E:503:1PE:H241	1.56	0.68
1:A:26:GLN:HB3	1:A:369:VAL:HG12	1.76	0.68
1:F:198:GLU:OE2	1:F:201:ARG:NH2	2.20	0.67
1:G:37:GLY:O	6:G:501:KYA:H5	1.94	0.67
1:B:257:LYS:HZ1	6:B:501:KYA:C9	2.08	0.67
1:C:37:GLY:C	6:C:501:KYA:H5	2.15	0.67
1:E:189:ASN:OD1	1:E:349:PHE:CD2	2.47	0.67
1:D:37:GLY:O	6:D:501:KYA:H5	1.96	0.66
1:E:33:ASP:HB3	1:E:36:ARG:CZ	2.26	0.66
1:H:161:ASP:HB3	1:H:196:SER:HB3	1.78	0.65
1:G:324:LEU:HD22	1:G:400:VAL:HG13	1.76	0.65
1:G:37:GLY:CA	6:G:501:KYA:H5	2.27	0.65
1:B:257:LYS:HE3	7:B:502:PMP:HNA2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:HH21	2:A:501:Q0P:C20	2.10	0.64
5:B:505:1PE:H142	1:C:46:LEU:HD23	1.80	0.64
1:E:190:PRO:HG3	1:E:392:ARG:HG3	1.80	0.64
1:B:46:LEU:HD23	5:B:505:1PE:H152	1.80	0.63
1:G:37:GLY:HA3	6:G:501:KYA:C9	2.28	0.63
1:C:139:TYR:CE1	6:C:501:KYA:H4	2.33	0.63
1:B:313:ARG:HG2	5:B:505:1PE:H222	1.82	0.62
5:A:505:1PE:H242	9:A:638:HOH:O	2.00	0.61
1:C:141:ARG:NE	6:C:501:KYA:O1	2.28	0.61
1:D:127:GLN:CD	1:D:127:GLN:H	2.04	0.61
1:D:323:ALA:O	1:D:327:GLU:HG3	2.01	0.61
1:C:7:SER:O	1:C:10:GLU:N	2.33	0.60
6:C:501:KYA:C4	7:C:502:PMP:H4A1	2.32	0.60
1:C:5:SER:O	1:C:5:SER:OG	2.11	0.60
1:E:400:VAL:CG2	1:E:401:PRO:HD3	2.31	0.60
1:D:375:GLU:HG3	1:D:378:ALA:HB2	1.84	0.60
1:F:3:PHE:CE1	1:F:14:LEU:HD21	2.36	0.60
1:B:218:ASP:OD2	7:B:502:PMP:N1	2.35	0.59
1:B:37:GLY:O	6:B:501:KYA:C9	2.50	0.59
1:D:384:LYS:NZ	5:D:505:1PE:H241	2.17	0.59
1:G:112:MET:CE	1:G:123:TRP:CB	2.81	0.59
1:E:33:ASP:HB3	1:E:36:ARG:NH2	2.18	0.59
1:H:189:ASN:OD1	1:H:349:PHE:CD2	2.56	0.59
1:C:324:LEU:HD22	1:C:400:VAL:HG13	1.84	0.59
1:H:360:ARG:HG3	1:H:388:ASP:OD1	2.02	0.59
1:E:190:PRO:CB	1:E:349:PHE:HB2	2.32	0.59
1:C:257:LYS:NZ	7:C:502:PMP:HNA2	2.01	0.58
1:G:349:PHE:HZ	6:G:501:KYA:H9	1.67	0.58
1:C:141:ARG:NH2	6:C:501:KYA:H6	2.16	0.58
1:G:349:PHE:HZ	6:G:501:KYA:C9	2.17	0.58
4:A:504:GOL:O1	1:F:360:ARG:NH1	2.37	0.57
1:G:37:GLY:HA3	6:G:501:KYA:H9	1.86	0.57
1:G:83:ALA:HB1	1:G:88:ILE:O	2.04	0.57
1:E:190:PRO:HB3	1:E:349:PHE:HB2	1.87	0.57
1:G:112:MET:HE2	1:G:123:TRP:HB2	1.86	0.57
1:B:73:HIS:HB2	4:B:503:GOL:H32	1.87	0.57
1:E:190:PRO:CB	1:E:349:PHE:CB	2.83	0.57
1:C:367:LYS:HE3	1:D:239:LEU:HD21	1.87	0.57
1:G:141:ARG:NE	6:G:501:KYA:O1	2.35	0.56
1:B:141:ARG:NH2	6:B:501:KYA:H6	2.19	0.56
1:A:36:ARG:HG2	2:A:501:Q0P:C23	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLY:O	6:C:501:KYA:C5	2.46	0.56
1:F:257:LYS:NZ	8:F:501:PLP:O4A	2.28	0.56
1:G:17:ARG:O	1:G:20:GLN:HG2	2.06	0.56
1:C:11:LEU:HD23	1:C:423:LEU:HD23	1.88	0.56
1:G:141:ARG:NH2	6:G:501:KYA:H6	2.20	0.56
1:B:367:LYS:HG2	1:G:197:TRP:CG	2.42	0.55
1:F:327:GLU:O	1:F:331:GLN:HG3	2.06	0.55
1:C:83:ALA:HB1	1:C:88:ILE:O	2.06	0.55
1:A:189:ASN:OD1	1:A:349:PHE:CD2	2.60	0.55
1:H:25:LEU:HD23	1:H:25:LEU:O	2.06	0.55
1:F:336:SER:OG	1:F:338:ILE:HG12	2.07	0.55
1:E:377:GLY:O	1:E:383:ARG:HA	2.07	0.54
1:D:10:GLU:O	1:D:14:LEU:HB2	2.08	0.54
1:B:334:SER:O	1:B:337:LYS:HD2	2.08	0.54
1:D:257:LYS:HZ1	6:D:501:KYA:H9	1.73	0.54
1:G:37:GLY:O	6:G:501:KYA:C5	2.55	0.54
1:A:131:LYS:HD3	1:A:154:ILE:HD11	1.89	0.54
1:G:257:LYS:HE2	7:G:502:PMP:N4A	2.23	0.54
1:F:201:ARG:NH1	1:F:205:GLN:OE1	2.40	0.54
1:E:293:ASN:OD1	1:E:296:ARG:HD2	2.09	0.53
1:D:327:GLU:O	1:D:331:GLN:HG3	2.09	0.53
1:E:133:LEU:HD22	1:E:156:ILE:HD11	1.90	0.53
1:C:7:SER:O	1:C:8:PRO:C	2.45	0.53
1:E:17:ARG:HA	1:E:20:GLN:HG2	1.89	0.53
1:E:364:ALA:HB1	1:H:201:ARG:CZ	2.39	0.53
1:F:133:LEU:HB2	1:F:181:MET:HG3	1.91	0.53
1:B:37:GLY:O	6:B:501:KYA:H9	2.09	0.53
1:C:26:GLN:HG2	1:C:369:VAL:HG12	1.90	0.53
1:E:190:PRO:HG3	1:E:392:ARG:CD	2.38	0.53
1:G:112:MET:HE1	1:G:123:TRP:HB2	1.89	0.53
1:H:324:LEU:HD22	1:H:400:VAL:HG13	1.92	0.52
1:C:7:SER:O	1:C:9:GLN:N	2.42	0.52
1:G:336:SER:OG	1:G:338:ILE:HG12	2.10	0.52
1:H:33:ASP:HB3	1:H:36:ARG:NH2	2.25	0.52
1:A:83:ALA:HB1	1:A:88:ILE:O	2.10	0.51
1:A:205:GLN:HG2	1:A:243:ALA:HB2	1.93	0.51
1:E:7:SER:OG	1:E:10:GLU:HB2	2.10	0.51
1:E:189:ASN:OD1	1:E:349:PHE:CE2	2.62	0.51
1:D:257:LYS:NZ	7:D:502:PMP:HNA2	2.08	0.51
1:H:72:GLN:HB3	1:H:279:LEU:HD22	1.93	0.51
1:E:3:PHE:O	1:E:6:LEU:HD11	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:SER:O	1:B:5:SER:OG	2.26	0.51
1:G:37:GLY:CA	6:G:501:KYA:C5	2.88	0.51
1:E:325:VAL:HG22	1:E:407:VAL:HG21	1.92	0.51
1:G:112:MET:HE1	1:G:123:TRP:CB	2.41	0.51
1:B:11:LEU:HD23	1:B:423:LEU:HD23	1.93	0.50
1:G:197:TRP:CH2	1:G:201:ARG:HD3	2.46	0.50
1:D:131:LYS:HD3	1:D:154:ILE:HD11	1.94	0.50
1:D:139:TYR:CE1	6:D:501:KYA:H4	2.46	0.50
1:D:382:TYR:CG	5:D:505:1PE:H242	2.46	0.50
1:F:316:GLN:HG3	9:F:740:HOH:O	2.11	0.50
1:C:424:ASN:N	1:C:424:ASN:OD1	2.35	0.50
1:G:37:GLY:HA3	6:G:501:KYA:C5	2.42	0.50
1:G:337:LYS:O	1:G:337:LYS:HG3	2.12	0.49
1:D:37:GLY:O	6:D:501:KYA:C5	2.60	0.49
1:B:9:GLN:O	1:B:13:ALA:N	2.36	0.49
6:B:501:KYA:H4	7:B:502:PMP:H4A1	1.93	0.49
1:C:168:ILE:HG12	1:C:181:MET:HE3	1.93	0.49
1:B:317:ILE:HD11	5:B:505:1PE:H131	1.94	0.49
1:A:330:ASP:OD1	1:A:334:SER:OG	2.26	0.49
1:F:161:ASP:HB3	1:F:196:SER:HB3	1.94	0.49
1:E:400:VAL:HG23	1:E:401:PRO:HD3	1.94	0.48
1:B:365:LEU:HD13	1:B:416:LEU:HD12	1.95	0.48
1:E:307:VAL:O	1:E:311:MET:HG2	2.13	0.48
1:G:3:PHE:CE1	1:G:14:LEU:HD21	2.49	0.48
1:B:14:LEU:O	1:B:17:ARG:HB3	2.13	0.48
1:A:139:TYR:OH	1:A:141:ARG:HD2	2.13	0.47
1:E:190:PRO:CG	1:E:392:ARG:HG3	2.44	0.47
1:D:141:ARG:HE	6:D:501:KYA:C3	2.28	0.47
1:C:19:GLN:OE1	1:C:19:GLN:HA	2.14	0.47
1:G:11:LEU:HD23	1:G:423:LEU:HD23	1.97	0.47
1:D:37:GLY:O	1:D:257:LYS:HE2	2.15	0.47
1:D:123:TRP:HB3	1:D:130:ILE:HG13	1.97	0.47
1:D:83:ALA:HB1	1:D:88:ILE:O	2.13	0.47
1:E:190:PRO:HG3	1:E:392:ARG:CG	2.44	0.47
1:H:373:VAL:HG21	1:H:410:LEU:HD13	1.96	0.47
1:A:3:PHE:CZ	1:A:14:LEU:HD21	2.50	0.47
1:D:161:ASP:OD1	1:D:161:ASP:N	2.45	0.47
1:C:257:LYS:HD3	1:C:348:TYR:CE1	2.49	0.47
1:D:377:GLY:O	1:D:383:ARG:HA	2.15	0.47
1:F:6:LEU:HD22	1:F:10:GLU:HB3	1.97	0.47
1:G:20:GLN:HG3	1:G:21:ASP:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HA	1:B:6:LEU:HD12	1.47	0.46
1:D:3:PHE:O	1:D:6:LEU:HD22	2.14	0.46
1:E:3:PHE:HA	1:E:6:LEU:HD21	1.97	0.46
1:D:325:VAL:HG22	1:D:407:VAL:HG21	1.98	0.46
1:F:136:VAL:HA	1:F:137:PRO:C	2.36	0.46
1:E:23:ALA:HA	1:E:26:GLN:HG3	1.97	0.46
1:E:336:SER:OG	1:E:338:ILE:HG12	2.16	0.46
1:A:285:LYS:NZ	1:B:102:GLU:HG3	2.31	0.46
1:B:336:SER:OG	1:B:338:ILE:HG12	2.16	0.46
1:H:384:LYS:NZ	5:H:503:1PE:H241	2.31	0.46
1:C:305:ASP:OD1	1:C:308:ARG:NH1	2.49	0.46
1:A:324:LEU:HD22	1:A:400:VAL:HG13	1.98	0.45
1:G:257:LYS:HE2	7:G:502:PMP:HNA2	1.80	0.45
1:A:377:GLY:O	1:A:383:ARG:HA	2.17	0.45
4:B:504:GOL:H12	9:B:607:HOH:O	2.16	0.45
1:E:400:VAL:HG22	1:E:401:PRO:HD3	1.99	0.45
1:A:309:LEU:HD12	1:D:312:LEU:HD12	1.98	0.45
1:D:226:LEU:HG	1:D:346:GLY:HA2	1.99	0.45
1:F:6:LEU:HD22	1:F:10:GLU:CB	2.46	0.45
1:F:285:LYS:HE2	1:G:106:ASP:OD1	2.16	0.45
1:E:257:LYS:HE3	8:E:501:PLP:O4A	2.17	0.45
1:C:384:LYS:HZ1	4:C:504:GOL:H11	1.80	0.45
1:D:112:MET:HA	1:D:123:TRP:HB2	1.99	0.45
1:F:377:GLY:O	1:F:383:ARG:HA	2.17	0.45
1:B:7:SER:OG	1:B:10:GLU:OE1	2.35	0.44
1:E:50:LEU:HD11	1:E:259:THR:HB	1.98	0.44
5:B:505:1PE:H132	5:B:505:1PE:H141	1.72	0.44
1:G:355:LEU:HD12	1:G:356:PRO:HD2	1.98	0.44
1:B:257:LYS:HE3	7:B:502:PMP:N4A	2.30	0.44
1:H:180:GLY:HA2	1:H:214:ARG:O	2.17	0.44
1:E:189:ASN:CG	1:E:349:PHE:CE2	2.90	0.44
1:A:307:VAL:O	1:A:311:MET:HG2	2.18	0.44
1:B:136:VAL:HA	1:B:137:PRO:C	2.38	0.44
6:D:501:KYA:C4	7:D:502:PMP:H4A1	2.46	0.44
1:B:112:MET:HA	1:B:123:TRP:HB2	1.99	0.44
1:C:205:GLN:HG2	1:C:243:ALA:HB2	2.00	0.44
1:H:345:LYS:HD3	1:H:345:LYS:HA	1.62	0.44
4:B:503:GOL:H31	9:B:620:HOH:O	2.18	0.44
6:B:501:KYA:C8	7:B:502:PMP:H4A1	2.48	0.44
1:B:73:HIS:H	4:B:503:GOL:C3	2.31	0.43
1:G:29:LYS:HE3	1:G:29:LYS:HB2	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:GLY:O	1:B:383:ARG:HA	2.18	0.43
6:D:501:KYA:O1	4:D:504:GOL:O1	2.35	0.43
6:D:501:KYA:C3	4:D:504:GOL:HO1	2.31	0.43
1:B:161:ASP:HB2	1:B:196:SER:HB3	2.01	0.43
1:G:33:ASP:HB3	1:G:36:ARG:NH2	2.32	0.43
1:B:332:ARG:NH1	1:B:408:ASP:OD2	2.47	0.43
1:D:293:ASN:OD1	1:D:296:ARG:HD2	2.18	0.43
1:D:257:LYS:HD2	1:D:348:TYR:CZ	2.54	0.43
1:E:313:ARG:HH11	1:E:313:ARG:HD2	1.66	0.43
1:H:207:ARG:HA	1:H:207:ARG:CZ	2.48	0.43
1:B:71:GLY:HA3	4:B:503:GOL:H12	2.00	0.43
1:C:139:TYR:HE1	6:C:501:KYA:H4	1.79	0.43
1:G:139:TYR:CZ	1:G:141:ARG:HB2	2.53	0.43
1:H:30:LEU:O	1:H:370:GLY:HA3	2.18	0.43
1:B:83:ALA:HB1	1:B:88:ILE:O	2.18	0.43
1:C:168:ILE:CD1	1:C:181:MET:HE1	2.49	0.43
1:D:384:LYS:HZ2	5:D:505:1PE:H231	1.81	0.43
1:G:330:ASP:O	1:G:334:SER:OG	2.37	0.43
1:C:126:GLU:HG3	1:C:130:ILE:HD11	2.01	0.43
1:E:135:PRO:HA	1:E:156:ILE:O	2.18	0.43
1:E:3:PHE:N	1:E:3:PHE:CD2	2.87	0.43
1:H:377:GLY:O	1:H:383:ARG:HA	2.19	0.43
1:B:228:LEU:N	1:B:228:LEU:HD12	2.34	0.42
1:E:190:PRO:HB3	1:E:349:PHE:CG	2.54	0.42
1:F:18:HIS:HE1	9:F:730:HOH:O	2.02	0.42
1:F:3:PHE:O	1:F:6:LEU:HB2	2.19	0.42
1:D:257:LYS:HD2	1:D:348:TYR:CE2	2.53	0.42
1:G:25:LEU:HA	1:G:28:MET:HG3	2.00	0.42
1:A:417:ALA:O	1:A:421:THR:HG23	2.19	0.42
1:C:3:PHE:CZ	1:C:14:LEU:HD21	2.54	0.42
1:E:3:PHE:N	1:E:3:PHE:HD2	2.17	0.42
1:H:131:LYS:HD3	1:H:154:ILE:HD11	2.02	0.42
1:B:7:SER:O	1:B:10:GLU:HB3	2.20	0.42
1:C:25:LEU:HA	1:C:28:MET:HG3	2.01	0.42
1:E:3:PHE:CZ	1:E:14:LEU:HD21	2.54	0.42
1:E:190:PRO:HB3	1:E:349:PHE:HB3	1.99	0.42
1:E:36:ARG:HD3	1:E:36:ARG:HH11	1.73	0.42
1:F:142:HIS:NE2	1:F:218:ASP:OD2	2.49	0.42
1:A:232:ARG:NH2	9:A:613:HOH:O	2.51	0.42
1:D:135:PRO:HG3	1:D:181:MET:HE2	2.01	0.42
1:G:384:LYS:NZ	9:G:602:HOH:O	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:349:PHE:CZ	6:G:501:KYA:H9	2.51	0.42
1:C:377:GLY:O	1:C:383:ARG:HA	2.19	0.42
6:C:501:KYA:C8	7:C:502:PMP:H4A1	2.49	0.42
1:E:190:PRO:HG3	1:E:392:ARG:HD2	2.02	0.42
1:F:323:ALA:O	1:F:327:GLU:HG3	2.19	0.42
1:A:189:ASN:HA	1:A:190:PRO:HA	1.67	0.42
1:F:189:ASN:HA	1:F:190:PRO:HA	1.92	0.42
1:B:123:TRP:HB3	1:B:130:ILE:HG13	2.02	0.42
1:H:92:ASN:O	1:H:269:GLY:HA2	2.20	0.42
1:A:121:ARG:NH1	1:A:126:GLU:OE2	2.45	0.41
1:B:7:SER:HA	1:B:8:PRO:HD3	1.93	0.41
1:C:196:SER:O	1:C:200:VAL:HG23	2.20	0.41
1:C:257:LYS:HD3	1:C:348:TYR:CZ	2.55	0.41
1:D:36:ARG:HG2	1:D:36:ARG:H	1.61	0.41
5:E:503:1PE:H241	5:E:503:1PE:H231	1.76	0.41
1:G:94:ILE:HG21	1:G:94:ILE:HD13	1.83	0.41
1:A:190:PRO:HB3	1:A:349:PHE:CB	2.50	0.41
6:G:501:KYA:C4	7:G:502:PMP:H4A1	2.50	0.41
1:H:168:ILE:O	1:H:172:VAL:HG22	2.20	0.41
1:B:189:ASN:HA	1:B:190:PRO:HA	1.95	0.41
1:C:130:ILE:HD12	1:C:179:LYS:HG3	2.02	0.41
1:D:106:ASP:OD2	1:D:285:LYS:NZ	2.50	0.41
1:F:307:VAL:O	1:F:311:MET:HG2	2.21	0.41
1:A:133:LEU:HD23	1:A:154:ILE:HB	2.01	0.41
1:D:136:VAL:HA	1:D:137:PRO:C	2.41	0.41
1:E:161:ASP:HB3	1:E:196:SER:HB3	2.01	0.41
1:E:46:LEU:HD23	5:E:502:1PE:H241	2.02	0.41
1:F:135:PRO:HA	1:F:156:ILE:O	2.20	0.41
1:B:14:LEU:HA	1:B:14:LEU:HD12	1.78	0.41
1:E:313:ARG:NH1	5:E:503:1PE:H241	2.30	0.41
1:B:180:GLY:HA2	1:B:214:ARG:O	2.20	0.41
1:D:168:ILE:O	1:D:172:VAL:HG22	2.20	0.41
1:F:72:GLN:HB3	1:F:279:LEU:HD22	2.03	0.41
1:F:28:MET:HB3	1:F:28:MET:HE2	1.77	0.41
1:H:189:ASN:HA	1:H:190:PRO:HA	1.61	0.41
1:A:139:TYR:CZ	1:A:141:ARG:HB2	2.55	0.41
1:B:197:TRP:CH2	1:B:201:ARG:HD2	2.56	0.41
1:G:72:GLN:HB3	1:G:279:LEU:HD22	2.02	0.41
1:F:49:GLN:OE1	1:F:53:LEU:HD11	2.20	0.41
1:B:37:GLY:C	6:B:501:KYA:C5	2.79	0.41
1:G:168:ILE:O	1:G:172:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:LEU:HD23	1:H:154:ILE:HB	2.02	0.41
1:H:25:LEU:C	1:H:25:LEU:HD23	2.42	0.41
1:H:384:LYS:HZ2	5:H:503:1PE:H241	1.86	0.41
1:F:83:ALA:HB1	1:F:88:ILE:O	2.20	0.40
1:H:126:GLU:HG3	1:H:130:ILE:HD11	2.04	0.40
1:B:139:TYR:CZ	1:B:141:ARG:HB2	2.56	0.40
1:G:135:PRO:HA	1:G:156:ILE:O	2.20	0.40
1:B:106:ASP:OD2	1:B:285:LYS:HE2	2.20	0.40
1:B:324:LEU:HD21	1:B:404:ARG:HB2	2.03	0.40
1:H:11:LEU:HD21	1:H:422:LEU:HB3	2.03	0.40
1:H:18:HIS:CE1	1:H:415:LEU:HB3	2.56	0.40
1:A:133:LEU:HB2	1:A:181:MET:HG3	2.02	0.40
5:A:505:1PE:H252	5:A:505:1PE:H241	1.86	0.40
1:G:180:GLY:HA2	1:G:214:ARG:O	2.21	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	421/435 (97%)	411 (98%)	10 (2%)	0	100	100
1	B	421/435 (97%)	412 (98%)	9 (2%)	0	100	100
1	C	421/435 (97%)	414 (98%)	7 (2%)	0	100	100
1	D	427/435 (98%)	419 (98%)	8 (2%)	0	100	100
1	E	421/435 (97%)	413 (98%)	8 (2%)	0	100	100
1	F	420/435 (97%)	411 (98%)	9 (2%)	0	100	100
1	G	421/435 (97%)	412 (98%)	9 (2%)	0	100	100
1	H	414/435 (95%)	406 (98%)	8 (2%)	0	100	100
All	All	3366/3480 (97%)	3298 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	343/352 (97%)	342 (100%)	1 (0%)	92	96
1	B	343/352 (97%)	342 (100%)	1 (0%)	92	96
1	C	343/352 (97%)	337 (98%)	6 (2%)	60	73
1	D	347/352 (99%)	342 (99%)	5 (1%)	67	78
1	E	343/352 (97%)	340 (99%)	3 (1%)	78	87
1	F	342/352 (97%)	340 (99%)	2 (1%)	86	92
1	G	343/352 (97%)	339 (99%)	4 (1%)	71	82
1	H	336/352 (96%)	331 (98%)	5 (2%)	65	76
All	All	2740/2816 (97%)	2713 (99%)	27 (1%)	76	85

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	B	207	ARG
1	C	2	SER
1	C	26	GLN
1	C	28	MET
1	C	29	LYS
1	C	160	GLN
1	C	201	ARG
1	D	3	PHE
1	D	6	LEU
1	D	14	LEU
1	D	17	ARG
1	D	36	ARG
1	E	6	LEU
1	E	10	GLU
1	E	207	ARG

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Mol	Chain	Res	Type
1	F	207	ARG
1	F	232	ARG
1	G	17	ARG
1	G	19	GLN
1	G	28	MET
1	G	29	LYS
1	H	26	GLN
1	H	160	GLN
1	H	207	ARG
1	H	334	SER
1	H	337	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	205	GLN
1	H	19	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

34 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$
4	GOL	A	504	-	5,5,5	0.81	0	5,5,5	0.95	0
3	PO4	G	503	-	4,4,4	1.03	0	6,6,6	0.56	0
6	KYA	B	501	-	12,15,15	2.63	6 (50%)	16,21,21	2.88	6 (37%)
3	PO4	H	502	-	4,4,4	0.85	0	6,6,6	0.53	0
6	KYA	G	501	-	12,15,15	1.98	4 (33%)	16,21,21	1.55	5 (31%)
5	1PE	D	505	-	15,15,15	0.53	0	14,14,14	0.39	0
4	GOL	B	504	-	5,5,5	1.36	0	5,5,5	0.80	0
4	GOL	A	503	-	5,5,5	1.09	0	5,5,5	0.75	0
6	KYA	C	501	-	12,15,15	2.59	3 (25%)	16,21,21	2.49	3 (18%)
4	GOL	C	504	-	5,5,5	1.08	0	5,5,5	0.63	0
3	PO4	C	503	-	4,4,4	0.96	0	6,6,6	0.70	0
3	PO4	A	502	-	4,4,4	1.16	0	6,6,6	0.82	0
4	GOL	B	503	-	5,5,5	1.18	0	5,5,5	1.01	0
7	PMP	G	502	-	16,16,16	0.95	1 (6%)	21,23,23	1.34	2 (9%)
5	1PE	H	503	-	6,6,15	0.47	0	5,5,14	0.38	0
8	PLP	F	501	-	16,16,16	1.20	2 (12%)	20,23,23	1.34	4 (20%)
3	PO4	D	503	-	4,4,4	0.85	0	6,6,6	0.91	0
5	1PE	B	505	-	15,15,15	0.52	0	14,14,14	0.63	0
4	GOL	G	507	-	5,5,5	1.45	1 (20%)	5,5,5	0.83	0
7	PMP	B	502	-	16,16,16	2.88	3 (18%)	21,23,23	1.21	1 (4%)
6	KYA	D	501	-	12,15,15	3.11	6 (50%)	16,21,21	2.96	4 (25%)
5	1PE	A	505	-	9,9,15	0.47	0	8,8,14	0.68	0
7	PMP	D	502	-	16,16,16	0.95	1 (6%)	21,23,23	1.45	2 (9%)
5	1PE	E	502	-	9,9,15	0.47	0	8,8,14	0.77	0
2	Q0P	A	501	-	27,31,31	1.69	5 (18%)	34,44,44	2.14	9 (26%)
4	GOL	G	505	-	5,5,5	1.38	1 (20%)	5,5,5	0.80	0
4	GOL	G	508	-	5,5,5	0.95	0	5,5,5	0.99	0
5	1PE	E	503	-	9,9,15	0.53	0	8,8,14	0.57	0
4	GOL	G	506	-	5,5,5	1.27	1 (20%)	5,5,5	1.05	0
4	GOL	D	504	-	5,5,5	1.12	0	5,5,5	0.92	0
8	PLP	E	501	-	16,16,16	1.21	2 (12%)	20,23,23	1.69	4 (20%)
8	PLP	H	501	-	16,16,16	1.18	2 (12%)	20,23,23	1.30	2 (10%)
7	PMP	C	502	-	16,16,16	1.04	1 (6%)	21,23,23	1.38	2 (9%)
3	PO4	G	504	-	4,4,4	0.90	0	6,6,6	0.65	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
4	GOL	A	504	-	-	0/4/4/4	-
5	1PE	H	503	-	-	1/4/4/13	-
6	KYA	B	501	-	-	0/0/4/4	0/2/2/2
6	KYA	G	501	-	-	0/0/4/4	0/2/2/2
5	1PE	D	505	-	-	10/13/13/13	-
4	GOL	B	504	-	-	0/4/4/4	-
4	GOL	A	503	-	-	4/4/4/4	-
6	KYA	C	501	-	-	0/0/4/4	0/2/2/2
4	GOL	C	504	-	-	2/4/4/4	-
5	1PE	E	502	-	-	6/7/7/13	-
8	PLP	F	501	-	-	2/8/8/8	0/1/1/1
7	PMP	G	502	-	-	5/8/8/8	0/1/1/1
4	GOL	B	503	-	-	4/4/4/4	-
5	1PE	B	505	-	-	7/13/13/13	-
4	GOL	G	507	-	-	4/4/4/4	-
7	PMP	B	502	-	-	5/8/8/8	0/1/1/1
6	KYA	D	501	-	-	0/0/4/4	0/2/2/2
5	1PE	A	505	-	-	6/7/7/13	-
7	PMP	D	502	-	-	5/8/8/8	0/1/1/1
2	Q0P	A	501	-	-	11/19/23/23	0/2/2/2
4	GOL	G	505	-	-	4/4/4/4	-
4	GOL	G	508	-	-	2/4/4/4	-
5	1PE	E	503	-	-	5/7/7/13	-
4	GOL	G	506	-	-	3/4/4/4	-
4	GOL	D	504	-	-	0/4/4/4	-
8	PLP	E	501	-	-	2/8/8/8	0/1/1/1
8	PLP	H	501	-	-	2/8/8/8	0/1/1/1
7	PMP	C	502	-	-	5/8/8/8	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	PMP	C3-C2	7.99	1.48	1.40
6	D	501	KYA	C1-C2	-7.31	1.30	1.42
6	C	501	KYA	C1-C2	-6.73	1.31	1.42
7	B	502	PMP	C5-C4	5.89	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	Q0P	C12-C13	5.62	1.57	1.46
6	B	501	KYA	C1-C2	-5.55	1.33	1.42
7	B	502	PMP	C3-C4	5.48	1.48	1.40
6	D	501	KYA	C2-N	-4.52	1.30	1.37
6	G	501	KYA	C1-C2	-4.49	1.35	1.42
6	B	501	KYA	C2-N	-3.78	1.31	1.37
6	C	501	KYA	C2-N	-3.69	1.31	1.37
6	C	501	KYA	C3-C1	-3.45	1.35	1.42
6	D	501	KYA	C3-C1	-3.39	1.35	1.42
6	D	501	KYA	C5-C2	-3.33	1.36	1.41
6	G	501	KYA	C2-N	-3.27	1.32	1.37
7	C	502	PMP	C2-N1	3.01	1.39	1.33
8	E	501	PLP	C2-N1	2.99	1.39	1.33
6	B	501	KYA	C3-C1	-2.88	1.36	1.42
2	A	501	Q0P	C19-C17	2.87	1.54	1.48
8	F	501	PLP	C2-N1	2.81	1.39	1.33
8	H	501	PLP	C2-N1	2.80	1.39	1.33
6	D	501	KYA	C4-C1	-2.79	1.36	1.42
7	D	502	PMP	C2-N1	2.78	1.39	1.33
7	G	502	PMP	C2-N1	2.72	1.39	1.33
6	B	501	KYA	C5-C2	-2.67	1.37	1.41
6	G	501	KYA	C3-C1	-2.63	1.37	1.42
2	A	501	Q0P	C24-N25	2.58	1.46	1.37
6	B	501	KYA	C6-C3	2.57	1.43	1.37
6	B	501	KYA	O1-C3	2.51	1.42	1.36
6	D	501	KYA	C7-N	-2.43	1.29	1.33
4	G	505	GOL	C1-C2	2.24	1.60	1.51
6	G	501	KYA	C5-C2	-2.24	1.38	1.41
4	G	506	GOL	O2-C2	-2.21	1.36	1.43
8	F	501	PLP	C6-N1	2.19	1.39	1.34
2	A	501	Q0P	C16-C17	2.15	1.54	1.51
8	H	501	PLP	C4-C4A	2.08	1.51	1.46
2	A	501	Q0P	C29-C02	-2.08	1.38	1.40
4	G	507	GOL	O2-C2	-2.06	1.37	1.43
8	E	501	PLP	C6-N1	2.06	1.38	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	501	KYA	C7-N-C2	9.26	124.95	118.06
2	A	501	Q0P	C15-N14-C13	8.26	128.60	117.40
6	C	501	KYA	C7-N-C2	7.64	123.74	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	KYA	C7-N-C2	6.46	122.87	118.06
6	B	501	KYA	C6-C7-N	-5.70	117.03	122.23
6	D	501	KYA	C6-C7-N	-4.80	117.85	122.23
6	C	501	KYA	C6-C7-N	-4.19	118.41	122.23
6	B	501	KYA	C6-C3-C1	-4.05	115.71	120.52
2	A	501	Q0P	C29-C12-C05	-4.02	115.17	118.26
7	D	502	PMP	C5-C6-N1	-3.91	117.31	123.82
2	A	501	Q0P	C01-C02-C29	-3.89	116.08	120.89
7	C	502	PMP	C6-C5-C4	3.88	120.86	118.12
8	E	501	PLP	O4A-C4A-C4	-3.79	116.65	124.91
6	B	501	KYA	O1-C3-C6	3.56	131.59	121.17
7	D	502	PMP	C6-C5-C4	3.44	120.55	118.12
8	E	501	PLP	O4P-C5A-C5	-3.34	102.99	109.35
7	C	502	PMP	C5-C6-N1	-3.30	118.32	123.82
7	G	502	PMP	C6-C5-C4	3.23	120.40	118.12
8	H	501	PLP	O4A-C4A-C4	-3.08	118.19	124.91
7	G	502	PMP	C5-C6-N1	-3.01	118.81	123.82
6	C	501	KYA	C1-C2-N	-2.99	119.64	122.81
6	D	501	KYA	C5-C2-C1	2.95	122.52	119.13
6	B	501	KYA	O1-C3-C1	-2.94	112.64	116.31
8	F	501	PLP	O4A-C4A-C4	-2.77	118.87	124.91
6	G	501	KYA	C7-N-C2	2.70	120.07	118.06
6	G	501	KYA	C6-C3-C1	-2.69	117.33	120.52
8	H	501	PLP	C5-C6-N1	-2.66	119.38	123.82
6	G	501	KYA	C4-C1-C3	-2.62	118.60	122.21
8	E	501	PLP	C5-C6-N1	-2.53	119.60	123.82
2	A	501	Q0P	C05-C04-N03	-2.47	119.71	123.82
2	A	501	Q0P	C05-C12-C13	2.44	125.58	121.56
8	F	501	PLP	C5-C6-N1	-2.41	119.80	123.82
2	A	501	Q0P	O07-C06-C05	-2.40	104.78	109.35
2	A	501	Q0P	C06-C05-C04	-2.40	115.43	119.37
2	A	501	Q0P	C29-C02-N03	2.37	123.83	120.77
8	F	501	PLP	C3-C4-C5	2.29	120.02	118.26
6	D	501	KYA	C1-C2-N	-2.25	120.42	122.81
8	E	501	PLP	C3-C4-C5	2.23	119.97	118.26
8	F	501	PLP	C3-C4-C4A	-2.21	116.76	119.90
6	G	501	KYA	C3-C1-C2	2.20	120.70	117.91
2	A	501	Q0P	C04-C05-C12	2.19	122.18	118.15
7	B	502	PMP	C6-N1-C2	2.16	123.17	119.17
6	G	501	KYA	C4-C1-C2	2.11	120.68	118.33
6	B	501	KYA	C9-C8-C4	-2.06	117.56	120.44

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-C3
4	A	503	GOL	C1-C2-C3-O3
4	A	503	GOL	O2-C2-C3-O3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
7	G	502	PMP	C5A-O4P-P-O1P
7	G	502	PMP	C5A-O4P-P-O2P
7	G	502	PMP	C5A-O4P-P-O3P
8	F	501	PLP	C3-C4-C4A-O4A
8	F	501	PLP	C5-C4-C4A-O4A
4	G	507	GOL	O1-C1-C2-C3
4	G	507	GOL	C1-C2-C3-O3
7	B	502	PMP	C5A-O4P-P-O1P
7	B	502	PMP	C5A-O4P-P-O2P
7	B	502	PMP	C5A-O4P-P-O3P
7	D	502	PMP	C5A-O4P-P-O1P
7	D	502	PMP	C5A-O4P-P-O3P
2	A	501	Q0P	C26-C15-C16-C17
2	A	501	Q0P	N14-C15-C16-C17
2	A	501	Q0P	C16-C17-C19-C24
2	A	501	Q0P	O18-C17-C19-C24
2	A	501	Q0P	C16-C15-N14-C13
2	A	501	Q0P	C26-C15-N14-C13
4	G	505	GOL	O1-C1-C2-C3
4	G	505	GOL	O2-C2-C3-O3
8	E	501	PLP	C3-C4-C4A-O4A
8	E	501	PLP	C5-C4-C4A-O4A
8	H	501	PLP	C3-C4-C4A-O4A
8	H	501	PLP	C5-C4-C4A-O4A
7	C	502	PMP	C5A-O4P-P-O2P
7	C	502	PMP	C5A-O4P-P-O3P
5	D	505	1PE	OH4-C13-C23-OH3
5	B	505	1PE	OH4-C13-C23-OH3
5	B	505	1PE	OH6-C15-C25-OH5
4	A	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
4	G	507	GOL	O2-C2-C3-O3
5	B	505	1PE	OH5-C14-C24-OH4
5	D	505	1PE	OH2-C12-C22-OH3
5	D	505	1PE	OH7-C16-C26-OH6
5	E	503	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
5	E	503	1PE	OH6-C15-C25-OH5
5	E	502	1PE	C23-C13-OH4-C24
5	E	502	1PE	OH4-C13-C23-OH3
5	E	503	1PE	OH5-C14-C24-OH4
4	B	503	GOL	C1-C2-C3-O3
4	G	505	GOL	C1-C2-C3-O3
4	G	508	GOL	O1-C1-C2-C3
5	H	503	1PE	OH4-C13-C23-OH3
7	C	502	PMP	C5-C4-C4A-N4A
5	E	502	1PE	C24-C14-OH5-C25
5	A	505	1PE	OH4-C13-C23-OH3
5	D	505	1PE	C23-C13-OH4-C24
7	C	502	PMP	C3-C4-C4A-N4A
4	G	505	GOL	O1-C1-C2-O2
7	C	502	PMP	C5A-O4P-P-O1P
5	B	505	1PE	OH2-C12-C22-OH3
5	D	505	1PE	OH6-C15-C25-OH5
5	D	505	1PE	OH5-C14-C24-OH4
4	G	508	GOL	C1-C2-C3-O3
7	G	502	PMP	C5-C4-C4A-N4A
7	B	502	PMP	C5-C4-C4A-N4A
4	B	503	GOL	O2-C2-C3-O3
4	G	507	GOL	O1-C1-C2-O2
5	A	505	1PE	C14-C24-OH4-C13
5	E	503	1PE	C23-C13-OH4-C24
2	A	501	Q0P	C06-O07-P08-O09
5	D	505	1PE	C25-C15-OH6-C26
5	D	505	1PE	C16-C26-OH6-C15
5	D	505	1PE	C24-C14-OH5-C25
7	D	502	PMP	C4-C5-C5A-O4P
4	G	506	GOL	O1-C1-C2-O2
4	G	506	GOL	O1-C1-C2-C3
5	E	503	1PE	C24-C14-OH5-C25
5	B	505	1PE	C16-C26-OH6-C15
7	D	502	PMP	C5-C4-C4A-N4A
5	A	505	1PE	C23-C13-OH4-C24
2	A	501	Q0P	C06-O07-P08-O11
5	A	505	1PE	C24-C14-OH5-C25
5	E	502	1PE	C15-C25-OH5-C14
5	A	505	1PE	C15-C25-OH5-C14
5	B	505	1PE	C13-C23-OH3-C22
5	D	505	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
7	B	502	PMP	C3-C4-C4A-N4A
5	B	505	1PE	C24-C14-OH5-C25
7	D	502	PMP	C6-C5-C5A-O4P
4	G	506	GOL	C1-C2-C3-O3
5	E	502	1PE	OH6-C15-C25-OH5
2	A	501	Q0P	C06-O07-P08-O10
2	A	501	Q0P	C29-C12-C13-N14
7	G	502	PMP	C3-C4-C4A-N4A
5	E	502	1PE	OH5-C14-C24-OH4
5	A	505	1PE	OH5-C14-C24-OH4
2	A	501	Q0P	C15-C16-C17-O18

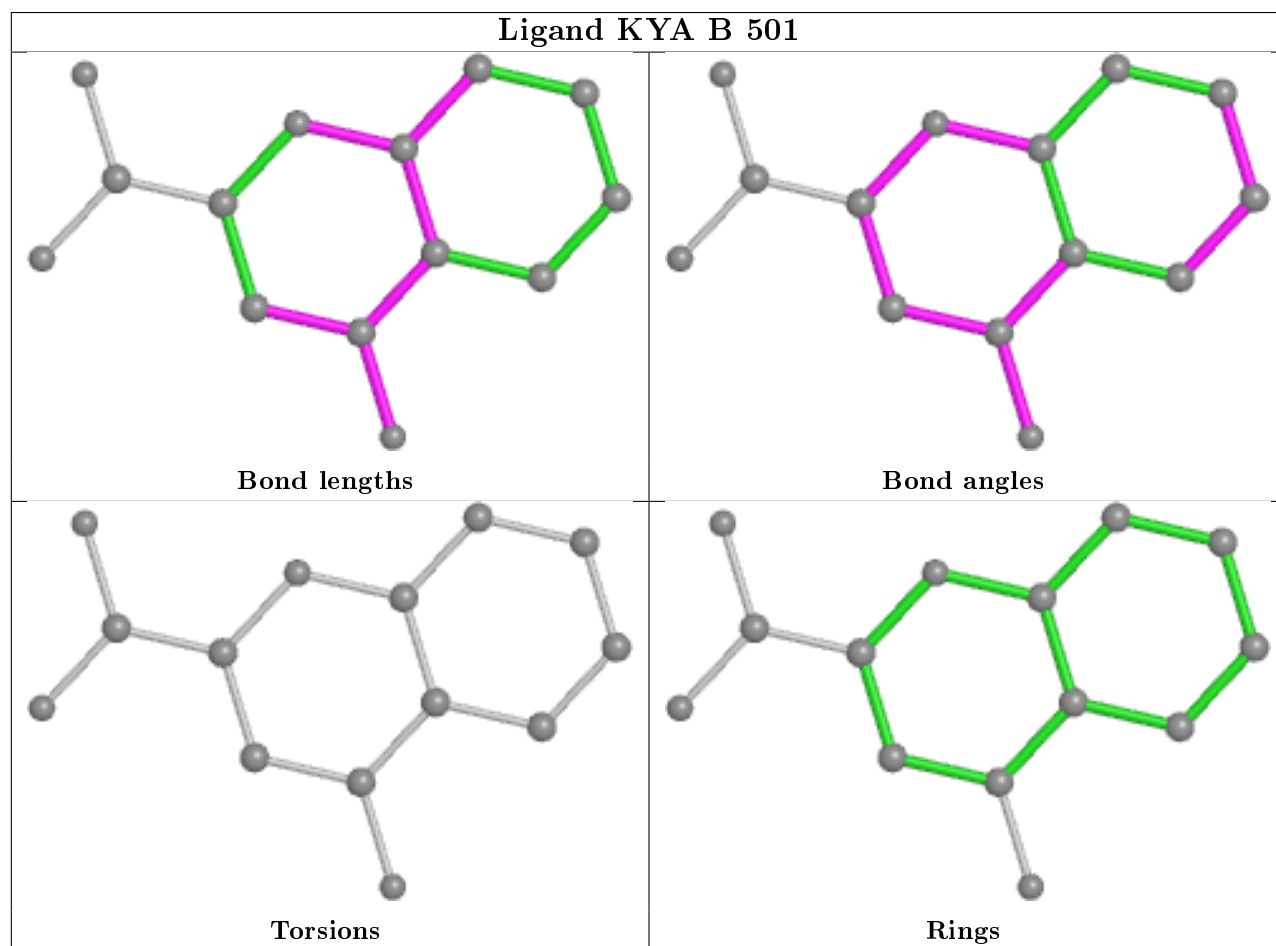
There are no ring outliers.

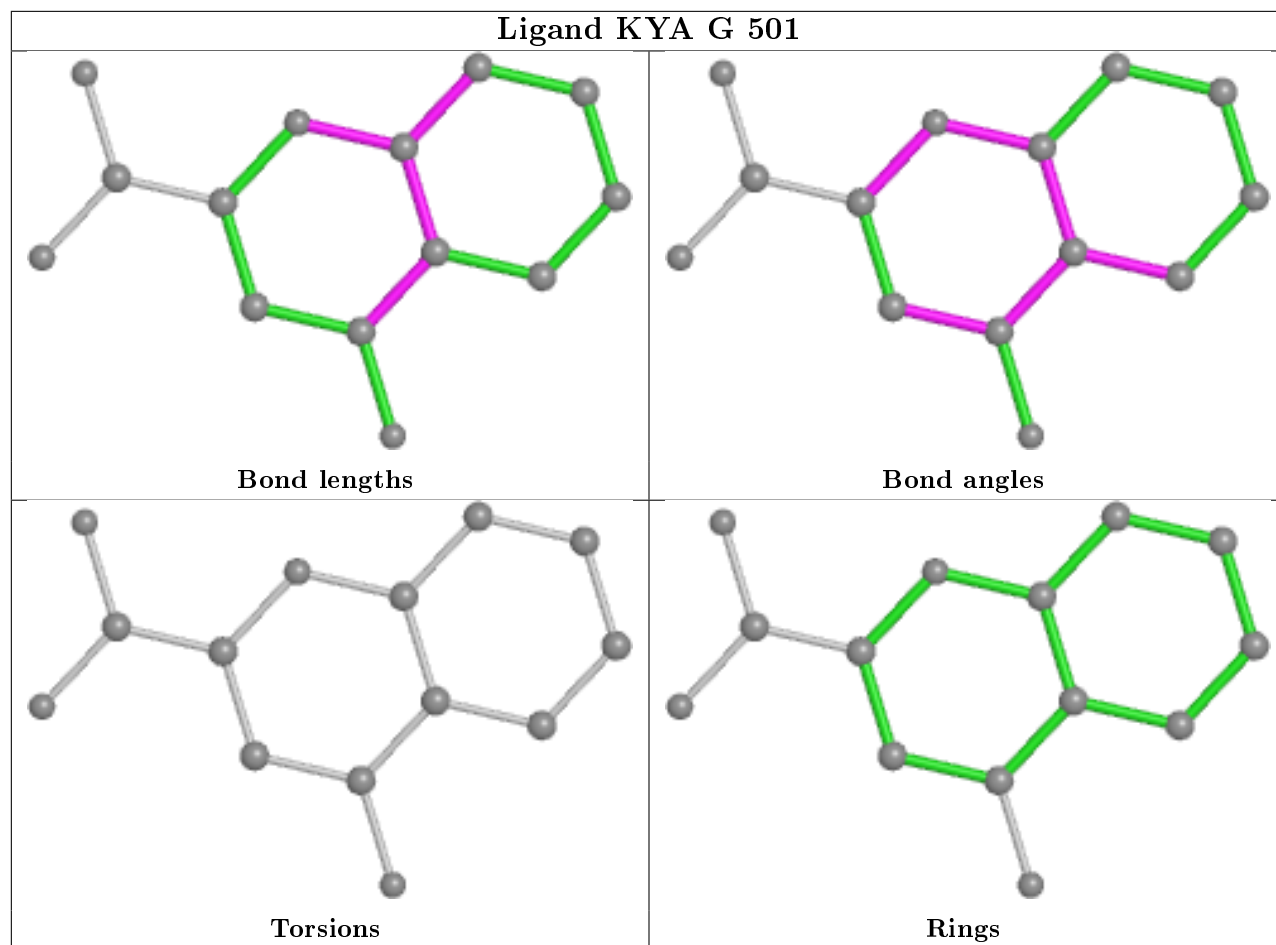
22 monomers are involved in 88 short contacts:

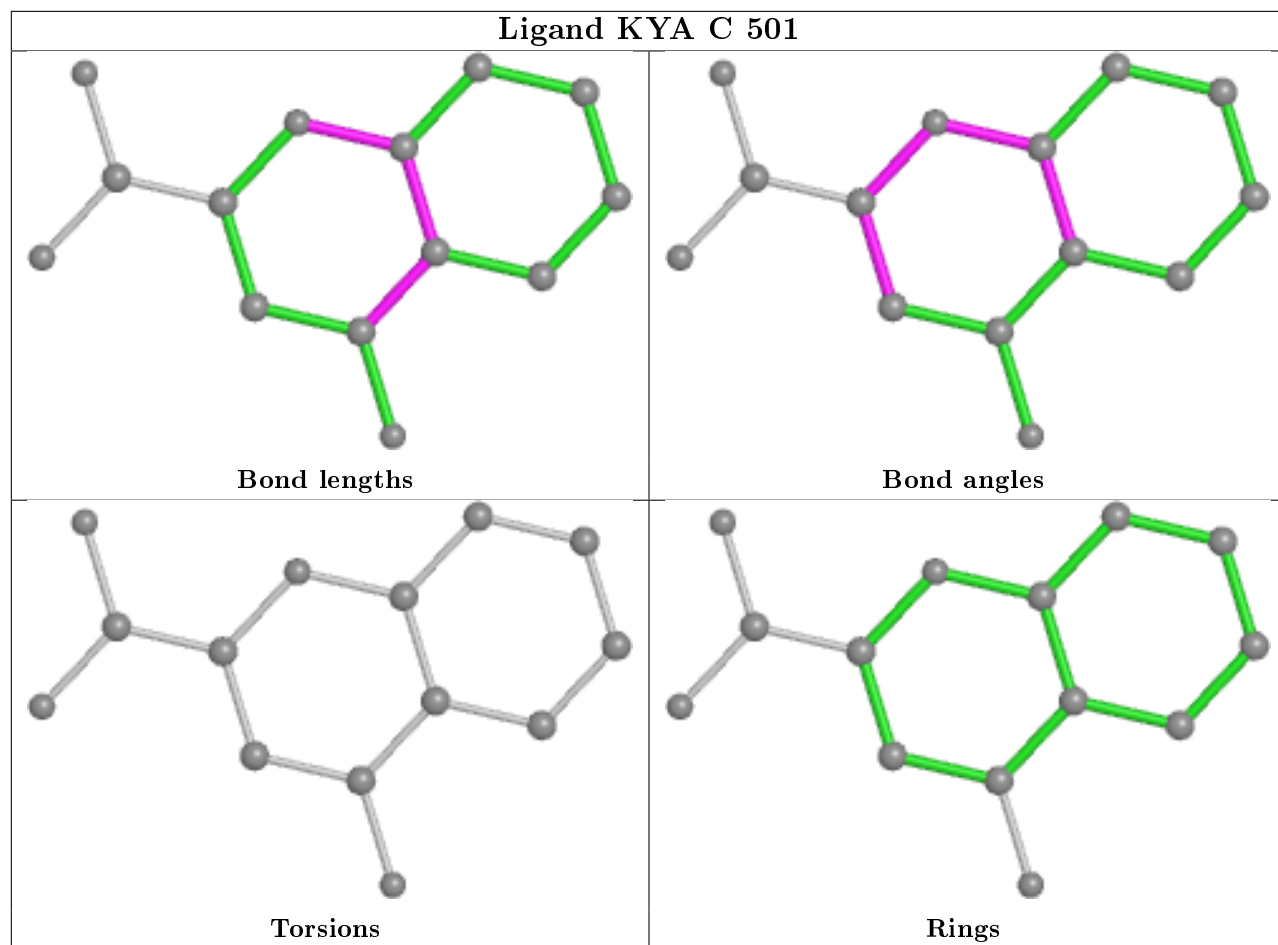
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	GOL	1	0
6	B	501	KYA	16	0
6	G	501	KYA	15	0
5	D	505	1PE	4	0
4	B	504	GOL	1	0
6	C	501	KYA	10	0
4	C	504	GOL	2	0
4	B	503	GOL	4	0
7	G	502	PMP	3	0
5	H	503	1PE	2	0
8	F	501	PLP	1	0
5	B	505	1PE	5	0
7	B	502	PMP	6	0
6	D	501	KYA	11	0
5	A	505	1PE	2	0
7	D	502	PMP	3	0
5	E	502	1PE	1	0
2	A	501	Q0P	2	0
5	E	503	1PE	3	0
4	D	504	GOL	2	0
8	E	501	PLP	1	0
7	C	502	PMP	3	0

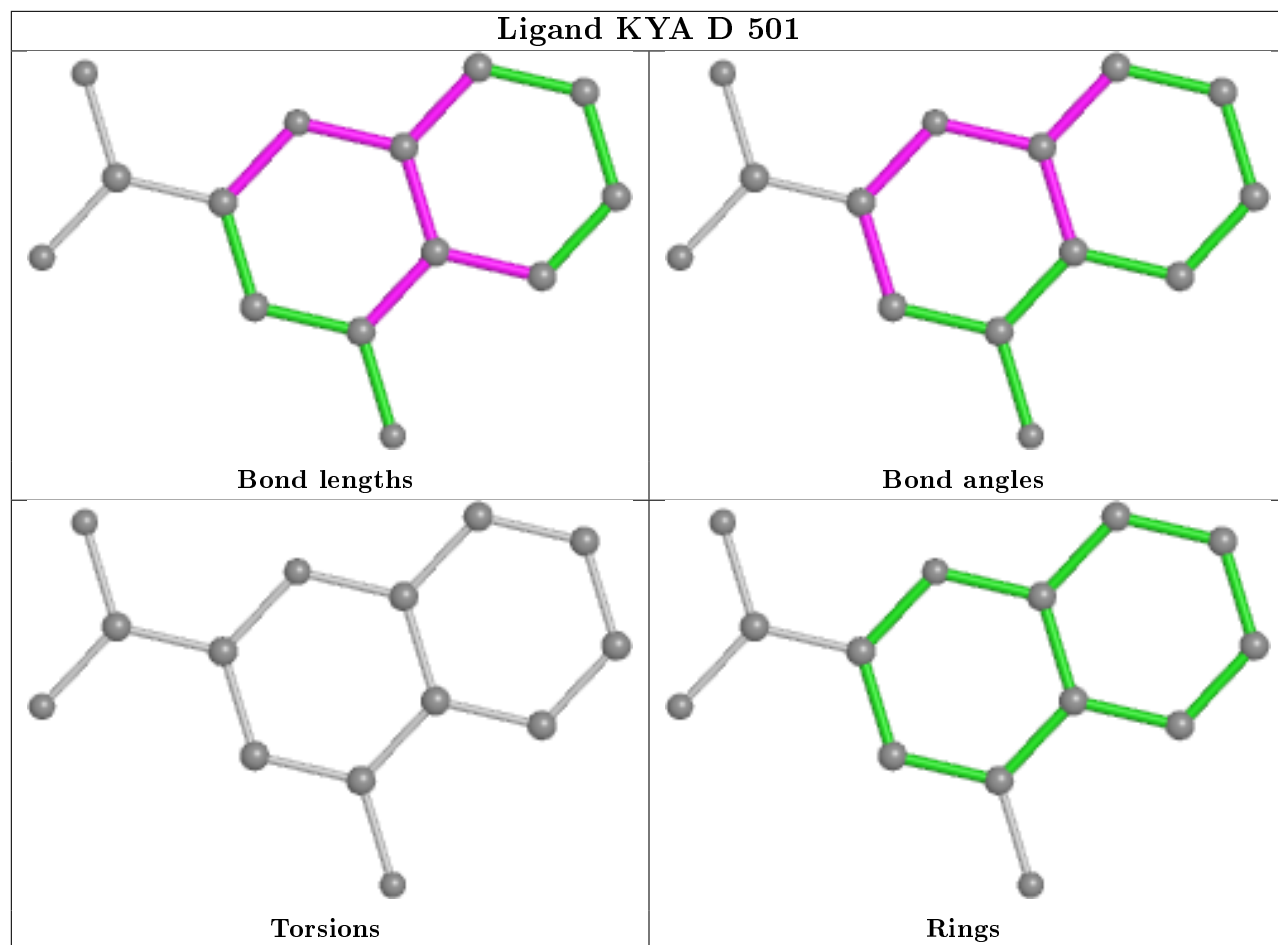
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

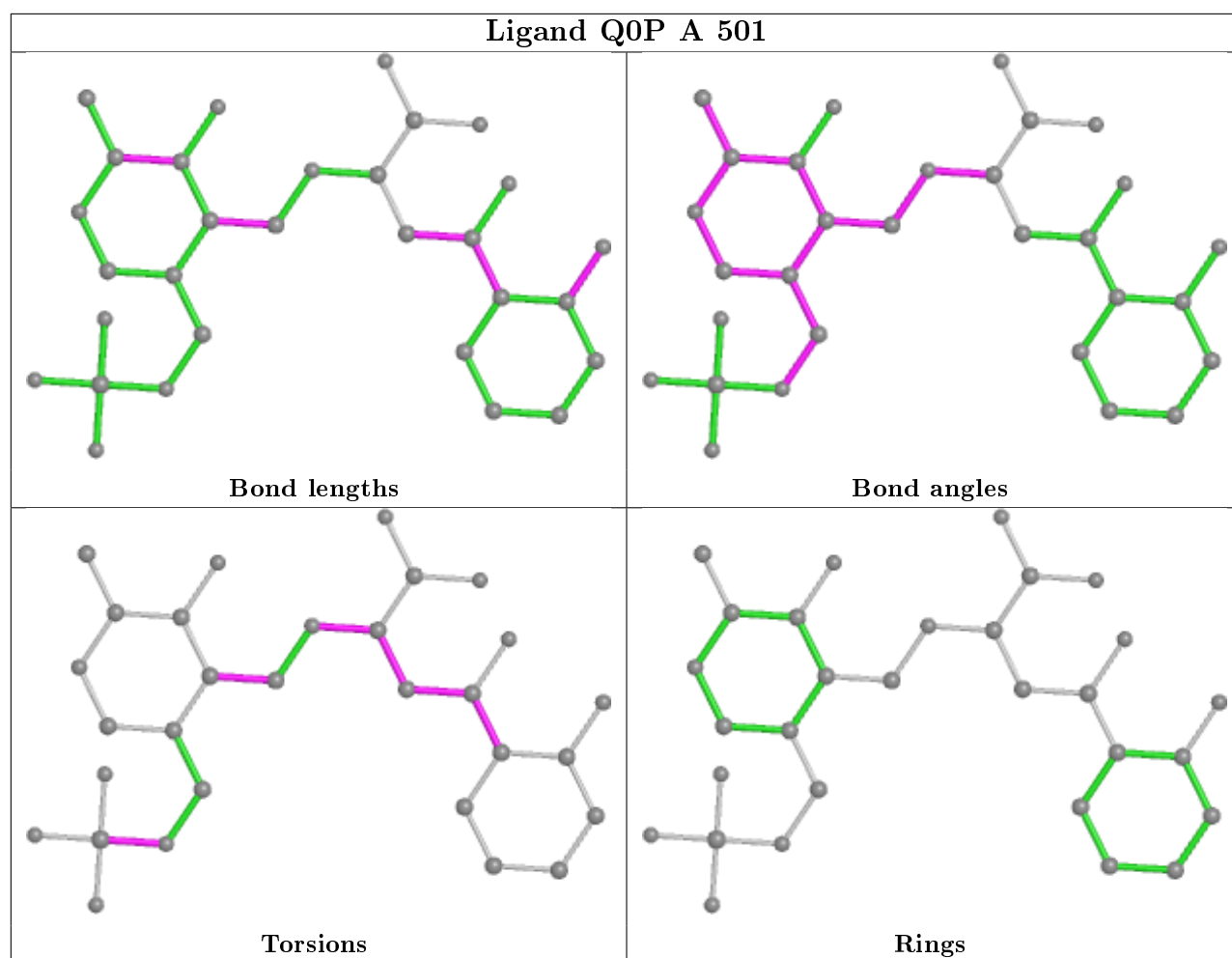
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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 ⓘ

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	423/435 (97%)	-0.21	18 (4%)	35	33	18, 28, 57, 78	1 (0%)
1	B	423/435 (97%)	-0.16	22 (5%)	27	25	20, 32, 64, 86	0
1	C	423/435 (97%)	-0.08	29 (6%)	16	15	20, 32, 63, 90	0
1	D	429/435 (98%)	-0.18	16 (3%)	41	39	20, 33, 53, 81	1 (0%)
1	E	423/435 (97%)	0.00	30 (7%)	16	14	21, 35, 65, 88	0
1	F	422/435 (97%)	-0.14	10 (2%)	59	57	23, 33, 54, 83	0
1	G	423/435 (97%)	0.22	38 (8%)	9	8	22, 35, 66, 81	0
1	H	416/435 (95%)	0.19	41 (9%)	7	6	22, 36, 74, 95	0
All	All	3382/3480 (97%)	-0.05	204 (6%)	21	20	18, 33, 64, 95	2 (0%)

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	12	ALA	8.8
1	C	6	LEU	8.0
1	H	11	LEU	7.5
1	E	5	SER	6.8
1	A	5	SER	6.7
1	C	9	GLN	6.5
1	H	14	LEU	6.5
1	H	422	LEU	6.3
1	G	423	LEU	6.2
1	A	6	LEU	6.2
1	C	14	LEU	6.2
1	H	421	THR	6.0
1	C	11	LEU	5.9
1	B	6	LEU	5.8
1	H	13	ALA	5.8
1	G	14	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	F	5	SER	5.3
1	E	9	GLN	5.2
1	H	16	ALA	5.2
1	E	6	LEU	5.2
1	F	4	ASP	5.2
1	H	9	GLN	5.2
1	H	368	ASP	5.2
1	H	15	HIS	5.2
1	H	419	THR	5.1
1	B	11	LEU	5.1
1	G	4	ASP	5.0
1	C	5	SER	5.0
1	G	20	GLN	5.0
1	E	11	LEU	5.0
1	B	4	ASP	5.0
1	G	5	SER	4.9
1	D	4	ASP	4.9
1	G	12	ALA	4.8
1	E	14	LEU	4.8
1	G	11	LEU	4.7
1	C	4	ASP	4.7
1	D	5	SER	4.6
1	H	355	LEU	4.6
1	H	23	ALA	4.6
1	G	8	PRO	4.5
1	E	16	ALA	4.3
1	C	8	PRO	4.3
1	A	7	SER	4.3
1	H	337	LYS	4.3
1	B	13	ALA	4.3
1	F	6	LEU	4.3
1	D	3	PHE	4.3
1	C	10	GLU	4.2
1	E	7	SER	4.2
1	E	4	ASP	4.1
1	A	9	GLN	4.1
1	G	6	LEU	4.1
1	B	9	GLN	4.0
1	F	9	GLN	4.0
1	G	7	SER	4.0
1	A	4	ASP	4.0
1	G	3	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	22	TYR	4.0
1	H	8	PRO	4.0
1	B	7	SER	4.0
1	G	22	TYR	3.9
1	B	3	PHE	3.9
1	H	339	ALA	3.9
1	H	418	ALA	3.9
1	E	8	PRO	3.9
1	C	20	GLN	3.9
1	C	17	ARG	3.8
1	G	421	THR	3.8
1	C	335	GLU	3.8
1	C	422	LEU	3.8
1	D	7	SER	3.8
1	E	335	GLU	3.7
1	C	13	ALA	3.7
1	D	17	ARG	3.7
1	C	16	ALA	3.7
1	B	2	SER	3.7
1	H	335	GLU	3.6
1	H	336	SER	3.6
1	A	11	LEU	3.6
1	D	6	LEU	3.6
1	H	412	THR	3.6
1	C	25	LEU	3.6
1	C	3	PHE	3.5
1	H	18	HIS	3.5
1	C	12	ALA	3.5
1	A	335	GLU	3.5
1	G	335	GLU	3.5
1	E	333	LEU	3.5
1	B	20	GLN	3.5
1	E	13	ALA	3.5
1	C	2	SER	3.5
1	E	12	ALA	3.4
1	E	17	ARG	3.4
1	B	422	LEU	3.4
1	H	416	LEU	3.4
1	F	3	PHE	3.3
1	C	7	SER	3.3
1	H	415	LEU	3.3
1	G	422	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	368	ASP	3.2
1	E	10	GLU	3.2
1	G	338	ILE	3.2
1	E	338	ILE	3.2
1	A	423	LEU	3.2
1	G	15	HIS	3.1
1	D	429	SER	3.1
1	H	17	ARG	3.1
1	E	422	LEU	3.1
1	E	3	PHE	3.1
1	H	127	GLN	3.1
1	B	335	GLU	3.0
1	C	423	LEU	3.0
1	D	430	SER	3.0
1	E	127	GLN	3.0
1	G	128	ASP	2.9
1	B	5	SER	2.9
1	C	355	LEU	2.9
1	F	12	ALA	2.9
1	D	128	ASP	2.9
1	C	424	ASN	2.8
1	A	14	LEU	2.8
1	F	7	SER	2.8
1	A	421	THR	2.8
1	E	330	ASP	2.8
1	B	16	ALA	2.8
1	B	14	LEU	2.8
1	B	423	LEU	2.8
1	H	331	GLN	2.8
1	G	127	GLN	2.8
1	C	418	ALA	2.8
1	G	17	ARG	2.8
1	B	10	GLU	2.8
1	C	336	SER	2.7
1	G	419	THR	2.7
1	E	331	GLN	2.7
1	A	27	GLY	2.7
1	F	8	PRO	2.7
1	F	20	GLN	2.7
1	G	9	GLN	2.7
1	G	337	LYS	2.7
1	D	9	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	338	ILE	2.6
1	E	336	SER	2.6
1	G	361	ARG	2.6
1	H	361	ARG	2.6
1	A	422	LEU	2.6
1	G	386	PRO	2.6
1	G	18	HIS	2.6
1	E	337	LYS	2.5
1	B	27	GLY	2.5
1	A	2	SER	2.5
1	C	27	GLY	2.5
1	A	10	GLU	2.4
1	H	128	ASP	2.4
1	E	339	ALA	2.4
1	D	422	LEU	2.4
1	F	13	ALA	2.4
1	B	337	LYS	2.4
1	D	2	SER	2.4
1	E	15	HIS	2.3
1	G	355	LEU	2.3
1	G	365	LEU	2.3
1	A	26	GLN	2.3
1	A	17	ARG	2.3
1	E	355	LEU	2.3
1	G	26	GLN	2.3
1	G	414	ALA	2.3
1	H	27	GLY	2.3
1	D	174	VAL	2.3
1	G	424	ASN	2.3
1	E	18	HIS	2.3
1	B	127	GLN	2.3
1	G	331	GLN	2.2
1	G	356	PRO	2.2
1	H	29	LYS	2.2
1	H	338	ILE	2.2
1	A	8	PRO	2.2
1	H	358	THR	2.2
1	E	2	SER	2.2
1	C	419	THR	2.2
1	H	360	ARG	2.1
1	B	421	THR	2.1
1	G	2	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	428	ALA	2.1
1	A	29	LYS	2.1
1	G	16	ALA	2.1
1	H	24	ALA	2.1
1	C	19	GLN	2.1
1	D	335	GLU	2.1
1	H	330	ASP	2.1
1	C	15	HIS	2.1
1	H	10	GLU	2.1
1	E	421	THR	2.1
1	H	414	ALA	2.1
1	B	12	ALA	2.0
1	G	375	GLU	2.0
1	D	8	PRO	2.0
1	H	25	LEU	2.0
1	H	423	LEU	2.0
1	C	417	ALA	2.0
1	E	334	SER	2.0
1	H	34	LEU	2.0
1	G	334	SER	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, 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	GOL	D	504	6/6	0.80	0.18	39,51,55,63	0
4	GOL	C	504	6/6	0.81	0.22	41,50,54,57	0
5	1PE	D	505	16/16	0.83	0.31	56,64,70,72	0

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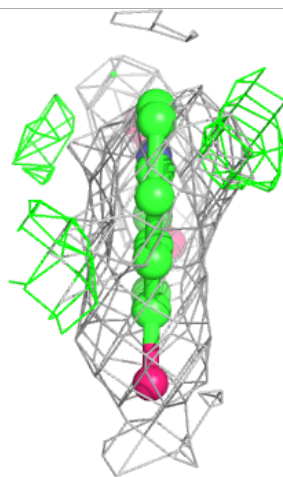
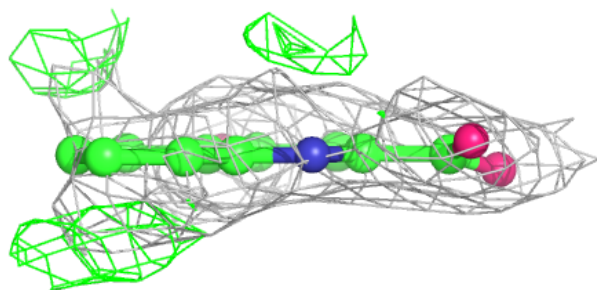
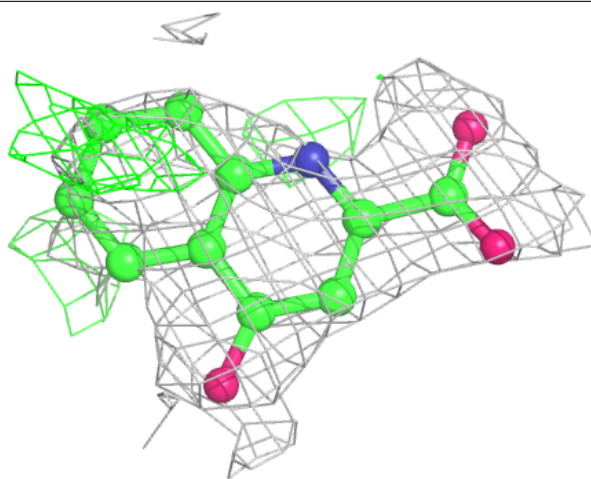
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	G	507	6/6	0.84	0.20	33,43,45,46	0
4	GOL	G	506	6/6	0.85	0.16	42,43,48,53	0
4	GOL	G	508	6/6	0.86	0.19	54,56,57,61	0
6	KYA	G	501	14/14	0.86	0.27	37,40,42,45	13
4	GOL	B	504	6/6	0.86	0.20	37,41,44,46	0
5	1PE	E	503	10/16	0.87	0.14	47,53,57,58	0
4	GOL	A	503	6/6	0.88	0.14	34,38,44,46	0
5	1PE	B	505	16/16	0.89	0.16	34,49,55,60	0
6	KYA	C	501	14/14	0.89	0.19	34,39,41,42	13
3	PO4	G	504	5/5	0.89	0.26	47,51,56,57	4
6	KYA	D	501	14/14	0.90	0.21	37,42,44,46	11
4	GOL	A	504	6/6	0.91	0.12	41,46,52,57	0
6	KYA	B	501	14/14	0.91	0.18	31,38,41,47	10
4	GOL	B	503	6/6	0.92	0.15	33,35,39,41	0
5	1PE	H	503	7/16	0.92	0.26	57,57,59,63	0
5	1PE	E	502	10/16	0.93	0.12	31,39,48,49	0
5	1PE	A	505	10/16	0.93	0.12	36,43,52,55	0
4	GOL	G	505	6/6	0.94	0.15	32,40,42,43	0
3	PO4	A	502	5/5	0.95	0.14	25,27,30,35	2
3	PO4	D	503	5/5	0.96	0.24	45,46,49,54	3
8	PLP	H	501	16/16	0.96	0.15	23,35,44,53	0
3	PO4	G	503	5/5	0.96	0.11	30,35,36,40	3
3	PO4	H	502	5/5	0.97	0.11	51,52,55,56	3
8	PLP	F	501	16/16	0.97	0.15	22,34,39,44	0
2	Q0P	A	501	30/30	0.97	0.16	20,29,39,43	17
8	PLP	E	501	16/16	0.97	0.12	26,37,44,52	0
7	PMP	B	502	16/16	0.97	0.15	20,32,36,39	0
7	PMP	C	502	16/16	0.97	0.14	24,32,38,38	0
7	PMP	G	502	16/16	0.97	0.14	22,37,41,48	0
7	PMP	D	502	16/16	0.98	0.12	23,33,40,43	0
3	PO4	C	503	5/5	0.98	0.13	38,38,42,43	4

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.

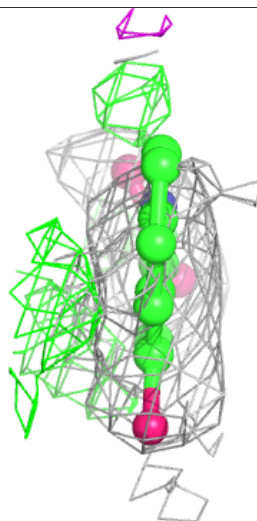
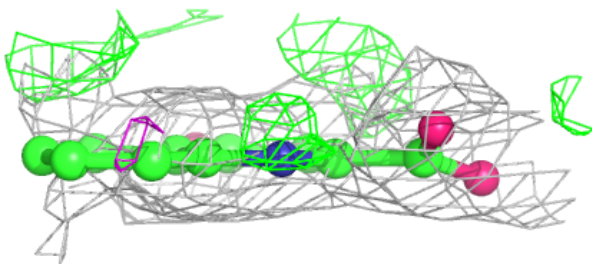
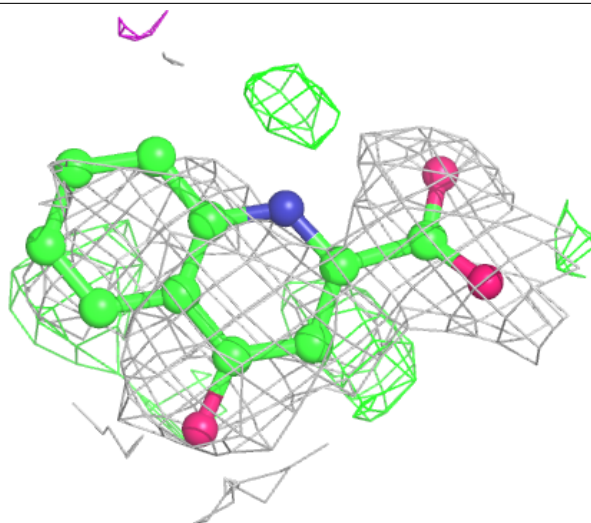
Electron density around KYA G 501:

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



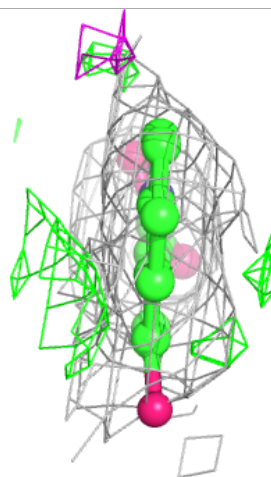
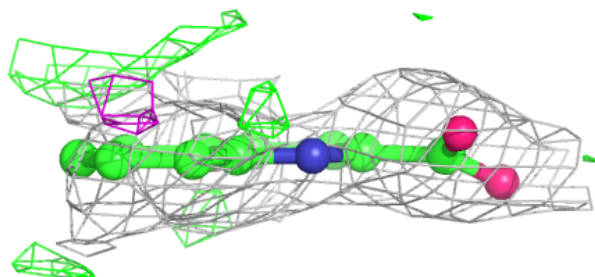
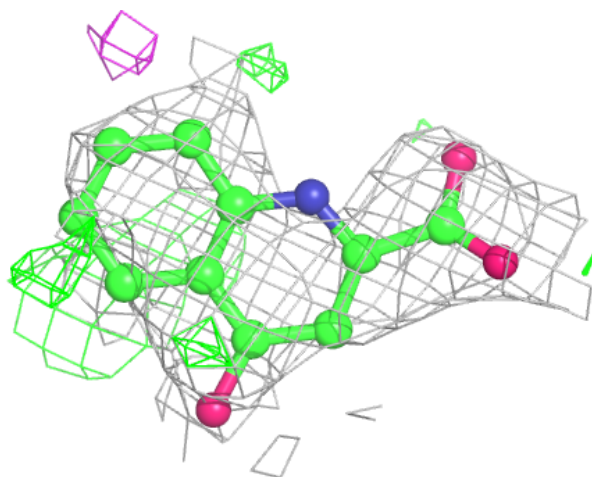
Electron density around KYA C 501:

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



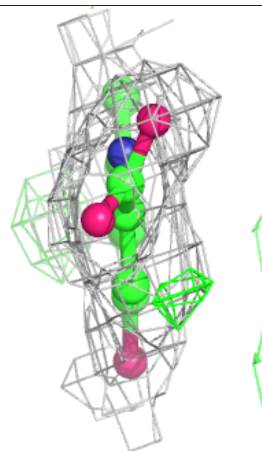
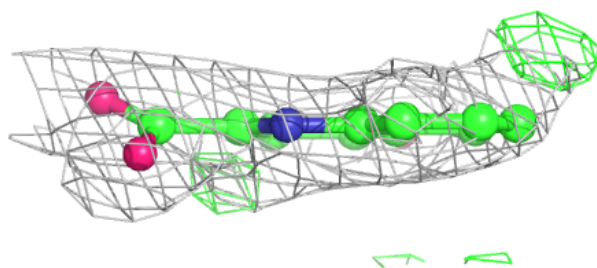
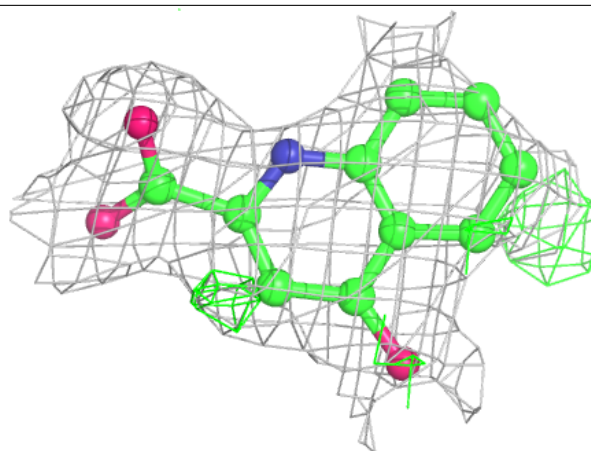
Electron density around KYA D 501:

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



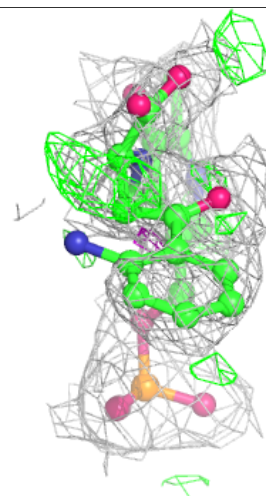
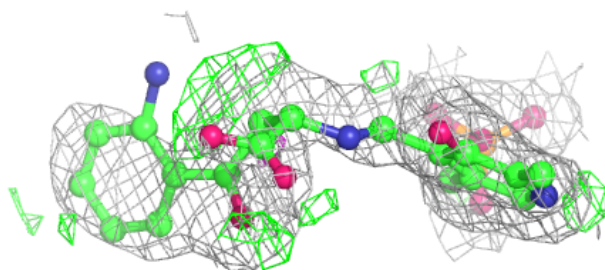
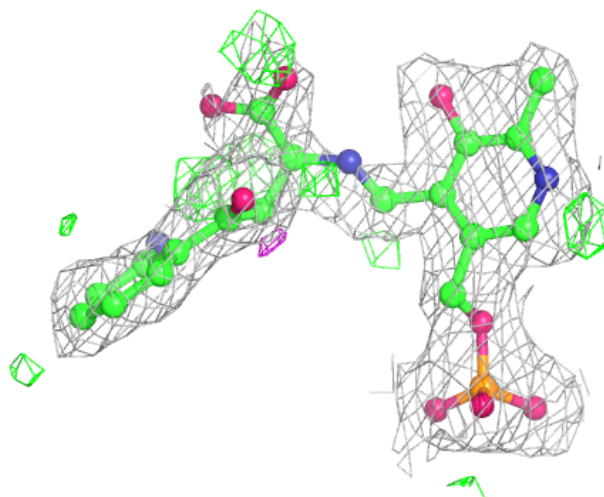
Electron density around KYA B 501:

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



Electron density around Q0P 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.