Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 12:18 AM EDT

PDB ID	:	4QAB
Title	:	X-RAY STRUCTURE of ACETYLCHOLINE BINDING PROTEIN (ACHBP) IN COMPLEX WITH 4-(MORPHOLIN-4-YL)-6-[4-(TRIFLUOROMETHYL)PHENYL]PYRIMIDIN-2-AMINE
Authors	:	Kaczanowska, K.; Harel, M.; Radic, Z.; Changeux, J.-P.; Finn, M.G.; Taylor, P.
Deposited on	:	2014-05-03
Resolution	:	2.98 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 (i) 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 (i)) were used in the production of this report:

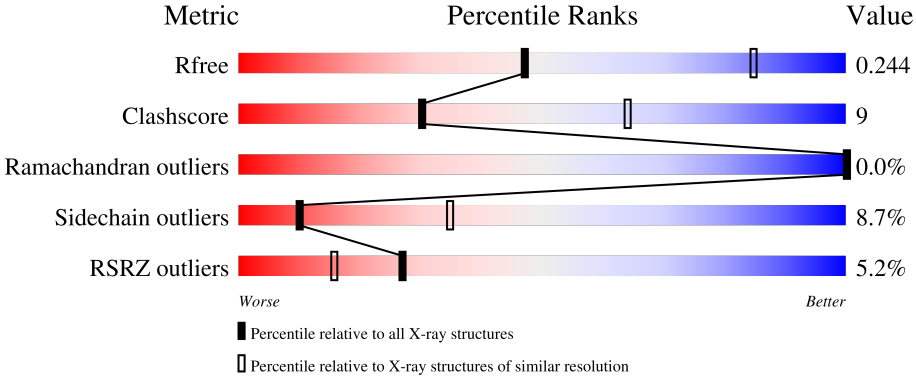
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 <=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	217	4% 76% 18% • •
1	B	217	3% 74% 17% • 6%
1	C	217	6% 76% 17% • 5%
1	D	217	6% 71% 24% • •
1	E	217	6% 77% 17% • 5%

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Mol	Chain	Length	Quality of chain
1	F	217	5% 73% 18% 5%
1	G	217	6% 73% 22%
1	H	217	3% 69% 24%
1	I	217	5% 75% 19%
1	J	217	7% 69% 23% 5%

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
3	NAG	G	302	-	-	-	X
3	NAG	I	302	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17236 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1673	1047	284	337	5	0	1	0
1	B	205	1650	1032	280	333	5	0	2	0
1	C	207	1665	1043	283	334	5	0	1	0
1	D	213	1711	1067	290	349	5	0	1	0
1	E	207	1664	1039	282	338	5	0	2	0
1	F	208	1689	1057	284	343	5	0	4	0
1	G	210	1693	1058	286	344	5	0	2	0
1	H	209	1690	1057	285	343	5	0	3	0
1	I	209	1694	1060	285	344	5	0	4	0
1	J	207	1676	1050	283	338	5	0	3	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P58154
A	-6	TYR	-	expression tag	UNP P58154
A	-5	LYS	-	expression tag	UNP P58154
A	-4	ASP	-	expression tag	UNP P58154
A	-3	ASP	-	expression tag	UNP P58154
A	-2	ASP	-	expression tag	UNP P58154
A	-1	ASP	-	expression tag	UNP P58154
A	0	LYS	-	expression tag	UNP P58154
B	-7	ASP	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	expression tag	UNP P58154
B	-5	LYS	-	expression tag	UNP P58154
B	-4	ASP	-	expression tag	UNP P58154
B	-3	ASP	-	expression tag	UNP P58154
B	-2	ASP	-	expression tag	UNP P58154
B	-1	ASP	-	expression tag	UNP P58154
B	0	LYS	-	expression tag	UNP P58154
C	-7	ASP	-	expression tag	UNP P58154
C	-6	TYR	-	expression tag	UNP P58154
C	-5	LYS	-	expression tag	UNP P58154
C	-4	ASP	-	expression tag	UNP P58154
C	-3	ASP	-	expression tag	UNP P58154
C	-2	ASP	-	expression tag	UNP P58154
C	-1	ASP	-	expression tag	UNP P58154
C	0	LYS	-	expression tag	UNP P58154
D	-7	ASP	-	expression tag	UNP P58154
D	-6	TYR	-	expression tag	UNP P58154
D	-5	LYS	-	expression tag	UNP P58154
D	-4	ASP	-	expression tag	UNP P58154
D	-3	ASP	-	expression tag	UNP P58154
D	-2	ASP	-	expression tag	UNP P58154
D	-1	ASP	-	expression tag	UNP P58154
D	0	LYS	-	expression tag	UNP P58154
E	-7	ASP	-	expression tag	UNP P58154
E	-6	TYR	-	expression tag	UNP P58154
E	-5	LYS	-	expression tag	UNP P58154
E	-4	ASP	-	expression tag	UNP P58154
E	-3	ASP	-	expression tag	UNP P58154
E	-2	ASP	-	expression tag	UNP P58154
E	-1	ASP	-	expression tag	UNP P58154
E	0	LYS	-	expression tag	UNP P58154
F	-7	ASP	-	expression tag	UNP P58154
F	-6	TYR	-	expression tag	UNP P58154
F	-5	LYS	-	expression tag	UNP P58154
F	-4	ASP	-	expression tag	UNP P58154
F	-3	ASP	-	expression tag	UNP P58154
F	-2	ASP	-	expression tag	UNP P58154
F	-1	ASP	-	expression tag	UNP P58154
F	0	LYS	-	expression tag	UNP P58154
G	-7	ASP	-	expression tag	UNP P58154
G	-6	TYR	-	expression tag	UNP P58154
G	-5	LYS	-	expression tag	UNP P58154

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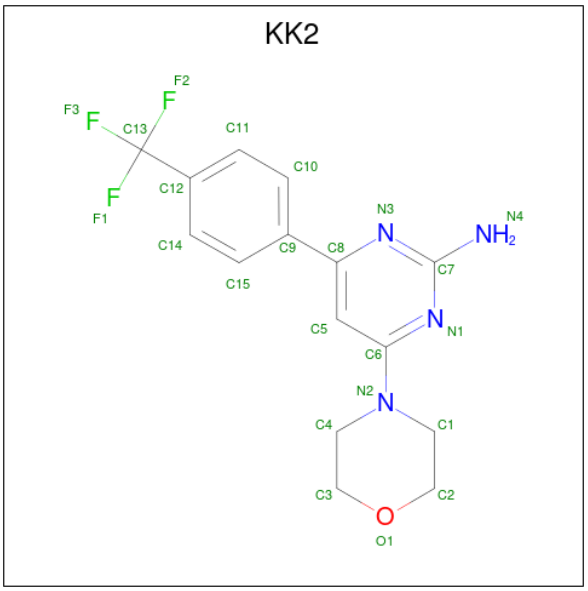
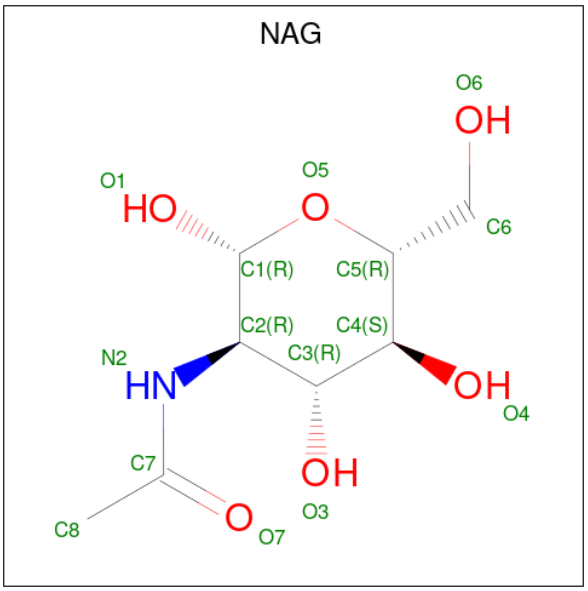
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP P58154
G	-3	ASP	-	expression tag	UNP P58154
G	-2	ASP	-	expression tag	UNP P58154
G	-1	ASP	-	expression tag	UNP P58154
G	0	LYS	-	expression tag	UNP P58154
H	-7	ASP	-	expression tag	UNP P58154
H	-6	TYR	-	expression tag	UNP P58154
H	-5	LYS	-	expression tag	UNP P58154
H	-4	ASP	-	expression tag	UNP P58154
H	-3	ASP	-	expression tag	UNP P58154
H	-2	ASP	-	expression tag	UNP P58154
H	-1	ASP	-	expression tag	UNP P58154
H	0	LYS	-	expression tag	UNP P58154
I	-7	ASP	-	expression tag	UNP P58154
I	-6	TYR	-	expression tag	UNP P58154
I	-5	LYS	-	expression tag	UNP P58154
I	-4	ASP	-	expression tag	UNP P58154
I	-3	ASP	-	expression tag	UNP P58154
I	-2	ASP	-	expression tag	UNP P58154
I	-1	ASP	-	expression tag	UNP P58154
I	0	LYS	-	expression tag	UNP P58154
J	-7	ASP	-	expression tag	UNP P58154
J	-6	TYR	-	expression tag	UNP P58154
J	-5	LYS	-	expression tag	UNP P58154
J	-4	ASP	-	expression tag	UNP P58154
J	-3	ASP	-	expression tag	UNP P58154
J	-2	ASP	-	expression tag	UNP P58154
J	-1	ASP	-	expression tag	UNP P58154
J	0	LYS	-	expression tag	UNP P58154

- Molecule 2 is 4-(morpholin-4-yl)-6-[4-(trifluoromethyl)phenyl]pyrimidin-2-amine (three-letter code: KK2) (formula: $C_{15}H_{15}F_3N_4O$).



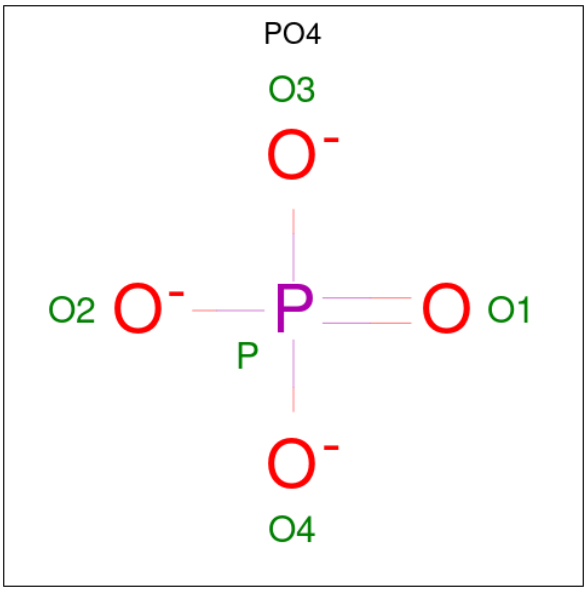
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	B	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	C	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	D	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	E	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	F	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	G	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	H	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	I	1	Total	C	F	N	O	0	0
			23	15	3	4	1		
2	J	1	Total	C	F	N	O	0	0
			23	15	3	4	1		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0
3	C	1	14	8	1	5	0	0
3	D	1	14	8	1	5	0	0
3	E	1	14	8	1	5	0	0
3	G	1	14	8	1	5	0	0
3	H	1	14	8	1	5	0	0
3	I	1	14	8	1	5	0	0
3	J	1	14	8	1	5	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	G	1	Total O P 5 4 1	0	0
4	H	1	Total O P 5 4 1	0	0
4	I	1	Total O P 5 4 1	0	0
4	J	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	3	Total O 3 3	0	0

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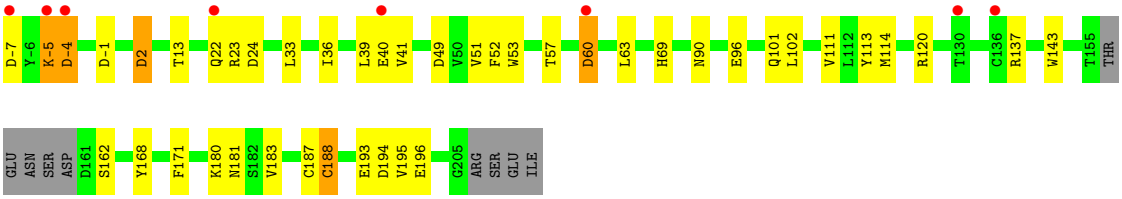
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	1	1	1	0	0
			Total	O		
5	D	3	3	3	0	0
			Total	O		
5	E	4	4	4	0	0
			Total	O		
5	F	3	3	3	0	0
			Total	O		
5	G	1	1	1	0	0
			Total	O		
5	I	2	2	2	0	0
			Total	O		
5	J	2	2	2	0	0

3 Residue-property plots (i)

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.

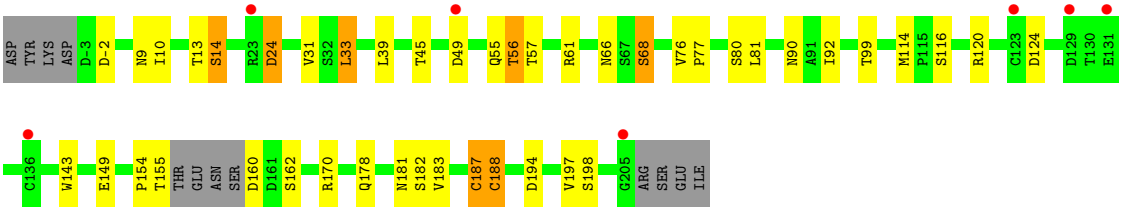
• Molecule 1: Acetylcholine-binding protein

Chain A:



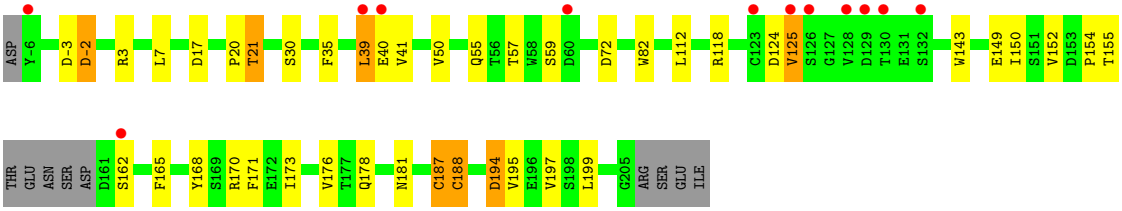
• Molecule 1: Acetylcholine-binding protein

Chain B:



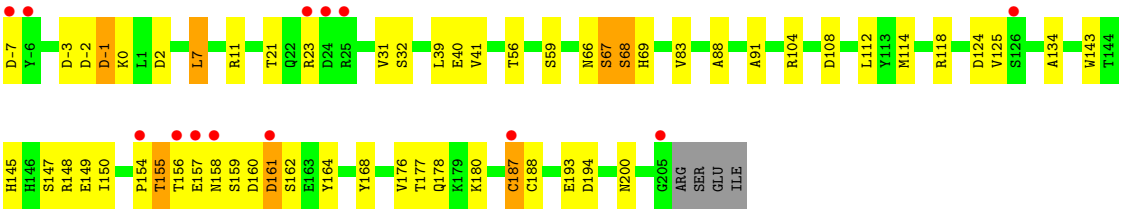
• Molecule 1: Acetylcholine-binding protein

Chain C:



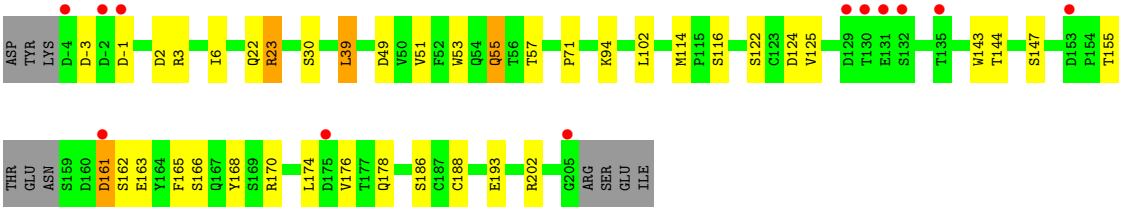
• Molecule 1: Acetylcholine-binding protein

Chain D:



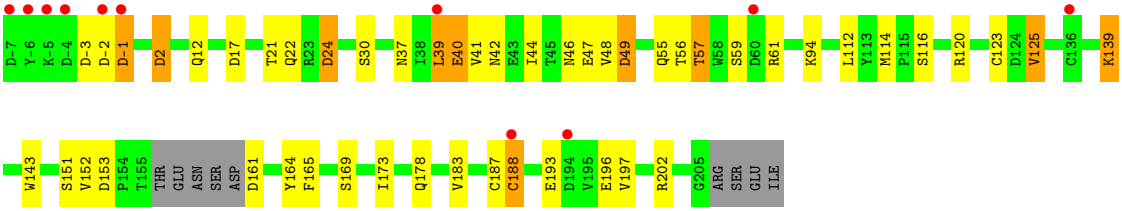
• Molecule 1: Acetylcholine-binding protein

Chain E:



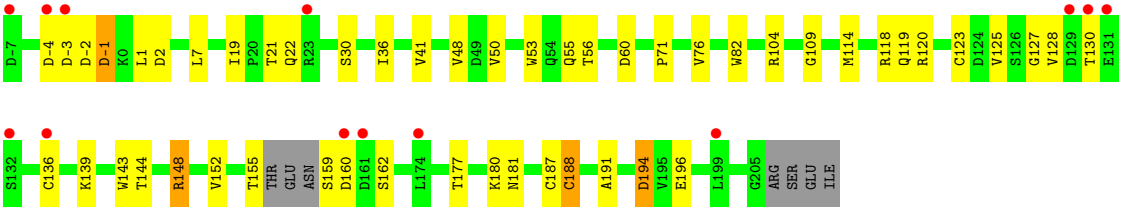
• Molecule 1: Acetylcholine-binding protein

Chain F:



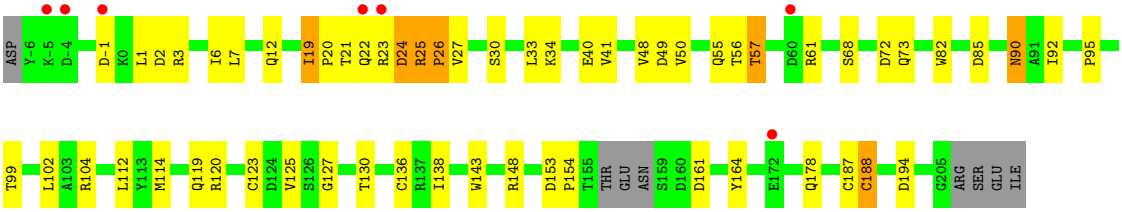
• Molecule 1: Acetylcholine-binding protein

Chain G:



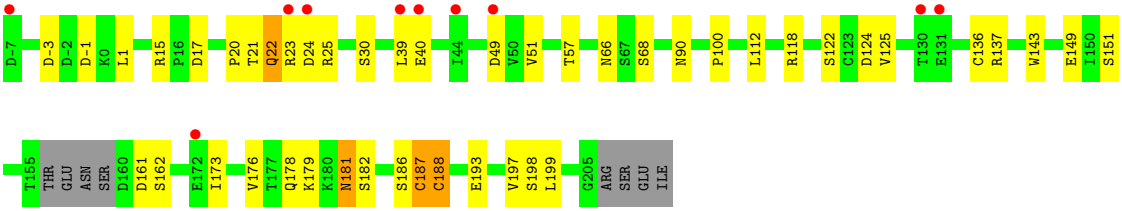
• Molecule 1: Acetylcholine-binding protein

Chain H:



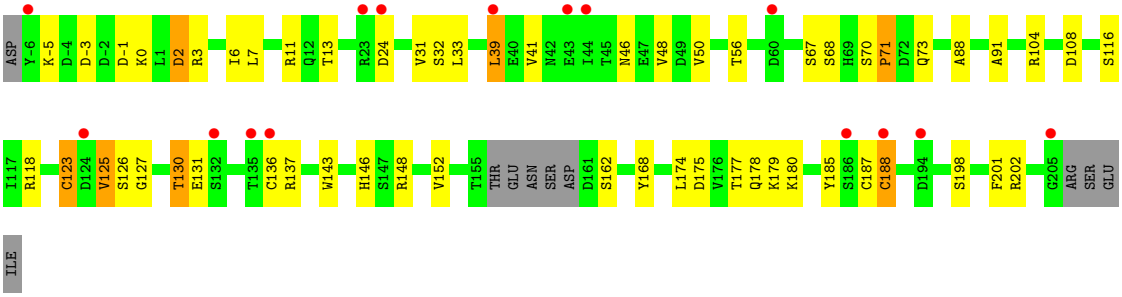
• Molecule 1: Acetylcholine-binding protein

Chain I:



• Molecule 1: Acetylcholine-binding protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.64Å 134.01Å 147.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.98 49.52 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.52-2.98) 97.4 (49.52-2.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	9.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.150 , 0.233 0.169 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17236	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, KK2, PO4

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	0.51	0/1712	0.60	0/2333
1	B	0.46	0/1691	0.60	0/2305
1	C	0.41	0/1704	0.58	0/2322
1	D	0.46	0/1751	0.58	0/2388
1	E	0.45	0/1705	0.59	0/2324
1	F	0.50	0/1737	0.59	0/2367
1	G	0.46	0/1735	0.59	0/2364
1	H	0.58	2/1735 (0.1%)	0.69	3/2364 (0.1%)
1	I	0.44	0/1746	0.59	0/2379
1	J	0.47	1/1721 (0.1%)	0.61	0/2345
All	All	0.48	3/17237 (0.0%)	0.60	3/23491 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	26	PRO	N-CD	5.11	1.55	1.47
1	J	71	PRO	N-CD	5.06	1.54	1.47
1	H	154	PRO	N-CD	5.04	1.54	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	153	ASP	C-N-CD	5.87	140.72	128.40
1	H	25	ARG	C-N-CD	5.72	140.42	128.40
1	H	19	ILE	C-N-CD	5.62	140.20	128.40

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	1673	0	1610	28	0
1	B	1650	0	1590	25	0
1	C	1665	0	1606	28	0
1	D	1711	0	1639	55	0
1	E	1664	0	1599	25	0
1	F	1689	0	1625	33	0
1	G	1693	0	1625	33	0
1	H	1690	0	1625	36	0
1	I	1694	0	1630	36	0
1	J	1676	0	1618	43	0
2	A	23	0	15	2	0
2	B	23	0	15	1	0
2	C	23	0	15	3	0
2	D	23	0	15	1	0
2	E	23	0	15	1	0
2	F	23	0	15	1	0
2	G	23	0	15	2	0
2	H	23	0	15	1	0
2	I	23	0	15	2	0
2	J	23	0	15	2	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
3	E	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	2	0
3	I	14	0	13	1	0
3	J	14	0	13	0	0
4	A	5	0	0	0	0
4	C	5	0	0	1	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	5	0	0	1	0
5	A	6	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	3	0	0	0	0
5	E	4	0	0	0	0
5	F	3	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0
All	All	17236	0	16434	312	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 9.

All (312) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:THR:CG2	1:D:178:GLN:HB2	1.43	1.47
1:D:156:THR:HG21	1:D:178:GLN:CB	1.59	1.31
1:J:123:CYS:SG	1:J:136:CYS:HB3	1.85	1.17
1:D:156:THR:HB	1:D:157:GLU:CG	1.76	1.16
1:F:21:THR:HG21	1:G:-2:ASP:HB3	1.14	1.12
1:C:162:SER:HB2	1:C:165:PHE:HB2	1.31	1.12
1:D:156:THR:CB	1:D:157:GLU:HG2	1.80	1.10
1:D:32:SER:HB2	1:D:155:THR:HG21	1.40	1.04
1:E:22:GLN:C	1:E:23:ARG:HG2	1.81	0.98
1:D:156:THR:HB	1:D:157:GLU:HG2	0.98	0.98
1:D:156:THR:CG2	1:D:178:GLN:CB	2.28	0.95
1:D:156:THR:HG23	1:D:178:GLN:NE2	1.83	0.93
1:H:26:PRO:HG3	1:H:148:ARG:O	1.67	0.93
1:F:21:THR:CG2	1:G:-2:ASP:HB3	2.00	0.87
1:J:123:CYS:SG	1:J:136:CYS:CB	2.62	0.87
1:F:21:THR:HG21	1:G:-2:ASP:CB	2.05	0.85
1:B:92:ILE:HD12	1:C:39:LEU:HD11	1.59	0.83
1:A:60:ASP:OD1	1:A:63:LEU:HD12	1.78	0.82
1:H:24:ASP:O	1:H:25:ARG:HG3	1.79	0.82
1:D:156:THR:HG23	1:D:178:GLN:HE21	1.44	0.80
1:A:39:LEU:HD11	1:A:51:VAL:HG23	1.63	0.79
1:D:32:SER:HB2	1:D:155:THR:CG2	2.14	0.78
1:C:162:SER:HB2	1:C:165:PHE:CB	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:HB2	1:D:176:VAL:CG2	2.14	0.77
1:D:156:THR:CG2	1:D:178:GLN:NE2	2.48	0.76
1:A:187:CYS:SG	1:A:188:CYS:N	2.58	0.76
1:I:187:CYS:SG	1:I:188:CYS:N	2.58	0.76
1:I:39:LEU:CD2	1:I:51:VAL:HG23	2.17	0.75
1:J:39:LEU:HD13	1:J:118:ARG:HE	1.51	0.75
1:A:40:GLU:H	1:A:49:ASP:HB3	1.53	0.74
1:H:34:LYS:HD2	1:H:164:TYR:HE1	1.53	0.73
1:J:136:CYS:SG	1:J:201:PHE:HE1	2.12	0.73
1:G:55:GLN:HA	1:G:114:MET:HG2	1.71	0.72
1:A:40:GLU:HB2	1:A:49:ASP:HB2	1.71	0.72
1:G:41:VAL:HG22	1:G:48:VAL:HG12	1.70	0.72
1:F:164:TYR:HE2	1:J:185:TYR:CD1	2.07	0.72
1:F:55:GLN:HA	1:F:114:MET:HG2	1.72	0.72
1:H:21:THR:HA	1:H:27:VAL:HG22	1.72	0.72
1:J:187:CYS:SG	1:J:188:CYS:N	2.65	0.69
1:E:22:GLN:O	1:E:23:ARG:HG2	1.93	0.69
1:J:39:LEU:HD22	1:J:118:ARG:NH2	2.08	0.69
1:D:161:ASP:HB2	1:D:176:VAL:HG21	1.75	0.69
1:F:30:SER:HB2	1:F:57:THR:HG23	1.76	0.68
1:A:23:ARG:O	1:A:24:ASP:HB2	1.94	0.68
1:I:39:LEU:O	1:I:40:GLU:HG3	1.95	0.67
1:D:39:LEU:C	1:D:40:GLU:HG3	2.15	0.67
1:I:39:LEU:HB2	1:I:49[A]:ASP:HB3	1.76	0.67
1:D:143:TRP:CE2	2:D:301:KK2:H15	2.30	0.67
1:H:143:TRP:CE2	2:H:301:KK2:H15	2.31	0.66
1:D:161:ASP:CB	1:D:176:VAL:CG2	2.74	0.66
1:E:55:GLN:HG3	1:E:114:MET:HG2	1.78	0.65
1:B:45:THR:HA	1:C:170:ARG:HD2	1.79	0.65
1:I:39:LEU:HD21	1:I:51:VAL:HG23	1.77	0.65
1:D:155:THR:HG23	1:D:155:THR:O	1.97	0.64
1:H:30:SER:HB2	1:H:57:THR:HG23	1.79	0.64
1:B:187:CYS:SG	1:B:188:CYS:N	2.71	0.63
1:G:187:CYS:SG	1:G:188:CYS:N	2.71	0.63
1:C:41:VAL:HG21	1:C:171:PHE:CZ	2.33	0.63
1:J:32:SER:O	1:J:33:LEU:HD23	1.99	0.63
1:G:19:ILE:HD12	1:G:21:THR:HG23	1.80	0.63
1:F:57:THR:HB	1:F:112:LEU:HD23	1.80	0.63
1:J:3:ARG:NH1	4:J:303:PO4:O2	2.32	0.62
3:H:302:NAG:O7	3:H:302:NAG:O3	2.11	0.62
1:D:159:SER:HB2	1:D:160:ASP:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ASP:CB	1:D:176:VAL:HG23	2.29	0.62
1:D:161:ASP:HB2	1:D:176:VAL:HG23	1.79	0.62
1:G:-1:ASP:HB2	1:G:2:ASP:HB2	1.82	0.61
1:I:30:SER:HB2	1:I:57:THR:HG23	1.82	0.61
1:I:39:LEU:HD23	1:I:51:VAL:HG23	1.82	0.60
1:B:55:GLN:HA	1:B:114:MET:HG2	1.83	0.60
1:J:41:VAL:HG13	1:J:125:VAL:HG11	1.83	0.60
1:G:-1:ASP:N	1:G:-1:ASP:OD2	2.34	0.60
1:E:22:GLN:HB3	1:E:23:ARG:NE	2.16	0.60
1:B:9:ASN:HD22	1:I:1:LEU:HD21	1.66	0.60
1:A:-1:ASP:HB3	1:A:2:ASP:HB2	1.84	0.60
1:H:85:ASP:HB2	1:I:100:PRO:HG2	1.83	0.60
1:C:162:SER:HB3	1:C:173:ILE:HD12	1.83	0.60
1:I:143:TRP:CE2	2:I:301:KK2:H15	2.36	0.60
1:A:24:ASP:HA	1:B:-2:ASP:HB3	1.85	0.59
1:E:174:LEU:HD11	1:E:202:ARG:HG2	1.84	0.59
1:D:156:THR:CG2	1:D:178:GLN:CG	2.80	0.59
1:J:39:LEU:HD22	1:J:118:ARG:HH21	1.68	0.59
1:B:143:TRP:CE2	2:B:301:KK2:H15	2.37	0.58
1:F:49:ASP:OD1	1:F:120:ARG:HG2	2.03	0.58
1:B:24:ASP:HA	1:C:-2:ASP:HB2	1.86	0.58
1:E:30:SER:HB3	1:E:57:THR:HG23	1.85	0.58
1:F:139:LYS:HG3	1:F:196:GLU:HG3	1.85	0.58
1:D:158:ASN:HA	1:D:159:SER:C	2.24	0.58
1:G:118:ARG:HE	1:G:120:ARG:HH12	1.50	0.58
1:H:34:LYS:HD2	1:H:164:TYR:CE1	2.38	0.58
1:I:137:ARG:NH1	1:I:198:SER:OG	2.37	0.57
1:C:143:TRP:CE2	2:C:301:KK2:H15	2.39	0.57
1:D:-1:ASP:OD2	1:D:-1:ASP:N	2.37	0.57
1:D:31:VAL:O	1:D:155:THR:HB	2.05	0.57
1:H:49[B]:ASP:OD1	1:H:120:ARG:NE	2.35	0.57
1:B:49[B]:ASP:CG	1:B:120:ARG:HG2	2.25	0.57
1:C:41:VAL:HG13	1:C:125:VAL:HG11	1.86	0.57
1:F:187:CYS:SG	1:F:188:CYS:N	2.77	0.57
1:J:136:CYS:SG	1:J:201:PHE:CE1	2.95	0.57
1:E:39:LEU:HD21	1:E:51:VAL:HG23	1.87	0.57
1:F:46:ASN:HB3	1:F:123:CYS:O	2.05	0.57
1:G:127:GLY:HA2	1:G:130:THR:HG23	1.87	0.57
1:J:137:ARG:HH12	1:J:179:LYS:NZ	2.03	0.57
1:D:154:PRO:HD3	1:D:180:LYS:HD2	1.87	0.56
1:I:17:ASP:OD2	1:J:11:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:LEU:HD21	1:I:51:VAL:CG2	2.35	0.56
1:E:55:GLN:HA	1:E:114:MET:HG2	1.88	0.56
1:H:21:THR:HA	1:H:27:VAL:CG2	2.35	0.56
1:J:39:LEU:HD13	1:J:118:ARG:NE	2.20	0.56
1:I:39:LEU:CD1	1:I:118:ARG:NH1	2.69	0.56
1:D:156:THR:HG21	1:D:178:GLN:HB2	0.62	0.56
1:F:47:GLU:HB3	1:F:120:ARG:HH21	1.71	0.56
1:J:185:TYR:OH	2:J:301:KK2:H1	2.06	0.56
1:B:178:GLN:HG2	1:B:197:VAL:HG22	1.88	0.55
1:C:20:PRO:HA	1:D:0:LYS:HD2	1.88	0.55
1:I:20:PRO:HA	1:J:0:LYS:HE3	1.89	0.55
1:H:-1:ASP:HB3	1:H:2:ASP:HB2	1.88	0.55
1:F:40:GLU:HB2	1:F:49:ASP:HB2	1.89	0.55
1:C:187:CYS:SG	1:C:188:CYS:N	2.80	0.55
1:F:41:VAL:HG13	1:F:125:VAL:HG11	1.89	0.54
1:H:26:PRO:HG3	1:H:148:ARG:C	2.28	0.54
1:I:23:ARG:HB3	1:I:25:ARG:HH21	1.72	0.54
1:J:123:CYS:HG	1:J:136:CYS:CB	2.20	0.54
2:C:301:KK2:H6	1:D:164:TYR:CD1	2.42	0.54
1:F:37:ASN:OD1	1:F:169:SER:HB2	2.07	0.54
1:D:155:THR:CG2	1:D:155:THR:O	2.54	0.54
1:F:24:ASP:HA	1:G:-2:ASP:HB2	1.90	0.54
1:J:146:HIS:CE1	1:J:148:ARG:HG3	2.43	0.54
1:D:156:THR:CG2	1:D:178:GLN:CD	2.76	0.54
1:D:41:VAL:CG1	1:D:125:VAL:HG11	2.37	0.54
1:G:148:ARG:HH22	1:G:191:ALA:H	1.54	0.54
1:J:88:ALA:HB3	1:J:91:ALA:HB2	1.90	0.53
1:H:55:GLN:HA	1:H:114:MET:HG2	1.88	0.53
3:H:302:NAG:HO3	3:H:302:NAG:C7	2.15	0.53
1:H:48:VAL:HG21	1:H:123:CYS:SG	2.49	0.52
1:J:41:VAL:HG22	1:J:48:VAL:HG23	1.91	0.52
1:J:131:GLU:O	1:J:202:ARG:NH1	2.42	0.52
1:H:41:VAL:HG22	1:H:48:VAL:HG12	1.90	0.52
1:B:31:VAL:HG22	1:B:56:THR:HG23	1.90	0.52
1:C:17:ASP:OD2	1:D:11:ARG:NH2	2.43	0.52
1:E:143:TRP:CE2	2:E:301:KK2:H15	2.44	0.52
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.44	0.52
1:G:60:ASP:O	1:G:109:GLY:HA3	2.08	0.52
1:I:149:GLU:OE2	1:J:3:ARG:NH2	2.43	0.52
1:J:137:ARG:HH12	1:J:179:LYS:HZ1	1.57	0.52
1:H:40:GLU:OE1	1:H:120:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:-1:ASP:HB3	1:J:2:ASP:HB2	1.91	0.51
1:I:22:GLN:CG	1:I:23:ARG:HD2	2.40	0.51
1:B:124:ASP:HB2	1:C:168:TYR:CE1	2.46	0.51
1:H:19:ILE:HG22	1:H:82:TRP:CZ2	2.46	0.51
1:H:123:CYS:O	1:H:125:VAL:HG23	2.10	0.51
1:I:23:ARG:CB	1:I:25:ARG:HH21	2.23	0.51
1:F:21:THR:CG2	1:G:-2:ASP:O	2.59	0.51
1:A:102:LEU:HB2	1:E:144:THR:HG21	1.92	0.51
1:I:39:LEU:HD12	1:I:118:ARG:NH1	2.25	0.51
1:C:154:PRO:HD3	1:C:195:VAL:HG22	1.92	0.51
1:F:164:TYR:HE2	1:J:185:TYR:HD1	1.55	0.50
1:H:90:ASN:HD21	1:H:138:ILE:HA	1.75	0.50
1:E:22:GLN:HB3	1:E:23:ARG:CZ	2.42	0.50
1:I:39:LEU:HB2	1:I:49[B]:ASP:HB2	1.92	0.50
1:J:152:VAL:O	1:J:180:LYS:NZ	2.42	0.50
1:B:181:ASN:HB3	1:B:194:ASP:OD1	2.12	0.50
1:I:161:ASP:OD2	1:I:176:VAL:HG21	2.11	0.50
1:H:41:VAL:HG13	1:H:125:VAL:HG11	1.93	0.50
1:F:143:TRP:CE2	2:F:301:KK2:H15	2.47	0.50
1:G:36:ILE:HD11	1:G:53:TRP:HB2	1.94	0.50
1:C:41:VAL:CG2	1:C:171:PHE:CZ	2.94	0.49
1:H:3:ARG:NH2	4:H:303:PO4:O1	2.27	0.49
1:E:162:SER:HA	1:E:165:PHE:HB3	1.94	0.49
1:A:39:LEU:HD11	1:A:51:VAL:CG2	2.38	0.49
1:D:187:CYS:SG	1:D:188:CYS:N	2.86	0.49
1:D:39:LEU:O	1:D:40:GLU:HG3	2.13	0.49
1:D:88:ALA:HB3	1:D:91:ALA:HB2	1.94	0.49
1:H:48:VAL:CG2	1:H:123:CYS:SG	3.00	0.49
1:I:66:ASN:ND2	3:I:302:NAG:H61	2.27	0.49
1:I:178:GLN:HG2	1:I:197:VAL:HG13	1.93	0.49
1:J:143:TRP:CE2	2:J:301:KK2:H15	2.48	0.49
1:G:144:THR:HG21	1:H:102:LEU:HB2	1.95	0.48
1:G:41:VAL:HG13	1:G:125:VAL:HG11	1.95	0.48
1:H:187:CYS:SG	1:H:188:CYS:N	2.86	0.48
1:A:41:VAL:HG21	1:A:171:PHE:CZ	2.48	0.48
1:D:39:LEU:HD12	1:D:118:ARG:HE	1.78	0.48
1:G:19:ILE:HG22	1:G:82:TRP:CZ2	2.49	0.48
1:I:124:ASP:HB2	1:J:168:TYR:CE1	2.49	0.48
1:A:33:LEU:HD22	1:A:52:PHE:CD1	2.48	0.48
1:D:66:ASN:OD1	1:D:68:SER:OG	2.32	0.48
1:J:108:ASP:OD1	1:J:108:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194[B]:ASP:OD1	1:A:195:VAL:N	2.46	0.47
1:H:22:GLN:O	1:H:23:ARG:C	2.51	0.47
1:J:33:LEU:H	1:J:178:GLN:HE22	1.63	0.47
1:G:139:LYS:HG2	1:G:196:GLU:HG3	1.95	0.47
1:G:118:ARG:HE	1:G:120:ARG:NH1	2.13	0.47
1:D:68:SER:O	1:D:69:HIS:ND1	2.47	0.47
1:G:143:TRP:CZ2	1:H:99:THR:HG21	2.50	0.47
1:H:112:LEU:HD23	1:H:114:MET:HE3	1.96	0.47
1:C:21:THR:HG21	1:D:-2:ASP:O	2.15	0.47
1:J:137:ARG:NH1	1:J:179:LYS:NZ	2.62	0.47
2:G:301:KK2:H6	1:H:164:TYR:CD2	2.50	0.47
1:E:147:SER:HB3	1:E:193:GLU:HG3	1.97	0.47
1:F:-1:ASP:HB3	1:F:2:ASP:HB2	1.97	0.47
1:A:39:LEU:CD1	1:A:51:VAL:HG23	2.40	0.46
1:A:60:ASP:OD1	1:A:63:LEU:CD1	2.58	0.46
1:E:39:LEU:HD23	1:E:49[A]:ASP:OD1	2.15	0.46
1:A:137:ARG:HD3	1:A:196:GLU:OE2	2.16	0.46
1:I:22:GLN:HG2	1:I:23:ARG:HD2	1.98	0.46
1:J:67:SER:HA	1:J:70:SER:HB2	1.98	0.46
1:D:156:THR:HG22	1:D:178:GLN:CD	2.35	0.46
1:E:161:ASP:O	1:E:162:SER:HB2	2.15	0.46
1:F:165:PHE:CD1	1:F:173:ILE:HD11	2.51	0.46
1:I:173:ILE:HG12	1:I:199:LEU:HD11	1.98	0.46
1:E:6:ILE:HD12	1:E:71:PRO:HG2	1.98	0.46
1:H:22:GLN:HE22	1:H:61:ARG:HH11	1.62	0.45
1:A:53:TRP:HE1	1:A:114:MET:HB3	1.82	0.45
1:D:149:GLU:OE2	1:E:3:ARG:NH2	2.49	0.45
1:D:161:ASP:CB	1:D:176:VAL:HG21	2.42	0.45
1:D:162:SER:O	1:D:162:SER:OG	2.33	0.45
1:G:60:ASP:O	1:G:109:GLY:CA	2.64	0.45
1:F:48:VAL:HG12	1:F:123:CYS:SG	2.56	0.45
1:I:57:THR:HB	1:I:112:LEU:HD23	1.98	0.45
1:F:41:VAL:CG1	1:F:125:VAL:HG11	2.46	0.45
1:A:22:GLN:O	1:A:23:ARG:HB2	2.16	0.45
1:A:101:GLN:HG2	1:A:113:TYR:OH	2.17	0.45
1:J:127:GLY:HA2	1:J:130:THR:HG23	1.99	0.45
1:H:95:PRO:HG3	1:H:119:GLN:NE2	2.31	0.45
1:A:143:TRP:CE2	2:A:301:KK2:H12	2.52	0.45
1:F:40:GLU:O	1:F:41:VAL:HG23	2.17	0.45
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.52	0.44
1:D:158:ASN:HB3	1:D:160:ASP:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:O	1:B:14:SER:HB3	2.17	0.44
1:I:1:LEU:HD12	1:I:1:LEU:HA	1.69	0.44
1:F:151:SER:HA	1:F:193[B]:GLU:OE1	2.17	0.44
1:A:180:LYS:HE3	1:A:193:GLU:OE1	2.17	0.44
1:B:49[B]:ASP:OD2	1:B:120:ARG:HG2	2.17	0.44
1:A:96:GLU:HG3	1:E:94:LYS:HD2	1.99	0.44
1:I:39:LEU:CB	1:I:49[A]:ASP:HB3	2.45	0.44
1:B:80:SER:O	1:B:81:LEU:HD23	2.18	0.44
1:D:159:SER:HA	1:D:160:ASP:HA	1.49	0.44
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.53	0.44
1:B:9:ASN:ND2	1:I:1:LEU:HD21	2.33	0.44
1:C:30:SER:HB3	1:C:155:THR:HG22	1.99	0.44
1:D:-7:ASP:N	1:D:67:SER:O	2.50	0.43
1:G:152:VAL:O	1:G:180:LYS:HE3	2.17	0.43
1:G:181:ASN:HB3	1:G:194[A]:ASP:OD2	2.18	0.43
1:A:-4:ASP:OD1	1:A:69:HIS:O	2.35	0.43
1:C:152:VAL:HG23	1:C:152:VAL:O	2.16	0.43
1:A:-7:ASP:OD1	1:A:-5:LYS:HB2	2.18	0.43
1:D:134:ALA:O	1:D:200:ASN:ND2	2.39	0.43
1:G:60:ASP:O	1:G:109:GLY:O	2.37	0.43
1:A:60:ASP:OD2	1:A:111:VAL:HG23	2.18	0.43
1:C:181:ASN:HB2	1:C:194:ASP:OD1	2.18	0.43
1:E:53:TRP:CZ2	1:E:114:MET:HE3	2.54	0.43
1:E:161:ASP:OD2	1:E:176:VAL:HG23	2.18	0.43
1:D:145:HIS:HB2	1:D:150:ILE:HD12	2.01	0.43
1:F:39:LEU:HD12	1:F:49:ASP:HB3	2.00	0.43
1:F:42:ASN:OD1	1:F:44:ILE:HB	2.19	0.43
1:G:143:TRP:CE2	2:G:301:KK2:H15	2.53	0.43
1:B:39:LEU:O	1:B:170:ARG:NH1	2.52	0.43
1:C:35:PHE:CZ	1:C:199:LEU:HD22	2.53	0.43
1:C:176:VAL:HG22	1:C:199:LEU:HD13	2.01	0.43
1:E:22:GLN:O	1:E:23:ARG:CG	2.65	0.43
2:A:301:KK2:H9	2:A:301:KK2:H1	1.85	0.42
1:H:2:ASP:O	1:H:6:ILE:HG13	2.19	0.42
1:H:73:GLN:NE2	1:H:104:ARG:HH21	2.17	0.42
1:J:174:LEU:HD21	1:J:202:ARG:HG2	2.00	0.42
1:J:46:ASN:OD1	1:J:125:VAL:HG23	2.19	0.42
1:J:73:GLN:HG3	1:J:104:ARG:HH21	1.84	0.42
1:D:7:LEU:HD22	1:D:11:ARG:HE	1.83	0.42
1:J:-5:LYS:HE2	1:J:-5:LYS:HB3	1.78	0.42
1:D:157:GLU:OE2	1:D:177:THR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:GLN:HG2	1:F:197:VAL:HG22	2.01	0.42
1:I:22:GLN:HG3	1:I:23:ARG:HD2	2.00	0.42
1:C:3:ARG:NH2	4:C:303:PO4:O3	2.37	0.42
1:F:152:VAL:HG22	1:F:193[A]:GLU:CG	2.50	0.42
1:G:159:SER:HA	1:G:160:ASP:HA	1.74	0.42
1:F:40:GLU:C	1:F:41:VAL:HG23	2.40	0.42
1:I:151:SER:HB2	1:I:193:GLU:OE1	2.20	0.42
1:B:90:ASN:OD1	1:B:90:ASN:N	2.53	0.41
1:B:99:THR:HG23	1:B:116:SER:HB3	2.02	0.41
1:I:39:LEU:HD11	1:I:118:ARG:NH1	2.35	0.41
1:B:76:VAL:HG12	1:B:77:PRO:O	2.20	0.41
1:C:82:TRP:HZ2	1:C:150:ILE:HD11	1.85	0.41
1:D:156:THR:HB	1:D:157:GLU:CA	2.49	0.41
1:F:22:GLN:NE2	1:F:61:ARG:HD3	2.34	0.41
1:J:7:LEU:HD12	1:J:7:LEU:HA	1.86	0.41
1:B:33:LEU:HG	1:B:197:VAL:HG21	2.03	0.41
1:B:92:ILE:HD12	1:C:39:LEU:CD1	2.40	0.41
1:J:2:ASP:HB3	1:J:71:PRO:HD3	2.02	0.41
1:G:1:LEU:HD12	1:G:1:LEU:HA	1.87	0.41
1:G:48:VAL:HG22	1:G:123:CYS:SG	2.60	0.41
1:C:178:GLN:HG2	1:C:197:VAL:HG22	2.03	0.41
1:A:33:LEU:HD22	1:A:52:PHE:HD1	1.86	0.41
2:C:301:KK2:F3	1:D:104:ARG:HG3	2.11	0.41
1:G:-4:ASP:O	1:G:71:PRO:HA	2.21	0.41
1:G:143:TRP:CE2	1:H:99:THR:HG21	2.56	0.41
1:A:36:ILE:HB	1:A:51:VAL:O	2.21	0.41
1:C:-2:ASP:N	1:C:-2:ASP:OD1	2.53	0.41
1:H:33:LEU:H	1:H:178:GLN:HE22	1.69	0.41
1:E:102:LEU:HD23	1:E:102:LEU:HA	1.87	0.41
1:B:92:ILE:O	1:C:118:ARG:HD2	2.20	0.40
1:B:66:ASN:OD1	1:B:68:SER:OG	2.39	0.40
1:D:147:SER:HB3	1:D:193:GLU:HG3	2.04	0.40
1:F:48:VAL:CG1	1:F:123:CYS:SG	3.09	0.40
1:H:127:GLY:HA2	1:H:130:THR:HG23	2.03	0.40
2:I:301:KK2:F3	1:J:104:ARG:HG2	2.11	0.40
1:H:1:LEU:HD12	1:H:1:LEU:HA	1.81	0.40
1:J:6:ILE:HD11	1:J:71:PRO:HD2	2.03	0.40
1:G:7:LEU:CD1	1:G:76:VAL:HG22	2.51	0.40
1:I:90:ASN:OD1	1:I:90:ASN:N	2.54	0.40
1:J:146:HIS:HE1	1:J:148:ARG:HG3	1.87	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	205/217 (94%)	196 (96%)	9 (4%)	0	100	100
1	B	203/217 (94%)	196 (97%)	6 (3%)	1 (0%)	29	66
1	C	204/217 (94%)	198 (97%)	6 (3%)	0	100	100
1	D	212/217 (98%)	208 (98%)	4 (2%)	0	100	100
1	E	205/217 (94%)	204 (100%)	1 (0%)	0	100	100
1	F	208/217 (96%)	199 (96%)	9 (4%)	0	100	100
1	G	208/217 (96%)	204 (98%)	4 (2%)	0	100	100
1	H	208/217 (96%)	205 (99%)	3 (1%)	0	100	100
1	I	209/217 (96%)	208 (100%)	1 (0%)	0	100	100
1	J	206/217 (95%)	203 (98%)	3 (2%)	0	100	100
All	All	2068/2170 (95%)	2021 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	154	PRO

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	195/203 (96%)	183 (94%)	12 (6%)	18	50
1	B	193/203 (95%)	176 (91%)	17 (9%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	194/203 (96%)	176 (91%)	18 (9%)	9	31
1	D	200/203 (98%)	181 (90%)	19 (10%)	8	30
1	E	195/203 (96%)	178 (91%)	17 (9%)	10	35
1	F	198/203 (98%)	177 (89%)	21 (11%)	6	25
1	G	198/203 (98%)	181 (91%)	17 (9%)	10	35
1	H	198/203 (98%)	183 (92%)	15 (8%)	13	41
1	I	199/203 (98%)	182 (92%)	17 (8%)	10	36
1	J	196/203 (97%)	177 (90%)	19 (10%)	8	29
All	All	1966/2030 (97%)	1794 (91%)	172 (9%)	10	35

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	LYS
1	A	-4	ASP
1	A	2	ASP
1	A	13	THR
1	A	57	THR
1	A	60	ASP
1	A	90	ASN
1	A	120	ARG
1	A	162	SER
1	A	181	ASN
1	A	183	VAL
1	A	188	CYS
1	B	13	THR
1	B	14	SER
1	B	24	ASP
1	B	33	LEU
1	B	56	THR
1	B	57	THR
1	B	61	ARG
1	B	68	SER
1	B	149	GLU
1	B	155	THR
1	B	160	ASP
1	B	162	SER
1	B	182	SER
1	B	183	VAL

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Mol	Chain	Res	Type
1	B	187	CYS
1	B	188	CYS
1	B	198	SER
1	C	-3	ASP
1	C	-2	ASP
1	C	7	LEU
1	C	21	THR
1	C	39	LEU
1	C	40	GLU
1	C	50	VAL
1	C	55	GLN
1	C	57	THR
1	C	59	SER
1	C	72[A]	ASP
1	C	72[B]	ASP
1	C	112	LEU
1	C	125	VAL
1	C	149	GLU
1	C	187	CYS
1	C	188	CYS
1	C	194	ASP
1	D	-3	ASP
1	D	-1	ASP
1	D	2	ASP
1	D	7	LEU
1	D	21	THR
1	D	23	ARG
1	D	56	THR
1	D	59	SER
1	D	67	SER
1	D	68	SER
1	D	83	VAL
1	D	108	ASP
1	D	112	LEU
1	D	114	MET
1	D	148	ARG
1	D	155	THR
1	D	161	ASP
1	D	187	CYS
1	D	194	ASP
1	E	-3	ASP
1	E	-1	ASP

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Mol	Chain	Res	Type
1	E	2	ASP
1	E	23	ARG
1	E	39	LEU
1	E	55	GLN
1	E	116	SER
1	E	122	SER
1	E	125	VAL
1	E	155	THR
1	E	161	ASP
1	E	163	GLU
1	E	166	SER
1	E	170	ARG
1	E	178	GLN
1	E	186	SER
1	E	188	CYS
1	F	-3	ASP
1	F	-2	ASP
1	F	-1	ASP
1	F	2	ASP
1	F	12	GLN
1	F	24	ASP
1	F	39	LEU
1	F	40	GLU
1	F	49	ASP
1	F	56	THR
1	F	57	THR
1	F	59	SER
1	F	94	LYS
1	F	116	SER
1	F	125	VAL
1	F	139	LYS
1	F	153	ASP
1	F	161	ASP
1	F	183	VAL
1	F	188	CYS
1	F	202	ARG
1	G	-3	ASP
1	G	-1	ASP
1	G	22	GLN
1	G	30	SER
1	G	50	VAL
1	G	56	THR

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Mol	Chain	Res	Type
1	G	104	ARG
1	G	119	GLN
1	G	128	VAL
1	G	136	CYS
1	G	148	ARG
1	G	155	THR
1	G	162	SER
1	G	177	THR
1	G	188	CYS
1	G	194[A]	ASP
1	G	194[B]	ASP
1	H	7	LEU
1	H	12	GLN
1	H	20	PRO
1	H	24	ASP
1	H	50	VAL
1	H	56	THR
1	H	57	THR
1	H	68	SER
1	H	72	ASP
1	H	90	ASN
1	H	92	ILE
1	H	136	CYS
1	H	161	ASP
1	H	188	CYS
1	H	194	ASP
1	I	-3	ASP
1	I	-1	ASP
1	I	15	ARG
1	I	21	THR
1	I	22	GLN
1	I	24	ASP
1	I	68	SER
1	I	122	SER
1	I	125	VAL
1	I	136	CYS
1	I	162	SER
1	I	179	LYS
1	I	181	ASN
1	I	182	SER
1	I	186	SER
1	I	187	CYS

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Mol	Chain	Res	Type
1	I	188	CYS
1	J	-3	ASP
1	J	2	ASP
1	J	13	THR
1	J	24	ASP
1	J	31	VAL
1	J	39	LEU
1	J	50	VAL
1	J	56	THR
1	J	68	SER
1	J	116	SER
1	J	123	CYS
1	J	125	VAL
1	J	126	SER
1	J	130	THR
1	J	162	SER
1	J	175	ASP
1	J	177	THR
1	J	188	CYS
1	J	198	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	B	9	ASN
1	D	178	GLN
1	H	22	GLN
1	H	55	GLN
1	I	181	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	NAG	C	302	1	14,14,15	0.43	0	17,19,21	1.78	3 (17%)
4	PO4	D	303	-	4,4,4	1.00	0	6,6,6	0.35	0
2	KK2	J	301	-	25,25,25	0.73	0	36,36,36	1.24	4 (11%)
3	NAG	G	302	1	14,14,15	0.37	0	17,19,21	0.75	1 (5%)
4	PO4	G	303	-	4,4,4	0.91	0	6,6,6	0.49	0
2	KK2	B	301	-	25,25,25	1.12	3 (12%)	36,36,36	1.36	6 (16%)
3	NAG	B	302	1	14,14,15	0.53	0	17,19,21	1.97	4 (23%)
3	NAG	E	302	1	14,14,15	0.52	0	17,19,21	1.26	1 (5%)
3	NAG	A	302	1	14,14,15	0.62	0	17,19,21	1.36	2 (11%)
2	KK2	D	301	-	25,25,25	1.01	1 (4%)	36,36,36	1.30	3 (8%)
3	NAG	I	302	1	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
4	PO4	C	303	-	4,4,4	1.02	0	6,6,6	0.61	0
4	PO4	E	304	-	4,4,4	0.83	0	6,6,6	0.51	0
2	KK2	H	301	-	25,25,25	1.20	2 (8%)	36,36,36	1.49	8 (22%)
2	KK2	G	301	-	25,25,25	1.00	0	36,36,36	1.40	5 (13%)
3	NAG	D	302	1	14,14,15	0.48	0	17,19,21	1.12	1 (5%)
2	KK2	E	301	-	25,25,25	1.09	2 (8%)	36,36,36	1.37	5 (13%)
4	PO4	H	303	-	4,4,4	1.04	0	6,6,6	0.64	0
4	PO4	J	303	-	4,4,4	1.03	0	6,6,6	0.41	0
3	NAG	H	302	1	14,14,15	0.30	0	17,19,21	0.62	0
2	KK2	A	301	-	25,25,25	1.31	3 (12%)	36,36,36	1.29	4 (11%)
4	PO4	A	303	-	4,4,4	0.95	0	6,6,6	0.48	0
4	PO4	I	303	-	4,4,4	1.06	0	6,6,6	0.59	0
2	KK2	F	301	-	25,25,25	1.42	4 (16%)	36,36,36	1.41	6 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	E	303	-	4,4,4	0.88	0	6,6,6	0.69	0
2	KK2	I	301	-	25,25,25	0.96	0	36,36,36	1.68	7 (19%)
4	PO4	F	302	-	4,4,4	1.27	0	6,6,6	0.41	0
2	KK2	C	301	-	25,25,25	1.11	4 (16%)	36,36,36	1.44	5 (13%)
3	NAG	J	302	1	14,14,15	0.29	0	17,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	302	1	-	1/6/23/26	0/1/1/1
2	KK2	J	301	-	-	4/14/22/22	0/3/3/3
3	NAG	G	302	1	-	3/6/23/26	0/1/1/1
2	KK2	B	301	-	-	4/14/22/22	0/3/3/3
3	NAG	B	302	1	-	2/6/23/26	0/1/1/1
3	NAG	E	302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	302	1	-	4/6/23/26	0/1/1/1
2	KK2	D	301	-	-	4/14/22/22	0/3/3/3
3	NAG	I	302	1	-	4/6/23/26	0/1/1/1
2	KK2	H	301	-	-	4/14/22/22	0/3/3/3
2	KK2	G	301	-	-	5/14/22/22	0/3/3/3
3	NAG	D	302	1	-	3/6/23/26	0/1/1/1
2	KK2	E	301	-	-	4/14/22/22	0/3/3/3
3	NAG	H	302	1	-	5/6/23/26	0/1/1/1
2	KK2	A	301	-	-	4/14/22/22	0/3/3/3
2	KK2	F	301	-	-	4/14/22/22	0/3/3/3
2	KK2	I	301	-	-	4/14/22/22	0/3/3/3
2	KK2	C	301	-	-	4/14/22/22	0/3/3/3
3	NAG	J	302	1	-	3/6/23/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	KK2	C9-C8	3.45	1.54	1.48
2	A	301	KK2	C6-N2	3.33	1.44	1.37
2	F	301	KK2	C6-N2	2.96	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	KK2	C5-C6	2.45	1.43	1.39
2	H	301	KK2	C6-N2	2.43	1.42	1.37
2	F	301	KK2	C7-N4	2.40	1.38	1.33
2	D	301	KK2	C7-N1	2.38	1.39	1.35
2	B	301	KK2	C6-N2	2.36	1.42	1.37
2	F	301	KK2	C4-N2	2.33	1.50	1.46
2	A	301	KK2	C6-N1	2.29	1.37	1.34
2	H	301	KK2	C7-N4	2.23	1.38	1.33
2	B	301	KK2	C1-N2	2.16	1.50	1.46
2	B	301	KK2	C7-N4	2.10	1.38	1.33
2	E	301	KK2	C7-N4	2.08	1.38	1.33
2	C	301	KK2	C6-N2	2.07	1.41	1.37
2	E	301	KK2	C7-N3	2.06	1.39	1.35
2	C	301	KK2	C4-N2	2.05	1.49	1.46
2	C	301	KK2	C1-N2	2.02	1.49	1.46
2	C	301	KK2	C7-N4	2.01	1.37	1.33

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	NAG	C1-O5-C5	6.01	120.33	112.19
3	B	302	NAG	C1-O5-C5	4.83	118.74	112.19
3	B	302	NAG	O5-C5-C6	4.77	114.68	107.20
3	E	302	NAG	O5-C1-C2	-4.44	104.28	111.29
2	I	301	KK2	C7-N1-C6	-4.13	113.81	116.73
2	C	301	KK2	C1-N2-C6	-4.12	110.83	120.39
2	I	301	KK2	C10-C9-C8	4.11	127.77	121.28
2	A	301	KK2	C4-N2-C6	3.97	129.59	120.39
2	C	301	KK2	C3-C4-N2	3.62	116.70	110.02
2	F	301	KK2	C8-C5-C6	3.58	119.38	117.03
3	D	302	NAG	C1-O5-C5	3.58	117.04	112.19
2	B	301	KK2	C1-N2-C6	-3.57	112.10	120.39
2	I	301	KK2	C15-C9-C8	-3.51	115.75	121.28
2	E	301	KK2	C7-N1-C6	-3.48	114.27	116.73
2	H	301	KK2	C7-N1-C6	-3.43	114.31	116.73
2	G	301	KK2	C10-C9-C8	3.40	126.65	121.28
2	E	301	KK2	C4-N2-C6	3.37	128.21	120.39
2	G	301	KK2	C7-N1-C6	-3.36	114.35	116.73
2	D	301	KK2	C7-N1-C6	-3.35	114.36	116.73
3	A	302	NAG	C2-N2-C7	3.29	127.59	122.90
2	J	301	KK2	C4-N2-C6	3.26	127.95	120.39
2	F	301	KK2	C7-N1-C6	-3.25	114.43	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	KK2	C8-C5-C6	3.24	119.16	117.03
2	D	301	KK2	C8-C5-C6	3.21	119.14	117.03
2	A	301	KK2	C5-C8-C9	3.15	126.05	121.85
2	B	301	KK2	C8-C5-C6	3.13	119.08	117.03
2	D	301	KK2	C1-N2-C6	-3.08	113.24	120.39
2	G	301	KK2	C15-C9-C8	-3.04	116.49	121.28
2	H	301	KK2	C4-N2-C6	3.00	127.35	120.39
2	G	301	KK2	C1-N2-C6	-2.91	113.63	120.39
2	E	301	KK2	C8-C5-C6	2.91	118.94	117.03
2	C	301	KK2	C7-N1-C6	-2.89	114.69	116.73
2	C	301	KK2	C2-C1-N2	2.88	115.33	110.02
2	I	301	KK2	C1-N2-C6	-2.86	113.74	120.39
3	C	302	NAG	C3-C4-C5	2.84	115.31	110.24
2	F	301	KK2	C1-N2-C6	-2.82	113.84	120.39
2	H	301	KK2	C10-C9-C8	2.81	125.73	121.28
2	A	301	KK2	C9-C8-N3	-2.78	112.07	116.02
3	B	302	NAG	O5-C1-C2	2.74	115.61	111.29
2	F	301	KK2	C10-C9-C8	2.71	125.57	121.28
2	B	301	KK2	C7-N1-C6	-2.62	114.88	116.73
3	B	302	NAG	C3-C4-C5	2.61	114.90	110.24
2	B	301	KK2	C2-C1-N2	2.59	114.80	110.02
2	C	301	KK2	C8-C5-C6	2.54	118.70	117.03
2	B	301	KK2	C3-C4-N2	2.49	114.62	110.02
2	G	301	KK2	C3-C4-N2	2.45	114.55	110.02
2	F	301	KK2	C3-C4-N2	2.44	114.52	110.02
2	I	301	KK2	C3-C4-N2	2.40	114.46	110.02
2	H	301	KK2	C8-C5-C6	2.37	118.59	117.03
3	A	302	NAG	C1-C2-N2	2.33	114.47	110.49
2	J	301	KK2	C7-N1-C6	-2.32	115.09	116.73
2	A	301	KK2	C7-N1-C6	-2.32	115.09	116.73
2	H	301	KK2	C5-C8-C9	2.30	124.91	121.85
2	J	301	KK2	C1-N2-C6	-2.30	115.06	120.39
2	H	301	KK2	C3-C4-N2	2.29	114.24	110.02
2	J	301	KK2	C3-C4-N2	2.20	114.08	110.02
2	H	301	KK2	C15-C9-C8	-2.19	117.82	121.28
2	I	301	KK2	C11-C12-C13	2.19	123.44	119.97
3	C	302	NAG	O5-C5-C4	2.19	116.15	110.83
2	B	301	KK2	C10-C9-C8	2.09	124.58	121.28
2	H	301	KK2	C1-N2-C6	-2.07	115.58	120.39
3	G	302	NAG	C3-C4-C5	2.03	113.86	110.24
2	F	301	KK2	C4-N2-C6	2.02	125.08	120.39
3	I	302	NAG	C3-C4-C5	2.01	113.83	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	KK2	C2-C1-N2	2.01	113.73	110.02
2	E	301	KK2	C1-N2-C6	-2.00	115.74	120.39

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	KK2	N3-C8-C9-C10
2	G	301	KK2	N3-C8-C9-C10
2	H	301	KK2	N3-C8-C9-C15
2	J	301	KK2	N3-C8-C9-C15
3	A	302	NAG	C8-C7-N2-C2
3	A	302	NAG	O7-C7-N2-C2
3	D	302	NAG	C1-C2-N2-C7
3	D	302	NAG	C8-C7-N2-C2
3	D	302	NAG	O7-C7-N2-C2
3	H	302	NAG	C3-C2-N2-C7
3	J	302	NAG	C8-C7-N2-C2
3	J	302	NAG	O7-C7-N2-C2
2	A	301	KK2	N3-C8-C9-C15
2	D	301	KK2	N3-C8-C9-C15
2	B	301	KK2	C5-C8-C9-C15
2	H	301	KK2	C5-C8-C9-C15
2	A	301	KK2	N3-C8-C9-C10
2	B	301	KK2	N3-C8-C9-C10
2	B	301	KK2	N3-C8-C9-C15
2	C	301	KK2	N3-C8-C9-C10
2	C	301	KK2	N3-C8-C9-C15
2	F	301	KK2	N3-C8-C9-C15
2	G	301	KK2	N3-C8-C9-C15
2	H	301	KK2	N3-C8-C9-C10
2	I	301	KK2	N3-C8-C9-C10
2	J	301	KK2	N3-C8-C9-C10
2	A	301	KK2	C5-C8-C9-C10
2	A	301	KK2	C5-C8-C9-C15
2	B	301	KK2	C5-C8-C9-C10
2	C	301	KK2	C5-C8-C9-C10
2	C	301	KK2	C5-C8-C9-C15
2	D	301	KK2	C5-C8-C9-C10
2	D	301	KK2	C5-C8-C9-C15
2	F	301	KK2	C5-C8-C9-C10
2	F	301	KK2	C5-C8-C9-C15

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Mol	Chain	Res	Type	Atoms
2	G	301	KK2	C5-C8-C9-C10
2	G	301	KK2	C5-C8-C9-C15
2	H	301	KK2	C5-C8-C9-C10
2	J	301	KK2	C5-C8-C9-C10
2	E	301	KK2	N3-C8-C9-C15
2	F	301	KK2	N3-C8-C9-C10
2	I	301	KK2	N3-C8-C9-C15
2	E	301	KK2	C5-C8-C9-C10
2	E	301	KK2	C5-C8-C9-C15
2	J	301	KK2	C5-C8-C9-C15
2	E	301	KK2	N3-C8-C9-C10
2	I	301	KK2	C5-C8-C9-C10
2	I	301	KK2	C5-C8-C9-C15
3	E	302	NAG	C8-C7-N2-C2
3	E	302	NAG	O7-C7-N2-C2
3	B	302	NAG	O5-C5-C6-O6
3	I	302	NAG	O5-C5-C6-O6
3	A	302	NAG	C1-C2-N2-C7
3	I	302	NAG	C4-C5-C6-O6
3	B	302	NAG	C4-C5-C6-O6
3	J	302	NAG	O5-C5-C6-O6
3	H	302	NAG	C1-C2-N2-C7
3	H	302	NAG	O5-C5-C6-O6
3	G	302	NAG	C1-C2-N2-C7
3	I	302	NAG	C8-C7-N2-C2
3	C	302	NAG	C4-C5-C6-O6
3	H	302	NAG	C8-C7-N2-C2
3	I	302	NAG	O7-C7-N2-C2
3	G	302	NAG	C3-C2-N2-C7
3	H	302	NAG	O7-C7-N2-C2
3	A	302	NAG	C4-C5-C6-O6
2	G	301	KK2	N1-C6-N2-C4
3	G	302	NAG	C4-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	301	KK2	2	0
2	B	301	KK2	1	0
2	D	301	KK2	1	0
3	I	302	NAG	1	0

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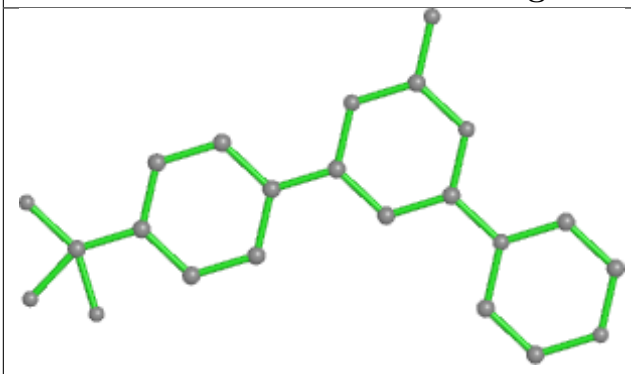
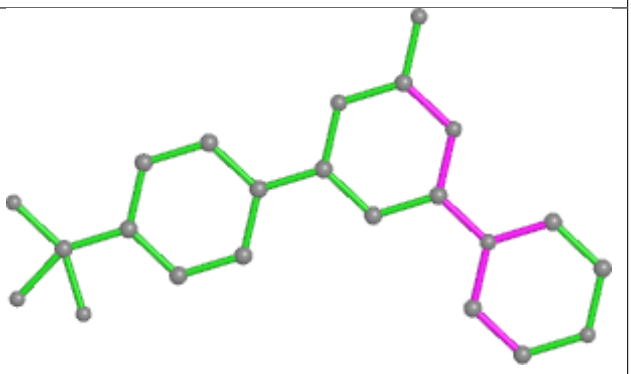
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	PO4	1	0
2	H	301	KK2	1	0
2	G	301	KK2	2	0
2	E	301	KK2	1	0
4	H	303	PO4	1	0
4	J	303	PO4	1	0
3	H	302	NAG	2	0
2	A	301	KK2	2	0
2	F	301	KK2	1	0
2	I	301	KK2	2	0
2	C	301	KK2	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand KK2 J 301



Bond lengths



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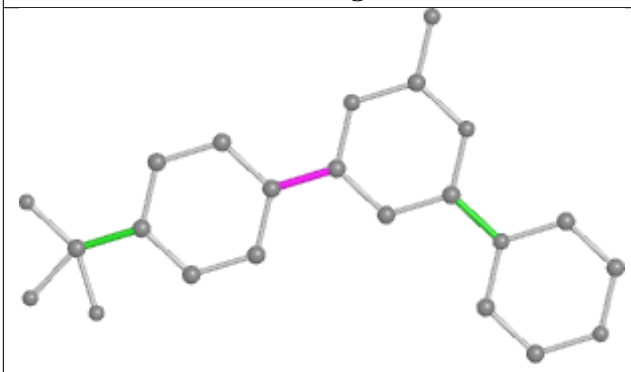
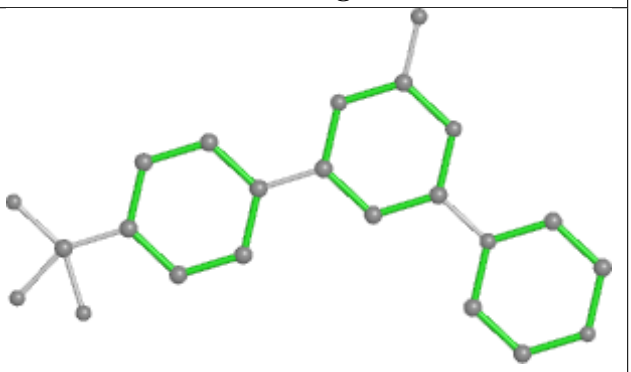
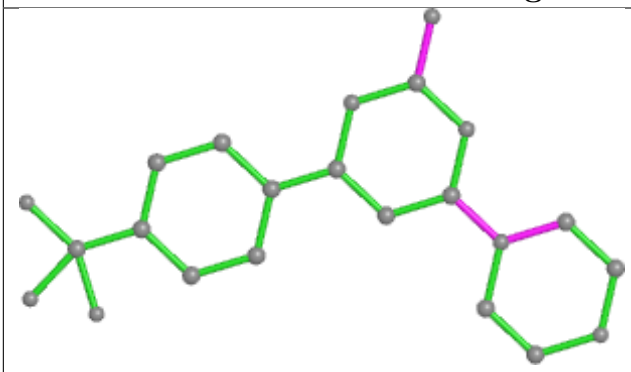


Torsions



Rings

Ligand KK2 B 301



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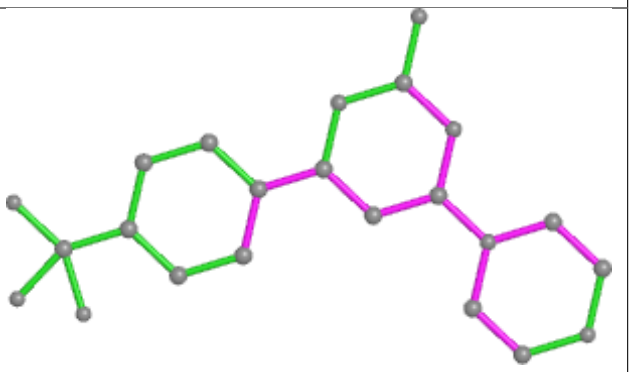

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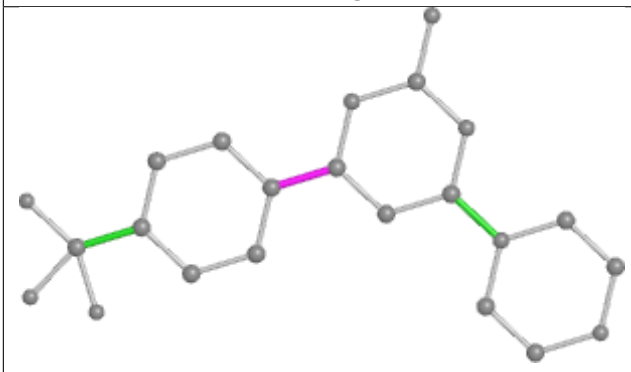

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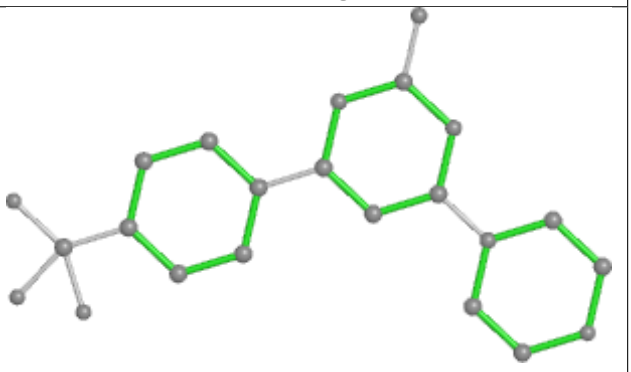
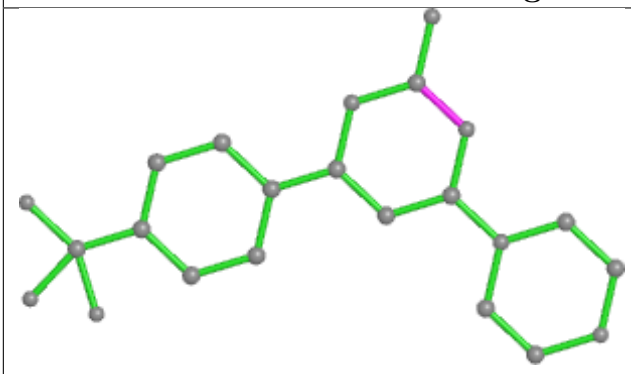


Rings

Ligand KK2 D 301



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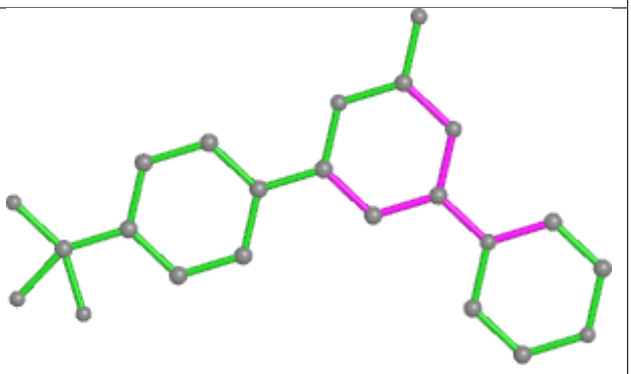
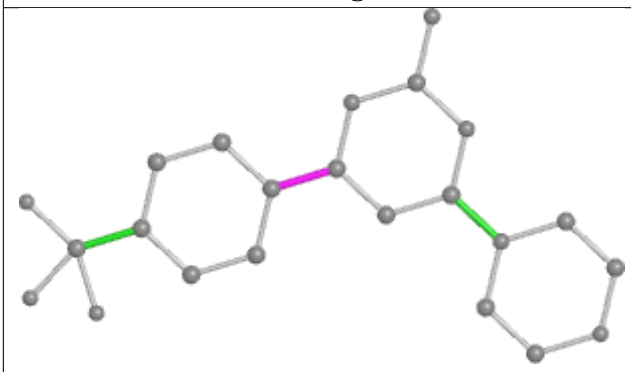


Bond angles



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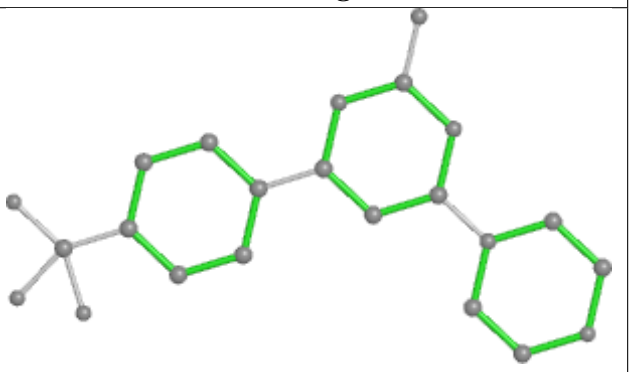
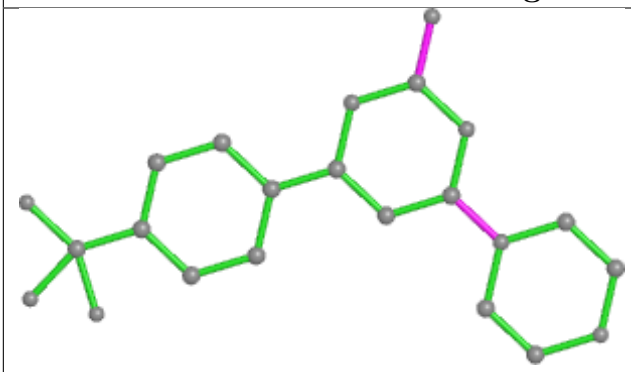


Rings

Ligand KK2 H 301



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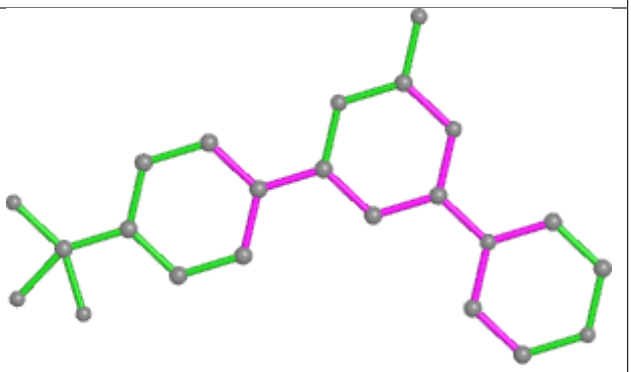
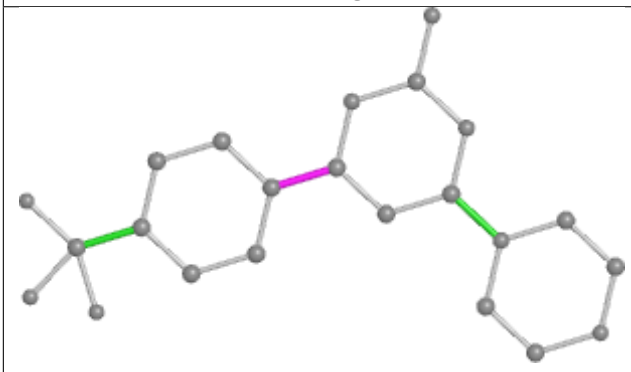


Bond angles



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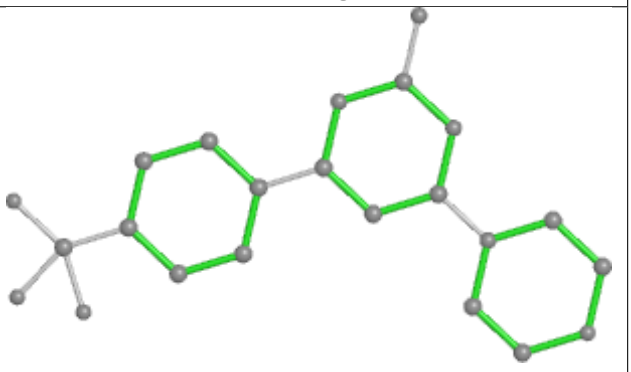
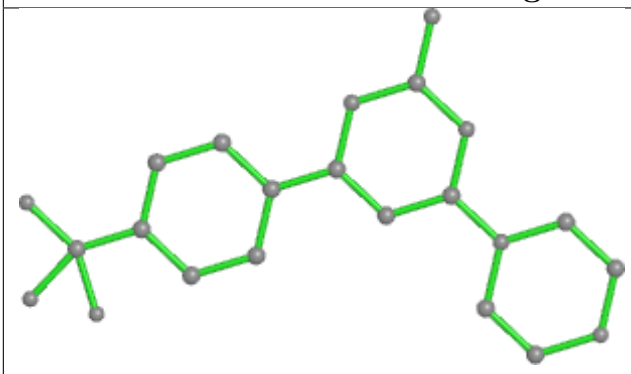


Rings

Ligand KK2 G 301



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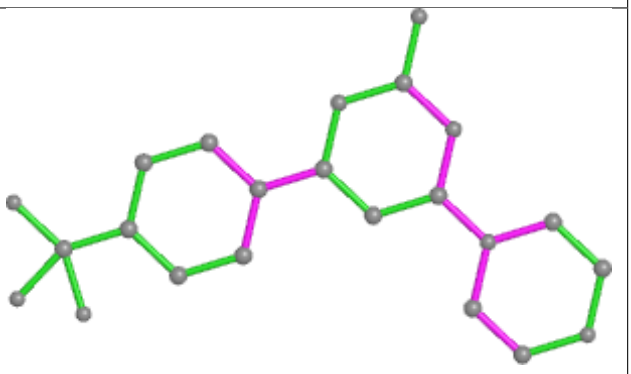

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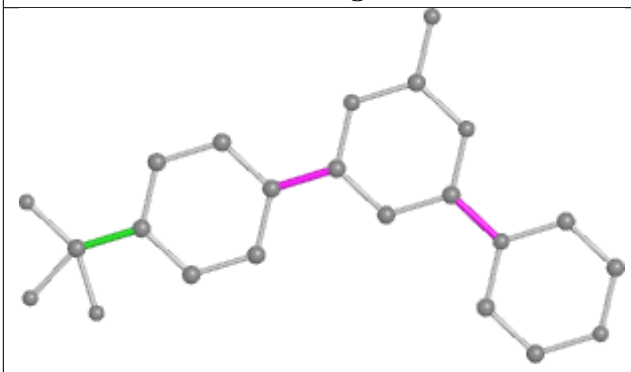

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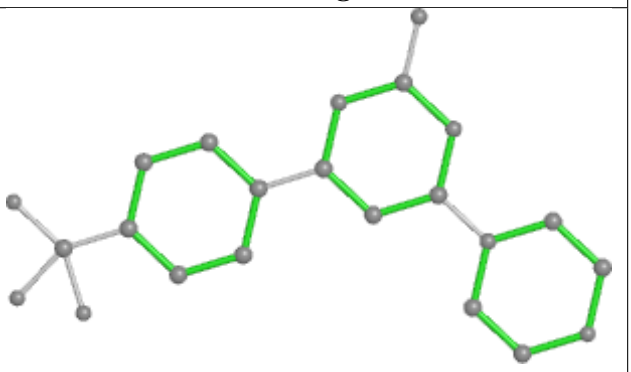
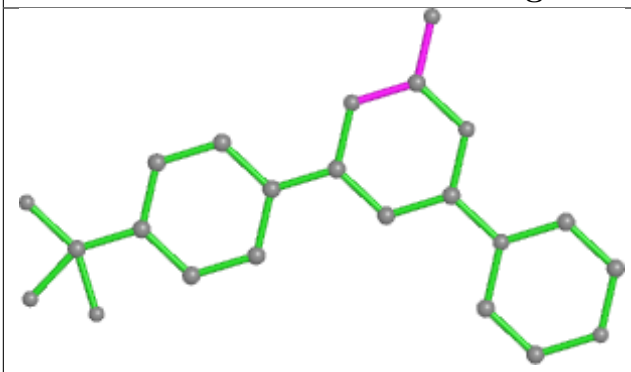


Rings

Ligand KK2 E 301



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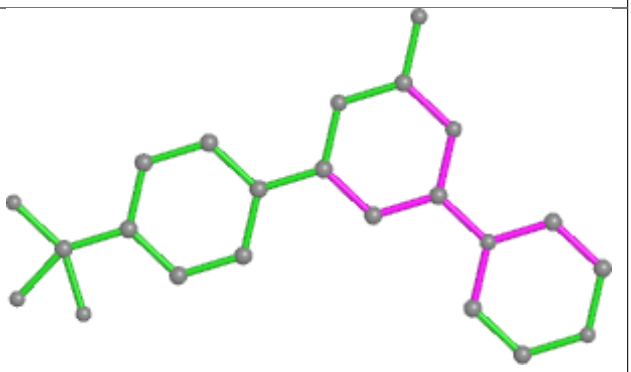
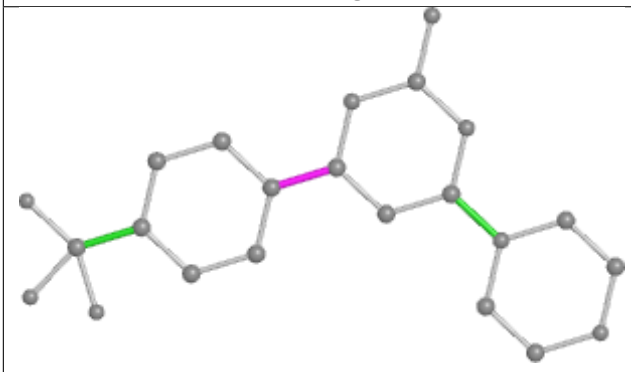
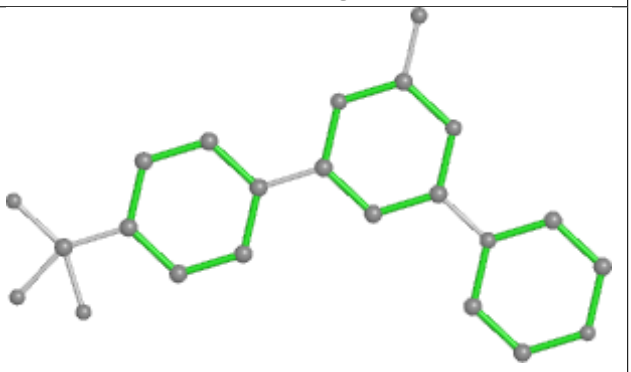


Bond angles

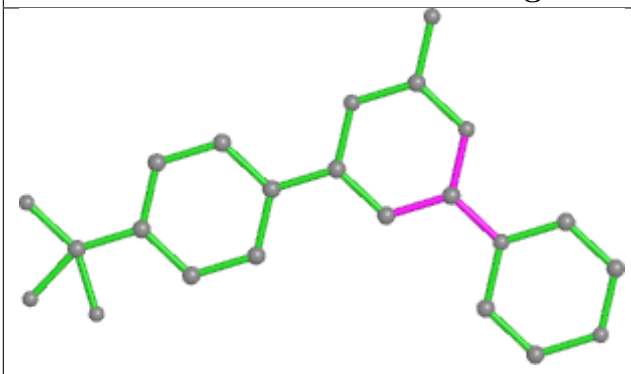


Torsions

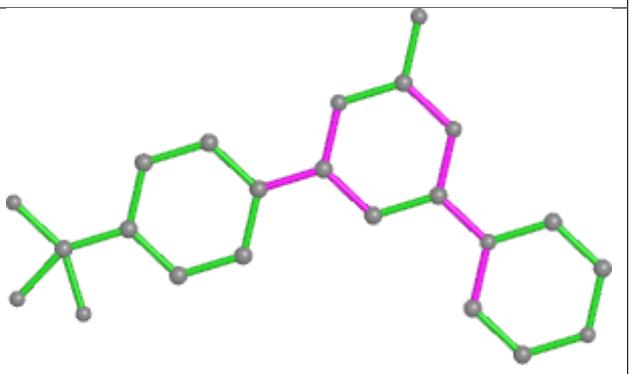


Rings

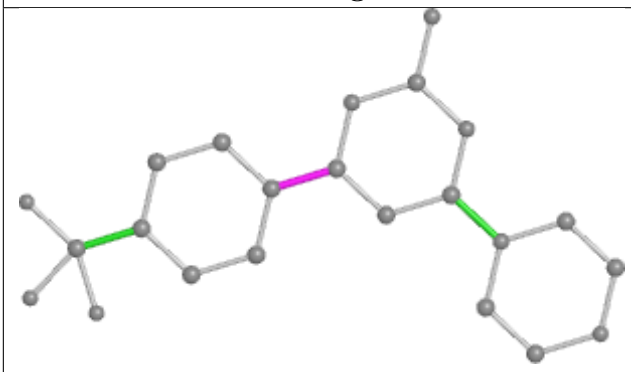
Ligand KK2 A 301



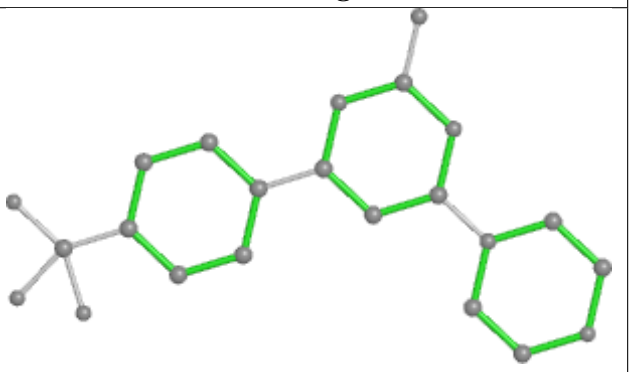
Bond lengths



Bond angles

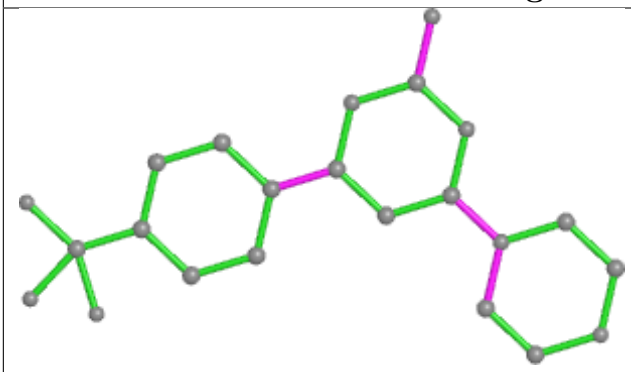


Torsions

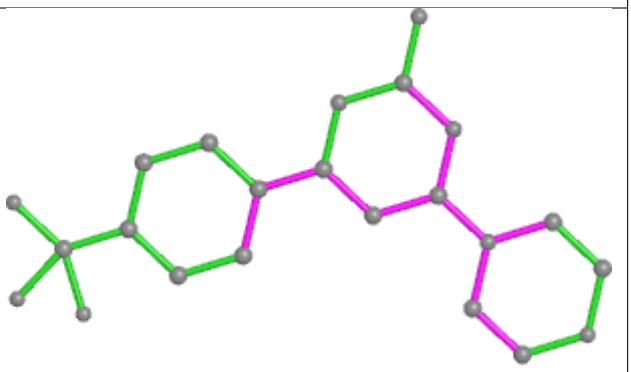


Rings

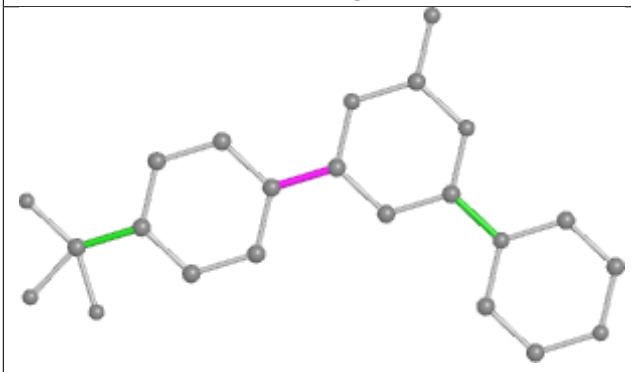
Ligand KK2 F 301



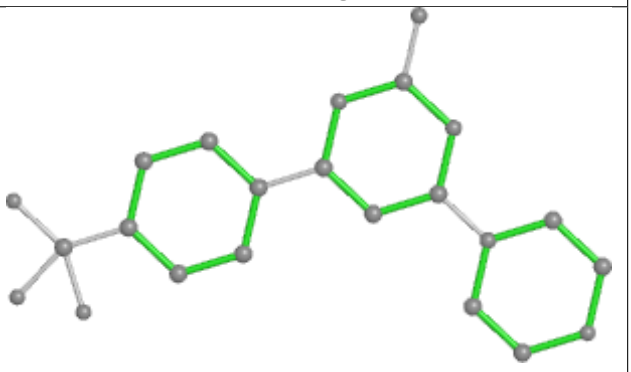
Bond lengths



Bond angles

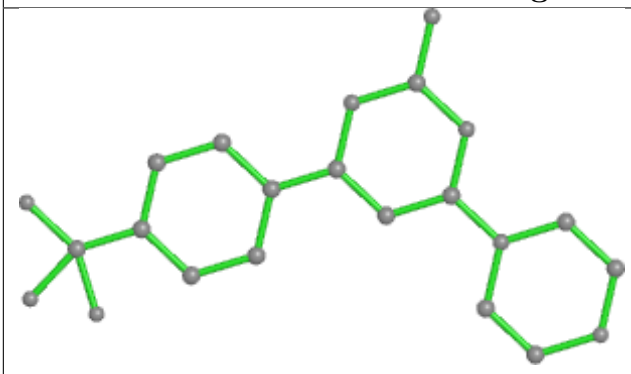


Torsions

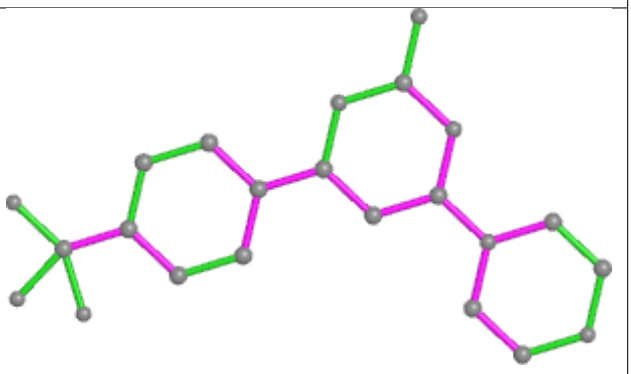


Rings

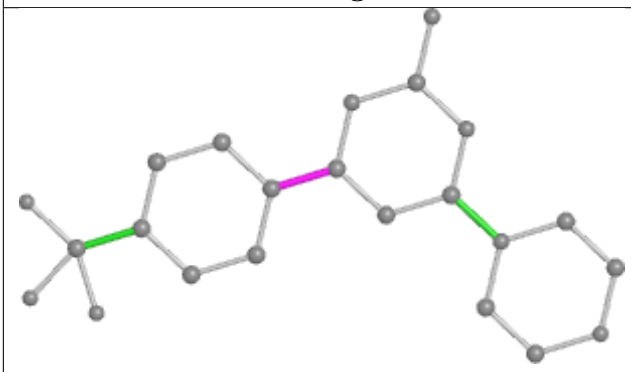
Ligand KK2 I 301



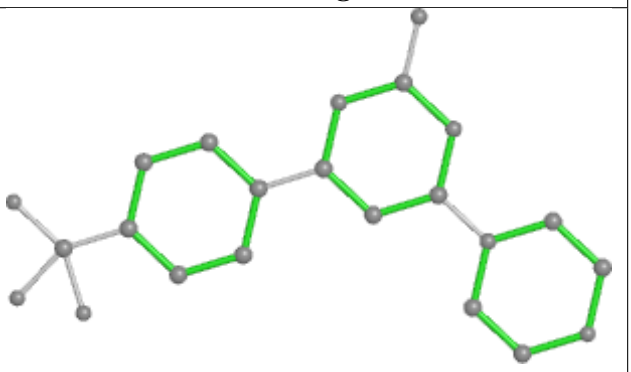
Bond lengths



Bond angles

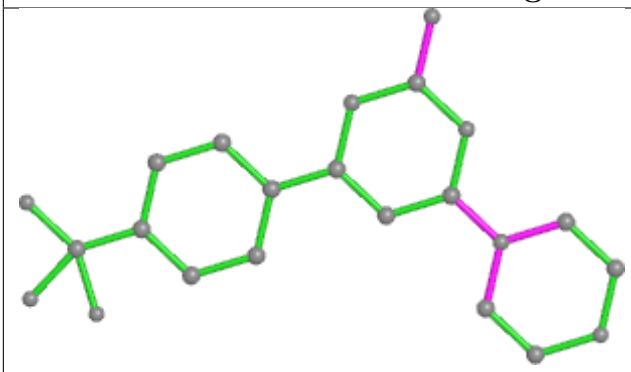


Torsions

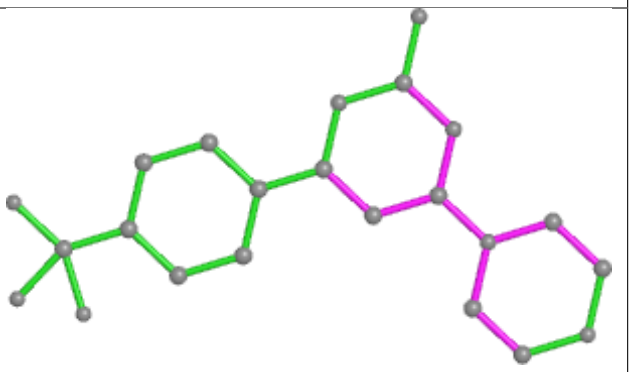


Rings

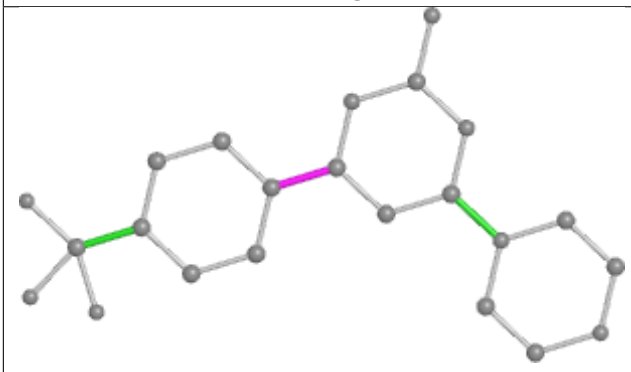
Ligand KK2 C 301



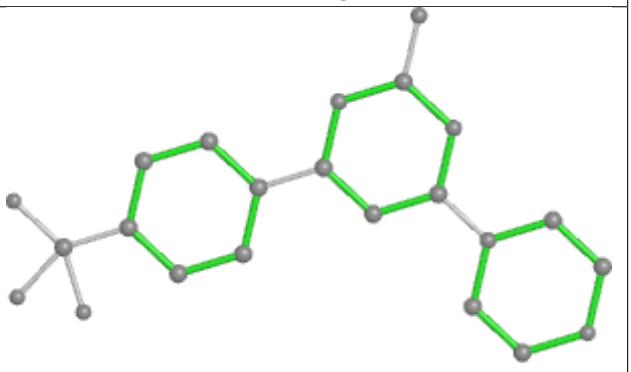
Bond lengths



Bond angles



Torsions



Rings

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	208/217 (95%)	0.20	8 (3%)	40	24	10, 24, 58, 85	0
1	B	205/217 (94%)	0.13	7 (3%)	45	27	8, 24, 54, 85	0
1	C	207/217 (95%)	0.27	12 (5%)	23	12	9, 27, 56, 76	0
1	D	213/217 (98%)	0.36	13 (6%)	21	11	10, 27, 61, 93	0
1	E	207/217 (95%)	0.25	12 (5%)	23	12	10, 24, 54, 70	0
1	F	208/217 (95%)	0.21	11 (5%)	26	15	9, 25, 55, 93	0
1	G	210/217 (96%)	0.28	13 (6%)	20	11	8, 25, 56, 99	0
1	H	209/217 (96%)	0.13	7 (3%)	46	28	9, 23, 53, 81	0
1	I	209/217 (96%)	0.19	10 (4%)	30	18	6, 23, 59, 80	0
1	J	207/217 (95%)	0.33	15 (7%)	15	8	8, 27, 59, 88	0
All	All	2083/2170 (95%)	0.24	108 (5%)	27	16	6, 25, 58, 99	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-6	TYR	7.4
1	H	22	GLN	6.0
1	D	-7	ASP	4.6
1	J	39	LEU	4.5
1	J	-6	TYR	4.4
1	G	160	ASP	4.2
1	B	136	CYS	4.2
1	A	60	ASP	4.1
1	G	-4	ASP	4.0
1	D	157	GLU	4.0
1	D	158	ASN	3.9
1	A	-5	LYS	3.8
1	D	24	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	24	ASP	3.7
1	G	130	THR	3.6
1	C	162	SER	3.6
1	J	136	CYS	3.5
1	J	205	GLY	3.4
1	G	23	ARG	3.4
1	I	-7	ASP	3.4
1	D	154	PRO	3.4
1	F	-7	ASP	3.4
1	H	23	ARG	3.3
1	E	-2	ASP	3.3
1	C	130	THR	3.3
1	G	132	SER	3.3
1	C	129	ASP	3.2
1	D	156	THR	3.2
1	D	161	ASP	3.1
1	I	44	ILE	3.0
1	C	125	VAL	3.0
1	G	136	CYS	3.0
1	D	25	ARG	3.0
1	A	-4	ASP	3.0
1	I	39	LEU	3.0
1	F	60[A]	ASP	3.0
1	J	186	SER	3.0
1	G	129	ASP	2.9
1	J	132	SER	2.9
1	D	23	ARG	2.9
1	C	-6	TYR	2.9
1	F	-6	TYR	2.9
1	F	-2	ASP	2.9
1	I	40	GLU	2.8
1	G	-3	ASP	2.8
1	A	130	THR	2.8
1	E	-4	ASP	2.8
1	C	132	SER	2.8
1	J	44	ILE	2.7
1	B	123	CYS	2.7
1	E	131	GLU	2.7
1	A	-7	ASP	2.7
1	H	-5	LYS	2.7
1	J	60	ASP	2.7
1	I	23	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	126	SER	2.6
1	I	131	GLU	2.6
1	D	205	GLY	2.6
1	D	187	CYS	2.6
1	I	130	THR	2.5
1	E	130	THR	2.5
1	F	194[A]	ASP	2.5
1	H	60[A]	ASP	2.5
1	J	23	ARG	2.5
1	I	49[A]	ASP	2.4
1	H	-1	ASP	2.4
1	B	23	ARG	2.4
1	C	123	CYS	2.4
1	C	40	GLU	2.4
1	E	129	ASP	2.3
1	G	161	ASP	2.3
1	E	-1	ASP	2.3
1	C	128	VAL	2.3
1	A	136	CYS	2.3
1	E	161	ASP	2.3
1	B	131	GLU	2.3
1	J	24	ASP	2.3
1	F	188	CYS	2.2
1	G	-7	ASP	2.2
1	E	153	ASP	2.2
1	E	205	GLY	2.2
1	F	136	CYS	2.2
1	D	126	SER	2.2
1	J	188	CYS	2.2
1	F	-1	ASP	2.2
1	J	135	THR	2.2
1	E	175	ASP	2.2
1	G	174	LEU	2.2
1	E	135	THR	2.2
1	F	39	LEU	2.1
1	F	-5	LYS	2.1
1	C	60	ASP	2.1
1	J	194[A]	ASP	2.1
1	E	132	SER	2.1
1	B	49[A]	ASP	2.1
1	J	43	GLU	2.1
1	A	22	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	129	ASP	2.1
1	G	131	GLU	2.1
1	H	-4	ASP	2.1
1	A	40	GLU	2.1
1	H	172[A]	GLU	2.1
1	C	39	LEU	2.1
1	G	199	LEU	2.0
1	J	124	ASP	2.0
1	B	205	GLY	2.0
1	I	172[A]	GLU	2.0
1	F	-4	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	302	14/15	0.63	0.51	50,66,88,93	0
3	NAG	I	302	14/15	0.64	0.45	47,62,70,74	0
3	NAG	D	302	14/15	0.70	0.26	53,69,91,93	0
3	NAG	H	302	14/15	0.71	0.31	47,60,79,85	0
3	NAG	E	302	14/15	0.73	0.37	58,70,91,96	0
3	NAG	J	302	14/15	0.76	0.38	46,63,82,85	0
3	NAG	B	302	14/15	0.84	0.28	38,63,70,72	0
3	NAG	A	302	14/15	0.87	0.29	47,72,78,79	0
3	NAG	C	302	14/15	0.89	0.24	39,58,68,72	0
2	KK2	B	301	23/23	0.94	0.20	13,20,39,46	0
2	KK2	G	301	23/23	0.95	0.19	10,18,33,43	0
2	KK2	F	301	23/23	0.96	0.23	15,25,42,53	0

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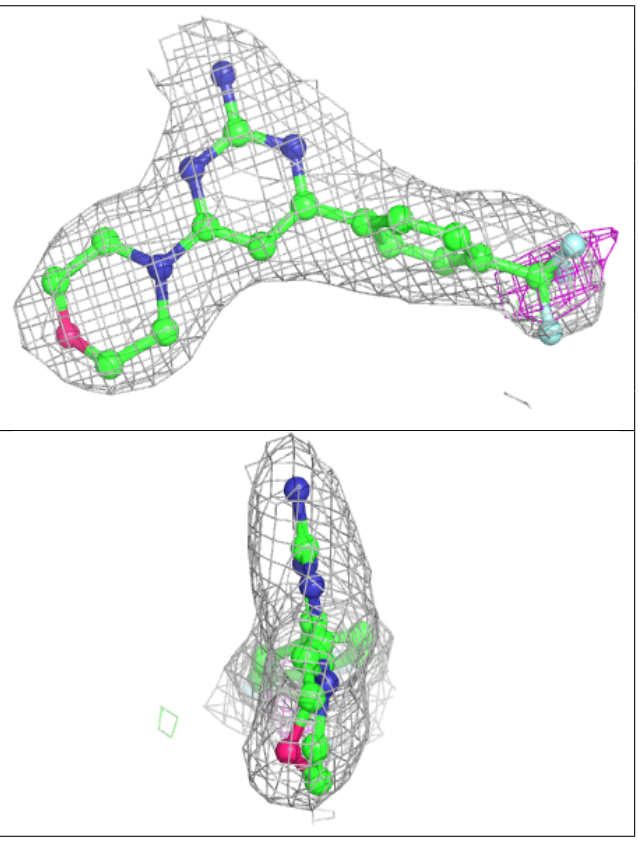
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KK2	A	301	23/23	0.96	0.23	13,22,40,50	0
2	KK2	H	301	23/23	0.96	0.18	15,24,29,32	0
2	KK2	I	301	23/23	0.96	0.22	14,20,30,32	0
2	KK2	J	301	23/23	0.96	0.23	14,27,40,45	0
2	KK2	C	301	23/23	0.96	0.20	15,26,40,44	0
2	KK2	D	301	23/23	0.96	0.20	16,22,37,46	0
2	KK2	E	301	23/23	0.97	0.18	11,14,36,49	0
4	PO4	A	303	5/5	0.99	0.14	9,15,15,18	0
4	PO4	C	303	5/5	0.99	0.15	7,9,10,16	0
4	PO4	D	303	5/5	0.99	0.13	13,14,18,18	0
4	PO4	E	303	5/5	0.99	0.14	10,12,14,15	0
4	PO4	E	304	5/5	0.99	0.13	13,15,16,18	0
4	PO4	F	302	5/5	0.99	0.18	13,16,19,22	0
4	PO4	G	303	5/5	0.99	0.16	10,13,13,14	0
4	PO4	H	303	5/5	0.99	0.14	10,10,12,23	0
4	PO4	I	303	5/5	0.99	0.15	8,9,10,14	0
4	PO4	J	303	5/5	0.99	0.16	10,10,13,17	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.

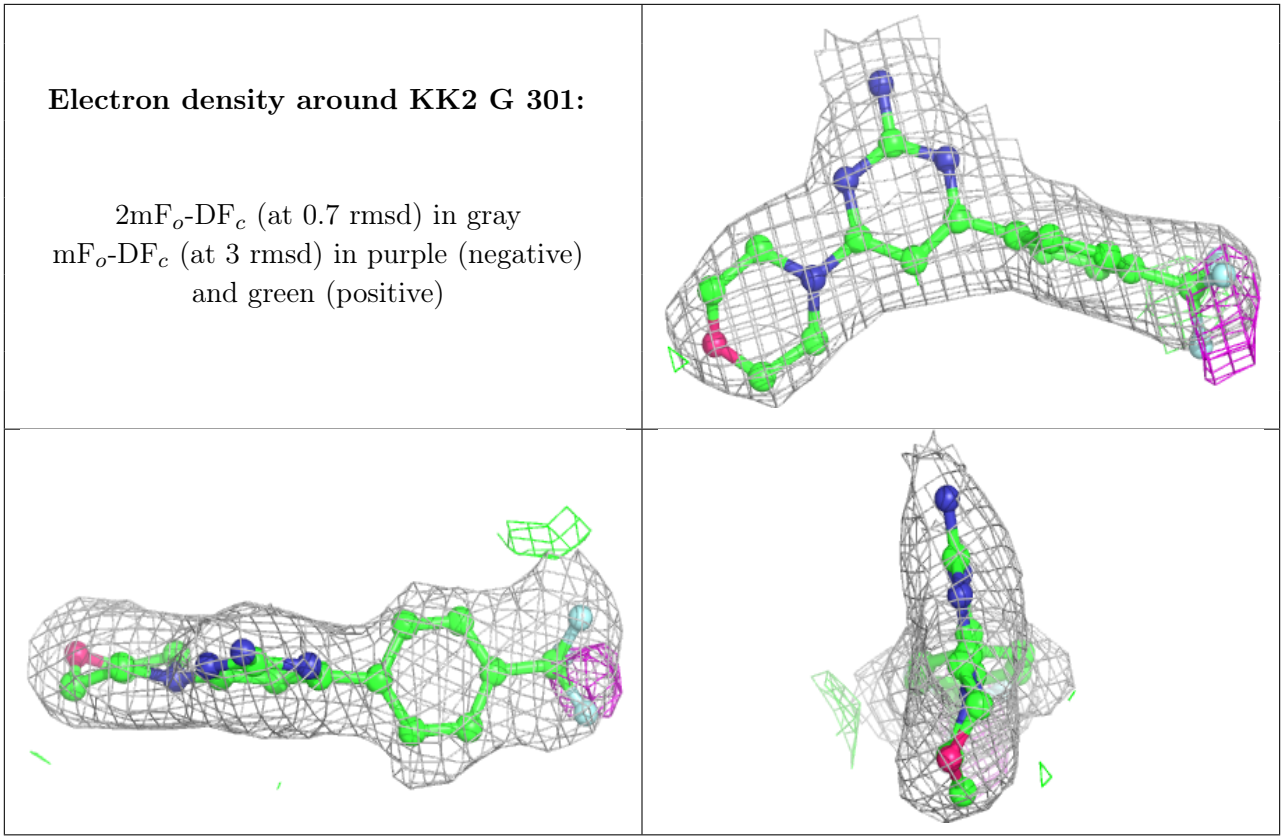
Electron density around KK2 B 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



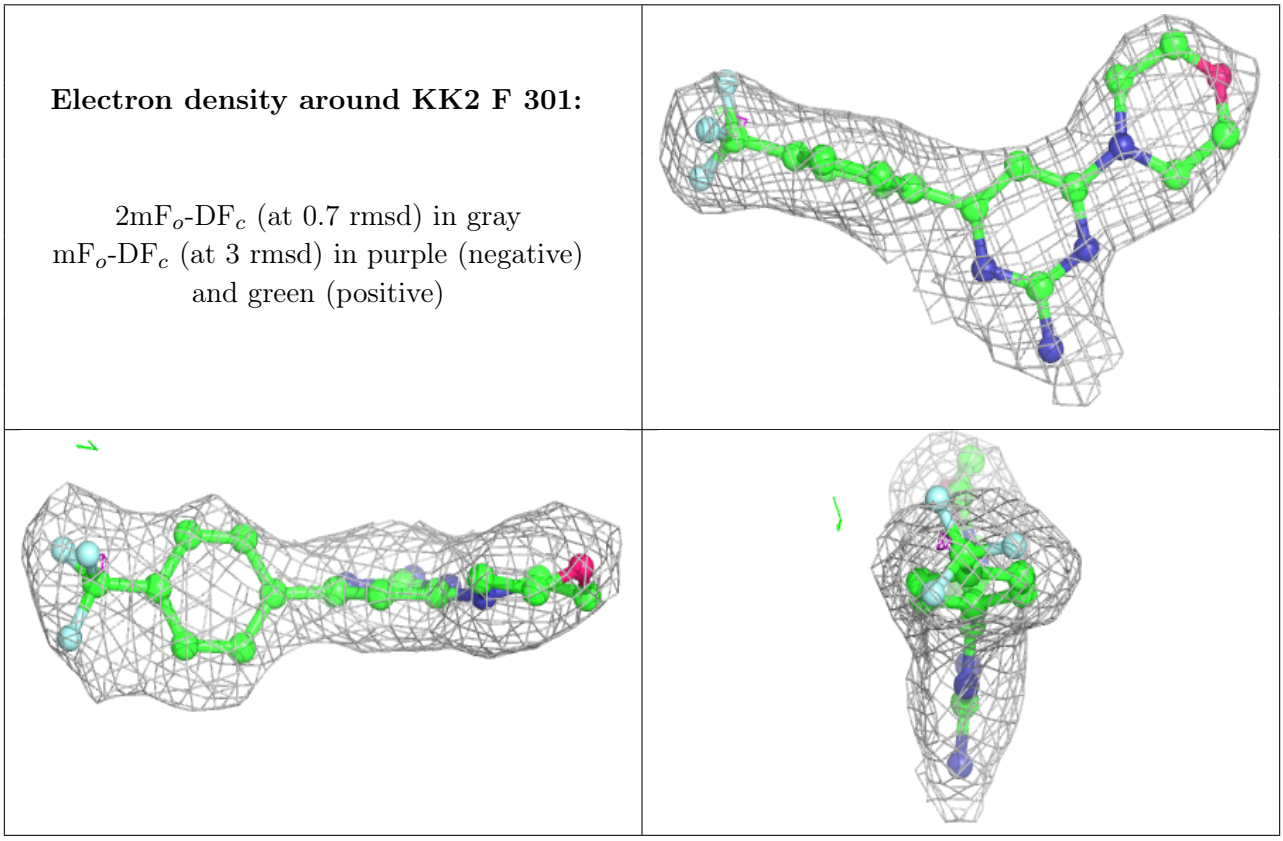
Electron density around KK2 G 301:

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



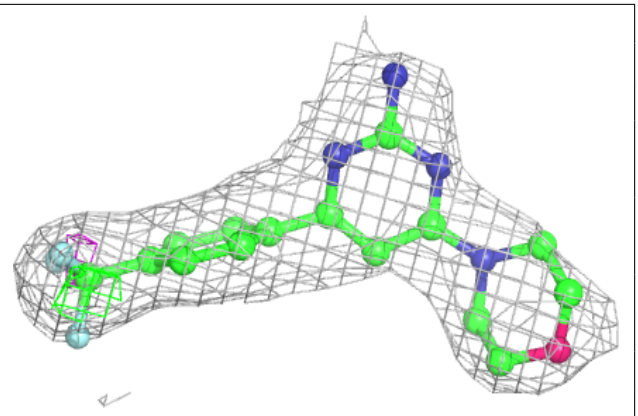
Electron density around KK2 F 301:

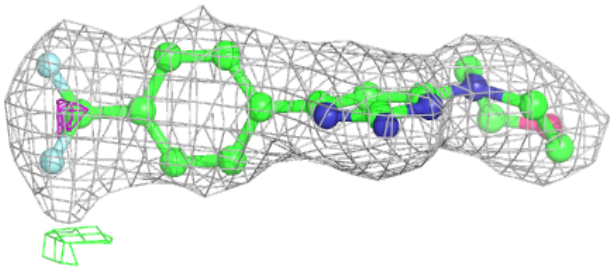
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

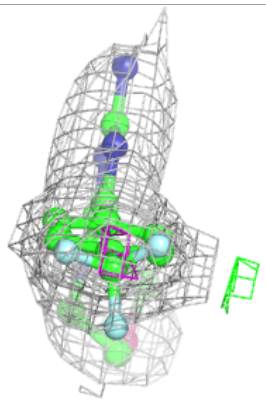


Electron density around KK2 A 301:

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

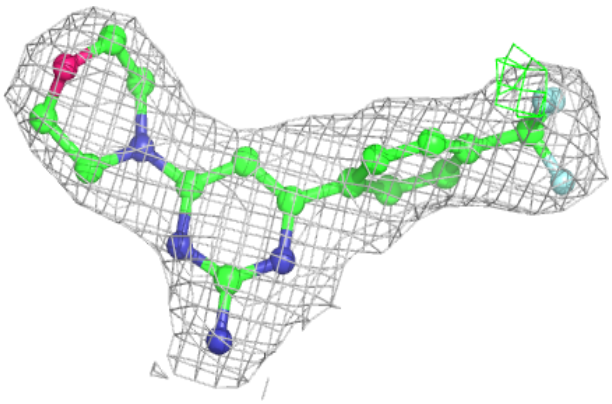


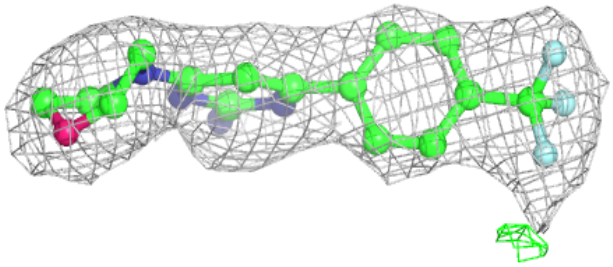


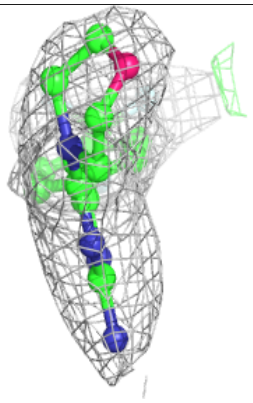


Electron density around KK2 H 301:

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

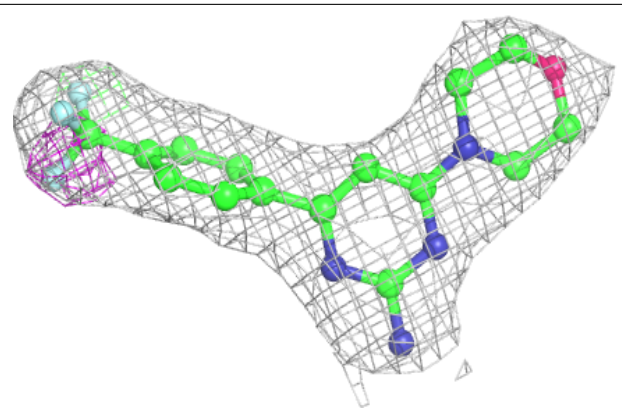


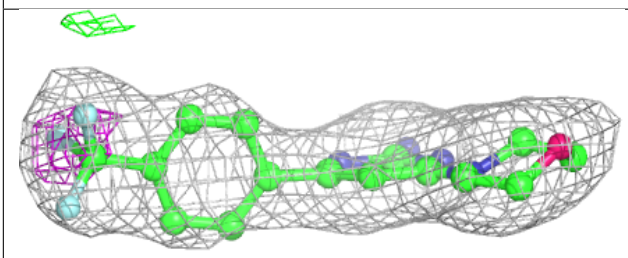


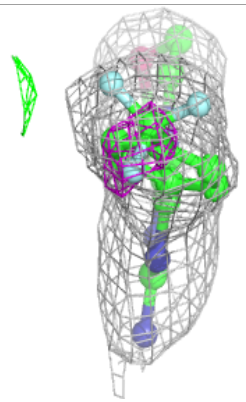


Electron density around KK2 I 301:

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

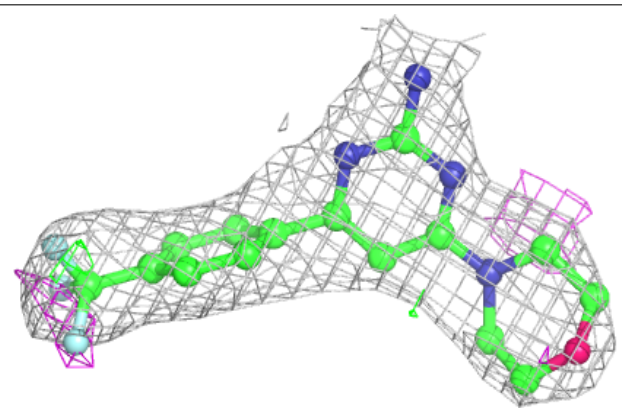


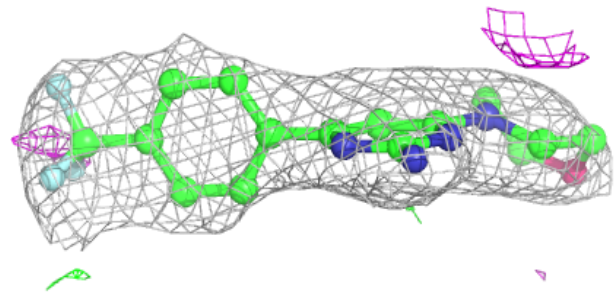


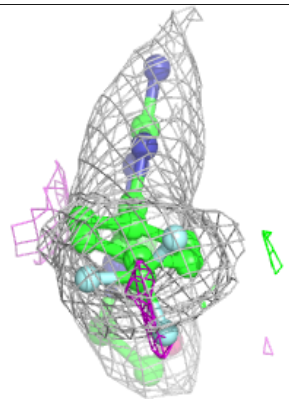


Electron density around KK2 J 301:

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

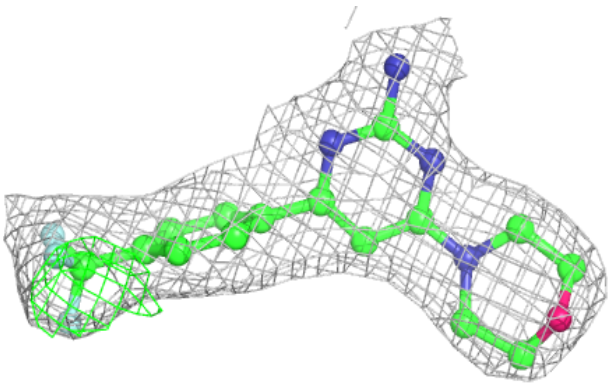


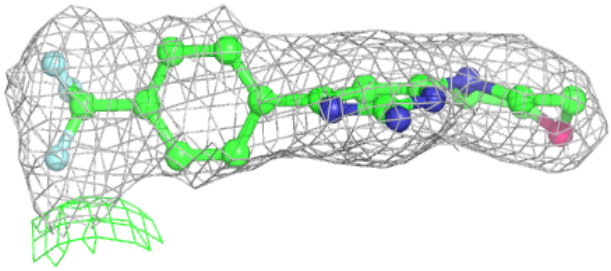


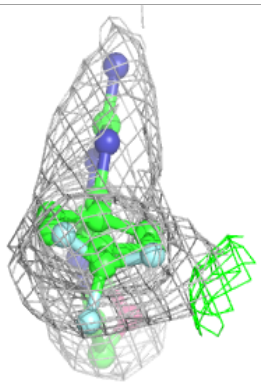


Electron density around KK2 C 301:

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

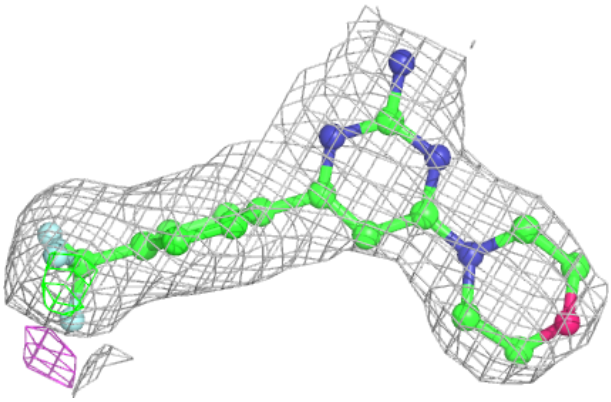


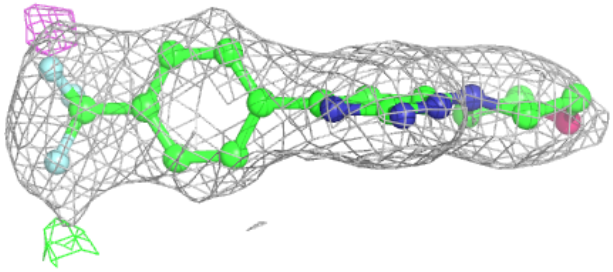


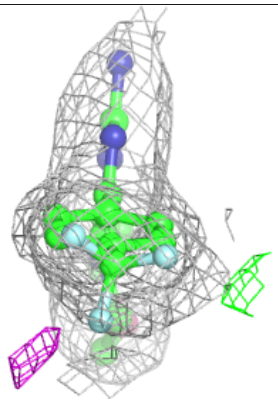


Electron density around KK2 D 301:

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

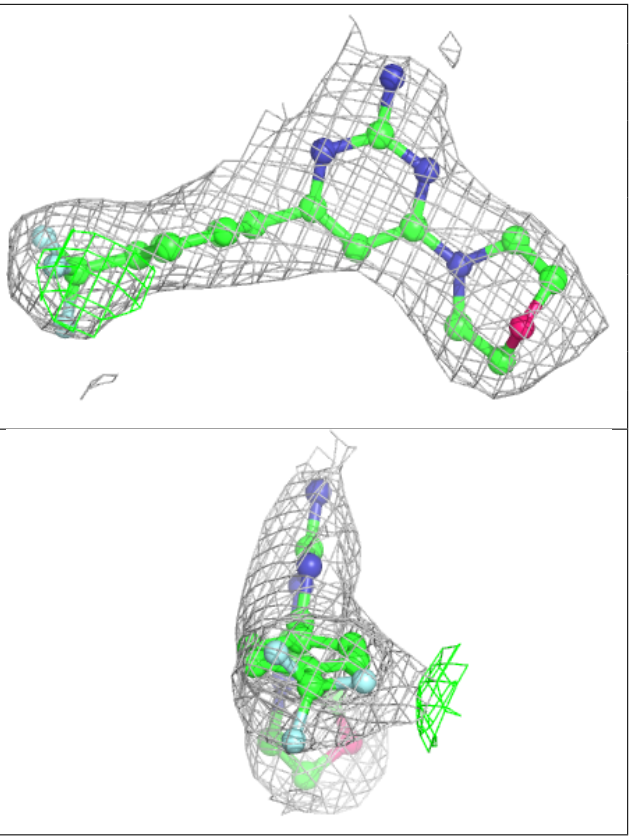






Electron density around KK2 E 301:

$2mF_o$-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.