Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:03 PM BST

PDB ID	:	5J5H
Title	:	X-RAY STRUCTURE OF ACETYLCHOLINE BINDING PROTEIN (ACHBP) IN COMPLEX WITH 6-(2-methoxyphenyl)-N4,N4-bis[(pyridin-2-yl)methyl]pyrimidine-2,4-diamine
Authors	:	Kaczanowska, K.; Harel, M.; Camacho Hernandez, A.G.; Taylor, P.
Deposited on	:	2016-04-02
Resolution	:	2.70 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:

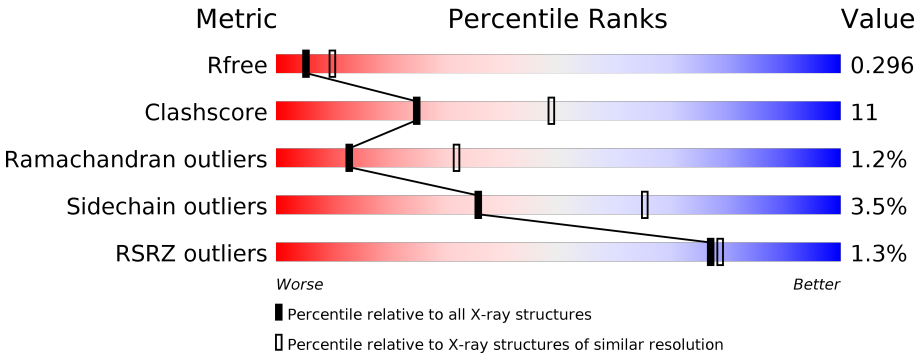
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	66% 25% 6%
1	B	218	2% 70% 25%
1	C	218	72% 20% 7%
1	D	218	69% 24% 5%
1	E	218	62% 28% 6%
1	F	218	3% 75% 22%

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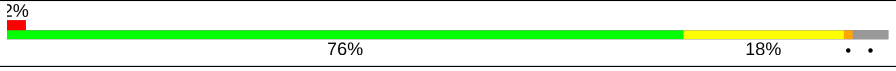
Mol	Chain	Length	Quality of chain
1	G	218	
1	H	218	
1	I	218	
1	J	218	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17280 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
1	A	204	Total	C	N	O	S	0	2	0
			1645	1030	282	328	5			
1	B	211	Total	C	N	O	S	0	0	0
			1694	1058	288	343	5			
1	C	203	Total	C	N	O	S	0	0	0
			1626	1019	278	324	5			
1	D	207	Total	C	N	O	S	0	1	0
			1665	1040	286	334	5			
1	E	206	Total	C	N	O	S	0	2	0
			1665	1041	287	332	5			
1	F	212	Total	C	N	O	S	0	0	0
			1702	1062	289	346	5			
1	G	212	Total	C	N	O	S	0	0	0
			1702	1062	289	346	5			
1	H	210	Total	C	N	O	S	0	0	0
			1682	1049	287	341	5			
1	I	202	Total	C	N	O	S	0	0	0
			1616	1013	277	321	5			
1	J	205	Total	C	N	O	S	0	1	0
			1648	1031	286	326	5			

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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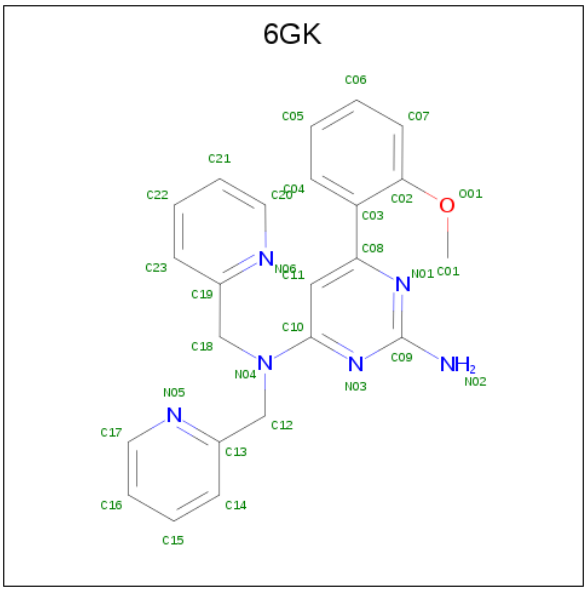
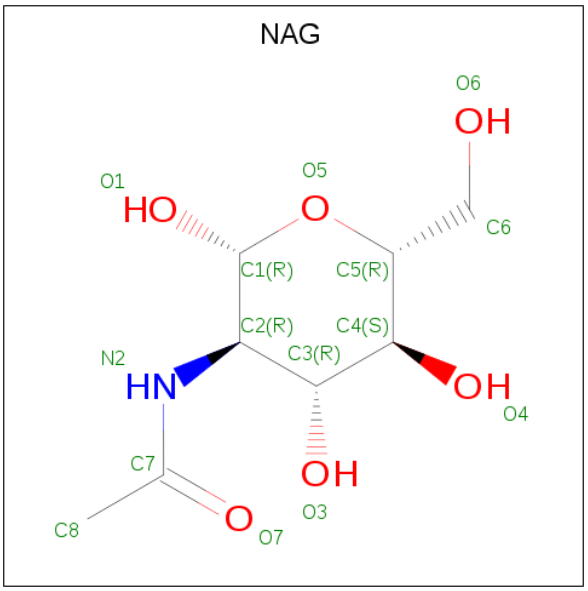
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP P58154
G	-3	ASP	-	expression tag	UNP P58154
G	-2	ASP	-	expression tag	UNP P58154
G	-1	ASP	-	expression tag	UNP P58154
G	0	LYS	-	expression tag	UNP P58154
H	-7	ASP	-	expression tag	UNP P58154
H	-6	TYR	-	expression tag	UNP P58154
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 6-(2-methoxyphenyl)-N 4 ,N 4 -bis[(pyridin-2-yl)methyl]pyrimidine-2,4-diamine (three-letter code: 6GK) (formula: $C_{23}H_{22}N_6O$).



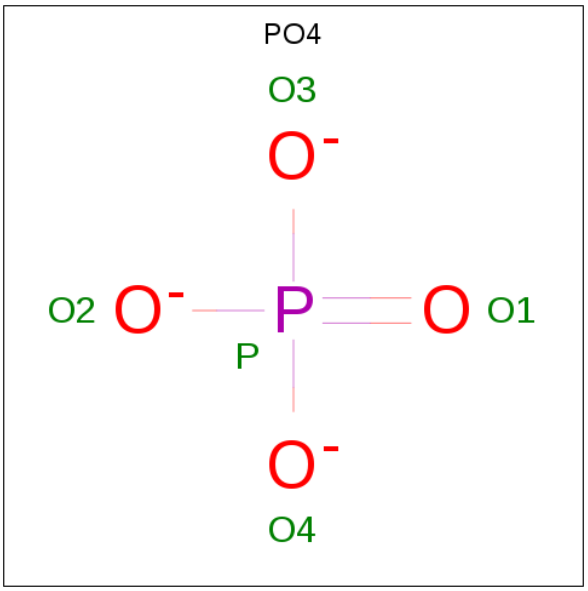
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	23	6	1		
2	B	1	Total	C	N	O	0	0
			30	23	6	1		
2	C	1	Total	C	N	O	0	0
			30	23	6	1		
2	D	1	Total	C	N	O	0	0
			30	23	6	1		
2	D	1	Total	C	N	O	0	0
			30	23	6	1		
2	F	1	Total	C	N	O	0	0
			30	23	6	1		
2	G	1	Total	C	N	O	0	0
			30	23	6	1		
2	G	1	Total	C	N	O	0	0
			30	23	6	1		
2	I	1	Total	C	N	O	0	0
			30	23	6	1		
2	J	1	Total	C	N	O	0	0
			30	23	6	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
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	I	1	Total C N O 14 8 1 5	0	0
3	J	1	Total C N O 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	A	1	Total O P 5 4 1	0	0
4	C	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	F	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0
4	F	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	12	Total O 12 12	0	0

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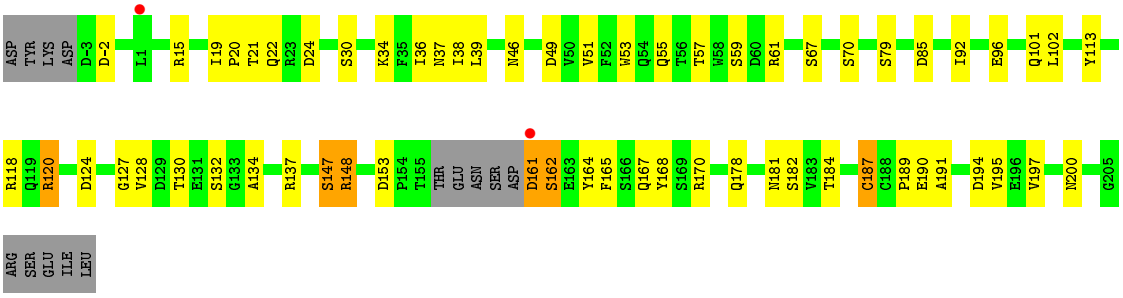
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	15	Total O 15 15	0	0
5	C	15	Total O 15 15	0	0
5	D	20	Total O 20 20	0	0
5	E	12	Total O 12 12	0	0
5	F	19	Total O 19 19	0	0
5	G	15	Total O 15 15	0	0
5	H	14	Total O 14 14	0	0
5	I	9	Total O 9 9	0	0
5	J	9	Total O 9 9	0	0

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.

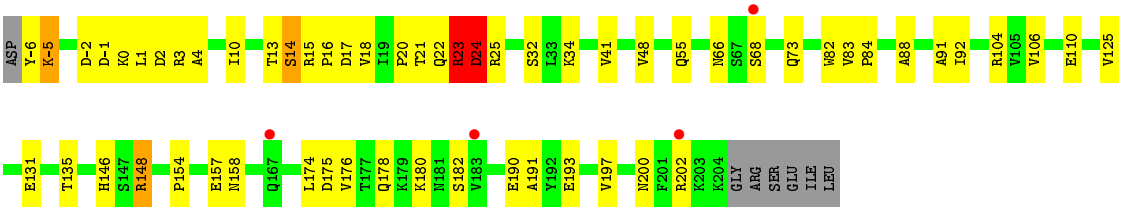
- Molecule 1: Acetylcholine-binding protein

Chain A:



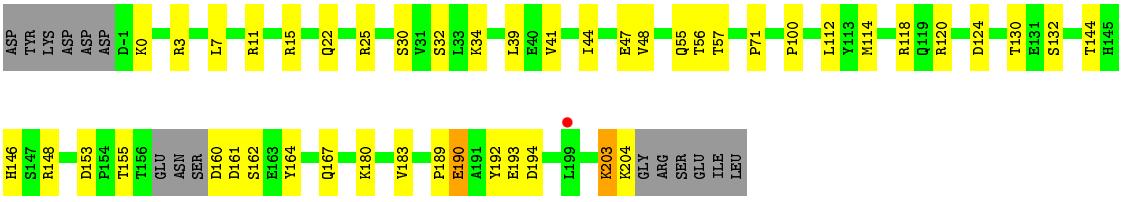
- Molecule 1: Acetylcholine-binding protein

Chain B:



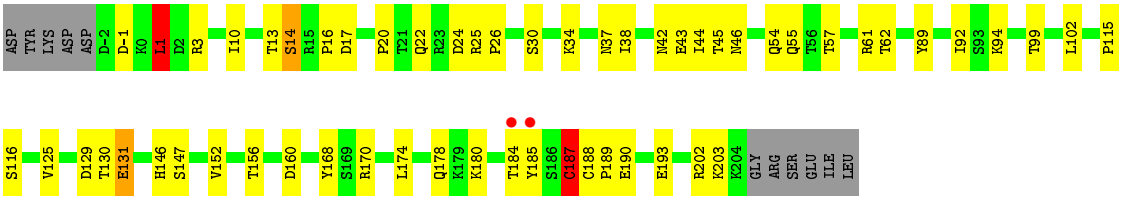
- Molecule 1: Acetylcholine-binding protein

Chain C:



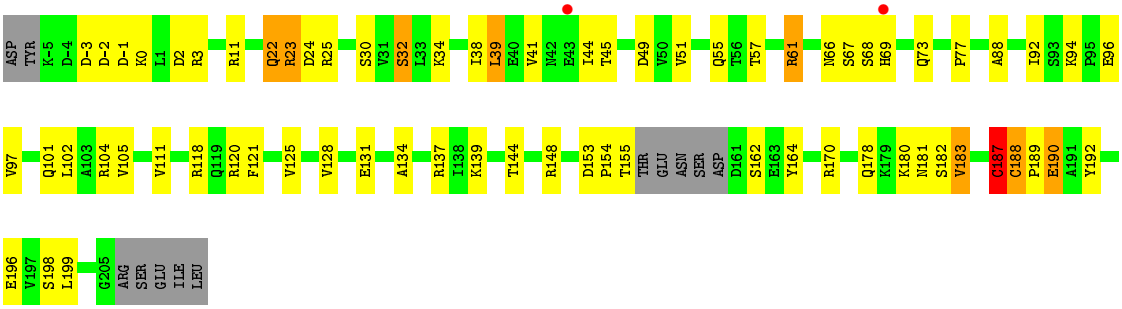
- Molecule 1: Acetylcholine-binding protein

Chain D:



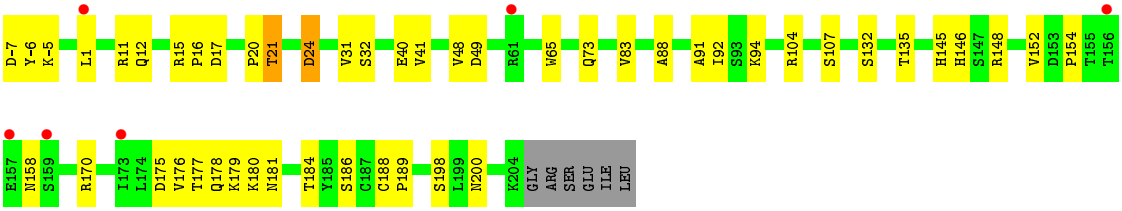
• Molecule 1: Acetylcholine-binding protein

Chain E:



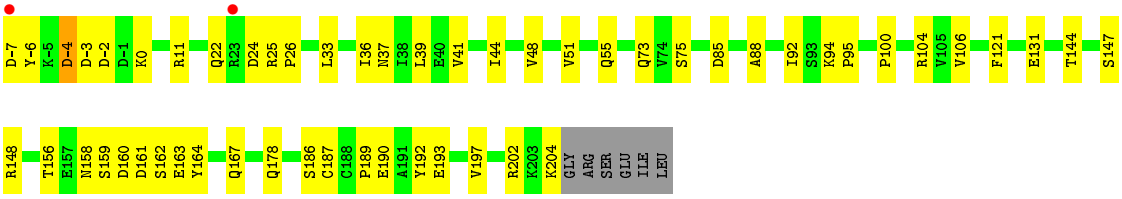
• Molecule 1: Acetylcholine-binding protein

Chain F:



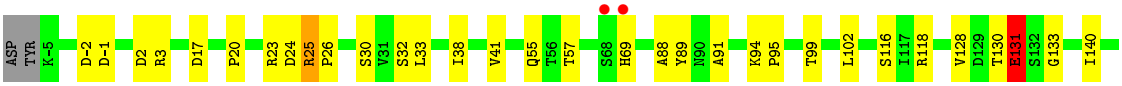
• Molecule 1: Acetylcholine-binding protein

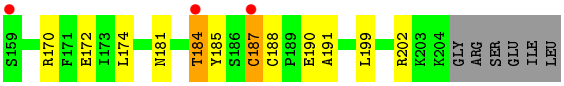
Chain G:



• Molecule 1: Acetylcholine-binding protein

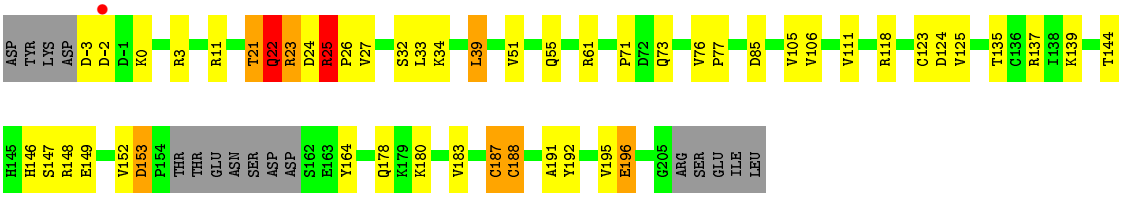
Chain H:





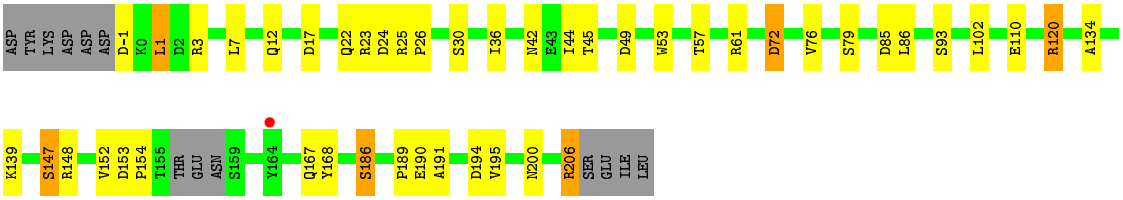
- Molecule 1: Acetylcholine-binding protein

Chain I:



- Molecule 1: Acetylcholine-binding protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.73Å 130.44Å 107.69Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	48.63 – 2.70 48.63 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.63-2.70) 95.6 (48.63-2.33)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.222 , 0.297 0.225 , 0.296	Depositor DCC
R_{free} test set	2004 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 15.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17280	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAG, 6GK

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	0.47	0/1686	0.64	1/2297 (0.0%)
1	B	0.55	1/1731 (0.1%)	0.73	3/2361 (0.1%)
1	C	0.50	0/1661	0.63	0/2265
1	D	0.52	0/1704	0.67	1/2324 (0.0%)
1	E	0.50	0/1703	0.64	0/2319
1	F	0.49	0/1739	0.61	0/2372
1	G	0.49	0/1739	0.63	0/2372
1	H	0.51	0/1718	0.66	0/2343
1	I	0.51	0/1651	0.73	4/2250 (0.2%)
1	J	0.49	0/1686	0.67	1/2296 (0.0%)
All	All	0.50	1/17018 (0.0%)	0.66	10/23199 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	24	ASP	CB-CG	5.36	1.63	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	23	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	B	23	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	I	25	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	161	ASP	CB-CG-OD1	6.59	124.23	118.30
1	I	25	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	I	23	ARG	CA-CB-CG	5.85	126.26	113.40
1	D	1	LEU	CA-CB-CG	-5.47	102.72	115.30
1	I	25	ARG	CB-CG-CD	5.45	125.78	111.60
1	J	1	LEU	CA-CB-CG	-5.10	103.58	115.30
1	B	25	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	131	GLU	Peptide
1	I	21	THR	Peptide
1	I	22	GLN	Peptide

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	1645	0	1595	43	0
1	B	1694	0	1628	41	0
1	C	1626	0	1576	40	0
1	D	1665	0	1611	40	0
1	E	1665	0	1613	54	0
1	F	1702	0	1632	38	0
1	G	1702	0	1632	41	0
1	H	1682	0	1619	34	0
1	I	1616	0	1565	43	0
1	J	1648	0	1603	38	0
2	A	30	0	0	0	0
2	B	30	0	0	1	0
2	C	30	0	0	3	0
2	D	60	0	0	2	0
2	F	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	60	0	0	1	0
2	I	30	0	0	0	0
2	J	30	0	0	0	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	F	14	0	13	0	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	0	0
3	J	14	0	13	0	0
4	A	10	0	0	1	0
4	C	10	0	0	1	0
4	D	5	0	0	0	0
4	F	15	0	0	0	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
4	J	5	0	0	0	0
5	A	12	0	0	1	0
5	B	15	0	0	0	0
5	C	15	0	0	3	0
5	D	20	0	0	0	0
5	E	12	0	0	0	0
5	F	19	0	0	0	0
5	G	15	0	0	3	0
5	H	14	0	0	0	0
5	I	9	0	0	0	0
5	J	9	0	0	1	0
All	All	17280	0	16204	359	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 11.

All (359) 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:I:23:ARG:HG2	1:I:25:ARG:HG2	1.43	0.98
1:B:131:GLU:HA	1:B:202:ARG:HD3	1.45	0.98
1:F:20:PRO:HA	1:G:0:LYS:HE2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:GLN:HG3	1:E:23:ARG:HB2	1.55	0.89
1:G:44:ILE:HG22	1:H:170:ARG:HD2	1.54	0.87
1:E:68:SER:HB3	1:E:69:HIS:HD2	1.38	0.86
1:I:23:ARG:CG	1:I:25:ARG:HG2	2.05	0.86
1:B:158:ASN:ND2	1:B:176:VAL:O	2.12	0.79
1:G:178:GLN:HG2	1:G:197:VAL:HG22	1.66	0.78
1:H:25:ARG:HG3	1:H:26:PRO:HD2	1.65	0.78
1:E:22:GLN:OE1	1:E:61:ARG:NH1	2.17	0.77
1:E:68:SER:HB3	1:E:69:HIS:CD2	2.21	0.76
1:H:3:ARG:NH2	4:H:302:PO4:O2	2.19	0.76
1:D:24:ASP:HA	1:E:-2:ASP:HB3	1.67	0.75
1:H:24:ASP:HA	1:I:-2:ASP:HB2	1.69	0.74
1:I:139:LYS:NZ	1:I:196:GLU:OE1	2.19	0.74
1:J:22:GLN:HE21	1:J:61:ARG:NH1	1.86	0.74
1:B:180:LYS:NZ	1:B:193:GLU:OE1	2.20	0.73
1:C:167:GLN:O	1:C:204:LYS:NZ	2.18	0.73
1:J:23:ARG:HD2	1:J:25:ARG:HB2	1.70	0.73
1:F:158:ASN:ND2	1:F:175:ASP:OD1	2.21	0.73
1:C:130:THR:HG22	1:C:132:SER:H	1.53	0.73
1:I:34:LYS:HG2	1:I:55:GLN:HE21	1.54	0.72
1:J:22:GLN:HE21	1:J:61:ARG:HH11	1.37	0.72
1:A:148:ARG:NH1	1:A:190:GLU:OE1	2.23	0.72
1:F:-7:ASP:OD1	1:F:-5:LYS:N	2.24	0.71
1:B:41:VAL:HG22	1:B:48:VAL:HG12	1.72	0.71
1:B:17:ASP:OD2	1:C:11:ARG:NH2	2.22	0.70
1:C:47:GLU:OE1	1:C:120:ARG:NH2	2.24	0.70
1:F:135:THR:OG1	1:F:200:ASN:ND2	2.26	0.69
1:J:147:SER:OG	1:J:191:ALA:O	2.10	0.69
1:F:11:ARG:NH2	1:J:17:ASP:OD2	2.25	0.69
1:G:73:GLN:HB3	1:G:106:VAL:HA	1.74	0.69
1:D:45:THR:HA	1:E:170:ARG:HD3	1.74	0.68
1:B:135:THR:OG1	1:B:200:ASN:ND2	2.27	0.68
1:J:22:GLN:O	1:J:24:ASP:N	2.25	0.68
1:E:137:ARG:NH1	1:E:198:SER:OG	2.27	0.68
1:E:23:ARG:HH21	1:E:25:ARG:HD3	1.59	0.68
1:C:189:PRO:O	1:C:190:GLU:HB2	1.93	0.67
1:E:187:CYS:SG	1:E:188:CYS:N	2.68	0.66
1:E:183:VAL:HG12	1:E:192:TYR:O	1.96	0.65
1:H:17:ASP:OD2	1:I:11:ARG:NH2	2.29	0.65
1:J:72:ASP:OD1	5:J:401:HOH:O	2.15	0.65
1:I:137:ARG:NH2	1:I:196:GLU:OE1	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:TYR:OH	5:G:401:HOH:O	2.14	0.65
1:C:146:HIS:ND1	1:C:190:GLU:HG3	2.13	0.64
1:G:22:GLN:NE2	1:G:26:PRO:O	2.31	0.64
1:B:158:ASN:ND2	1:B:175:ASP:OD1	2.26	0.64
1:J:148:ARG:NH2	1:J:190:GLU:OE1	2.30	0.64
1:I:187:CYS:SG	1:I:188:CYS:N	2.71	0.64
1:J:22:GLN:HB3	1:J:23:ARG:HG3	1.79	0.64
1:I:23:ARG:HH12	1:I:26:PRO:C	1.99	0.63
1:F:92:ILE:HB	1:G:39:LEU:HD11	1.81	0.63
1:A:178:GLN:HG2	1:A:197:VAL:HG13	1.80	0.63
1:H:174:LEU:HD21	1:H:202:ARG:HE	1.64	0.63
1:E:22:GLN:HG2	1:E:25:ARG:CZ	2.29	0.62
1:A:22:GLN:OE1	1:A:61:ARG:HG3	2.00	0.62
1:B:92:ILE:HB	1:C:39:LEU:HD11	1.81	0.62
1:D:22:GLN:HE22	1:D:61:ARG:HH11	1.47	0.61
1:H:131:GLU:HB3	1:H:202:ARG:HD2	1.83	0.60
1:G:55:GLN:NE2	2:G:301:6GK:N01	2.49	0.60
1:I:26:PRO:HB3	1:I:148:ARG:C	2.22	0.60
1:F:88:ALA:HB3	1:F:91:ALA:HB2	1.83	0.60
1:C:22:GLN:H	1:C:22:GLN:CD	2.05	0.59
1:E:131:GLU:H	1:E:131:GLU:CD	2.03	0.59
1:J:152:VAL:HG12	1:J:195:VAL:HG23	1.82	0.59
1:J:139:LYS:HE2	1:J:194:ASP:OD1	2.03	0.59
1:I:147:SER:OG	1:I:191:ALA:O	2.14	0.59
1:I:22:GLN:HB3	1:I:61:ARG:HD3	1.85	0.59
1:A:59:SER:HB3	5:A:409:HOH:O	2.03	0.58
1:H:130:THR:HG23	1:H:133:GLY:H	1.68	0.58
1:C:192:TYR:OH	5:C:401:HOH:O	2.17	0.58
1:B:23:ARG:NH1	1:B:24:ASP:OD2	2.36	0.58
1:A:24:ASP:HA	1:B:-2:ASP:HB2	1.86	0.58
1:A:20:PRO:HA	1:B:0:LYS:HD3	1.86	0.58
1:H:130:THR:OG1	1:H:131:GLU:N	2.37	0.58
1:A:37:ASN:OD1	1:A:38:ILE:N	2.37	0.57
1:J:167:GLN:NE2	1:J:168:TYR:OH	2.34	0.57
1:E:73:GLN:HB2	1:E:104:ARG:NH2	2.20	0.57
1:C:55:GLN:HG3	1:C:114:MET:SD	2.45	0.56
1:G:22:GLN:CD	1:G:22:GLN:H	2.08	0.56
1:H:-1:ASP:HB3	1:H:2:ASP:HB2	1.86	0.56
1:B:18:VAL:HG22	1:C:7:LEU:HD12	1.88	0.56
1:G:131:GLU:OE2	1:G:202:ARG:NH1	2.39	0.56
1:B:73:GLN:HG2	1:B:106:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:GLN:HB2	1:E:104:ARG:HH21	1.70	0.56
1:I:146:HIS:HB3	1:I:192:TYR:CE1	2.41	0.56
4:C:304:PO4:O4	1:D:3:ARG:NH2	2.33	0.55
1:E:67:SER:OG	1:E:67:SER:O	2.22	0.55
1:F:158:ASN:ND2	1:F:176:VAL:H	2.05	0.55
1:B:-1:ASP:HB3	1:B:2:ASP:HB2	1.89	0.55
1:F:-7:ASP:OD1	1:F:-6:TYR:N	2.40	0.55
1:E:39:LEU:HD11	1:E:51:VAL:HG23	1.88	0.55
1:E:49:ASP:OD2	1:E:118:ARG:NH2	2.40	0.55
1:C:203:LYS:NZ	5:C:403:HOH:O	2.39	0.54
1:G:-4:ASP:O	1:G:-2:ASP:N	2.41	0.54
1:A:39:LEU:HD11	1:E:92:ILE:HB	1.89	0.54
1:G:144:THR:HG21	1:H:102:LEU:HB2	1.90	0.54
1:E:25:ARG:HH22	1:E:61:ARG:HH12	1.55	0.54
1:I:22:GLN:CB	1:I:61:ARG:HD3	2.38	0.53
1:J:206:ARG:CZ	1:J:206:ARG:HB2	2.37	0.53
1:D:10:ILE:O	1:D:14:SER:HB3	2.08	0.53
1:C:41:VAL:HG22	1:C:48:VAL:HG12	1.90	0.53
4:A:304:PO4:O1	1:B:3:ARG:NH2	2.33	0.53
1:E:23:ARG:NH2	1:E:25:ARG:HD3	2.24	0.52
1:I:22:GLN:CD	1:I:23:ARG:HD2	2.29	0.52
1:F:170:ARG:HH21	1:J:45:THR:HG22	1.75	0.52
1:F:24:ASP:HA	1:G:-2:ASP:CB	2.39	0.52
1:H:30:SER:HB2	1:H:57:THR:CG2	2.40	0.52
1:C:55:GLN:HG2	2:C:301:6GK:C02	2.40	0.52
1:B:88:ALA:HB3	1:B:91:ALA:HB2	1.92	0.51
1:E:77:PRO:HA	1:E:102:LEU:HD23	1.92	0.51
1:F:17:ASP:OD2	1:G:11:ARG:NH2	2.34	0.51
1:I:105:VAL:HG22	1:I:111:VAL:HG22	1.91	0.51
1:I:32:SER:O	1:I:55:GLN:HG3	2.10	0.51
1:J:42:ASN:OD1	1:J:44:ILE:HG12	2.11	0.51
1:D:20:PRO:HA	1:E:0:LYS:HD2	1.93	0.51
1:I:27:VAL:N	1:I:149:GLU:O	2.44	0.51
1:C:44:ILE:O	1:D:170:ARG:HG3	2.11	0.51
1:E:30:SER:HB2	1:E:57:THR:HG22	1.93	0.51
1:I:34:LYS:HG2	1:I:55:GLN:NE2	2.24	0.51
1:A:34:LYS:HD2	1:A:164:TYR:CE2	2.45	0.51
1:B:174:LEU:HD12	1:B:200:ASN:OD1	2.10	0.50
1:D:152:VAL:O	1:D:180:LYS:HE2	2.10	0.50
1:E:153:ASP:OD1	1:E:180:LYS:NZ	2.44	0.50
1:F:148:ARG:NH2	1:G:-6:TYR:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:ILE:O	1:H:118:ARG:NH1	2.40	0.50
1:D:189:PRO:HG2	1:D:190:GLU:HG3	1.93	0.50
1:G:36:ILE:HD13	1:G:164:TYR:HB3	1.93	0.50
1:H:32:SER:HB3	1:H:55:GLN:HE21	1.76	0.50
1:A:170:ARG:NH1	1:E:45:THR:HG22	2.27	0.50
1:G:73:GLN:HG3	1:G:104:ARG:HH21	1.76	0.50
1:D:174:LEU:HD21	1:D:202:ARG:HG2	1.94	0.50
1:I:34:LYS:HB3	1:I:164:TYR:HD2	1.77	0.50
1:I:21:THR:HG22	1:I:27:VAL:HG23	1.94	0.50
1:A:130:THR:HG22	1:A:132:SER:H	1.77	0.49
1:A:96:GLU:HG3	1:E:94:LYS:HE2	1.93	0.49
1:J:49:ASP:HB2	1:J:120[B]:ARG:NH1	2.27	0.49
1:D:44:ILE:HG13	1:D:45:THR:N	2.26	0.49
1:F:41:VAL:HG22	1:F:48:VAL:HG23	1.93	0.49
1:I:144:THR:HG21	1:J:102:LEU:HB2	1.94	0.49
1:I:73:GLN:HG2	1:I:106:VAL:HA	1.94	0.49
1:D:42:ASN:O	1:D:125:VAL:HG11	2.12	0.49
1:H:174:LEU:HD21	1:H:202:ARG:NE	2.26	0.49
1:A:194:ASP:OD1	1:A:195:VAL:N	2.46	0.49
1:E:32:SER:HA	1:E:178:GLN:HE22	1.77	0.49
1:C:144:THR:HG21	1:D:102:LEU:HB2	1.94	0.49
1:C:55:GLN:HG2	2:C:301:6GK:C03	2.42	0.49
1:E:125:VAL:O	1:E:128:VAL:HG12	2.13	0.49
1:B:55:GLN:HB3	2:B:301:6GK:C07	2.42	0.49
1:H:41:VAL:HG11	1:H:128:VAL:HG21	1.95	0.49
1:D:55:GLN:HG2	2:D:301:6GK:C03	2.43	0.49
1:J:206:ARG:CG	1:J:206:ARG:HH11	2.26	0.48
1:D:17:ASP:OD2	1:E:11:ARG:NH2	2.44	0.48
1:E:139:LYS:HE3	1:E:196:GLU:OE1	2.12	0.48
1:D:30:SER:HB2	1:D:57:THR:CG2	2.44	0.48
1:A:170:ARG:HH11	1:E:45:THR:HG22	1.79	0.48
1:G:148:ARG:HD2	5:G:411:HOH:O	2.13	0.48
1:G:156:THR:HG22	1:G:158:ASN:HB2	1.96	0.48
1:I:21:THR:CG2	1:I:27:VAL:HG23	2.43	0.48
1:A:30:SER:HB2	1:A:57:THR:HG23	1.95	0.48
1:B:32:SER:HA	1:B:178:GLN:HE22	1.78	0.48
1:C:15:ARG:HH12	1:D:1:LEU:HD11	1.79	0.48
1:B:10:ILE:O	1:B:14:SER:HB3	2.13	0.48
1:C:34:LYS:HD3	1:C:164:TYR:CZ	2.49	0.48
1:F:73:GLN:HB2	1:F:104:ARG:NH2	2.28	0.48
1:C:160:ASP:OD1	1:C:161:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HG2	1:A:190:GLU:HG3	1.95	0.48
1:H:131:GLU:OE1	1:H:202:ARG:NH1	2.47	0.48
1:G:33:LEU:H	1:G:178:GLN:HE22	1.62	0.48
1:D:129:ASP:OD1	1:D:203:LYS:HE2	2.14	0.47
1:C:34:LYS:HD3	1:C:164:TYR:CE1	2.49	0.47
1:J:7:LEU:HD13	1:J:76:VAL:HG22	1.95	0.47
1:A:184:THR:HG22	1:A:191:ALA:HA	1.96	0.47
1:B:-6:TYR:CD2	1:B:-5:LYS:HG3	2.48	0.47
1:A:170:ARG:HD2	1:E:44:ILE:HG22	1.97	0.47
1:J:206:ARG:HG2	1:J:206:ARG:HH11	1.78	0.47
1:B:178:GLN:HG2	1:B:197:VAL:HG22	1.96	0.47
1:B:-1:ASP:O	1:B:3:ARG:HG3	2.14	0.47
1:D:22:GLN:HE22	1:D:61:ARG:NH1	2.12	0.47
1:E:22:GLN:HE21	1:E:23:ARG:HD3	1.79	0.47
1:I:22:GLN:O	1:I:24:ASP:N	2.43	0.47
1:B:82:TRP:CZ3	1:B:84:PRO:HD3	2.49	0.47
1:G:167:GLN:O	1:G:204:LYS:NZ	2.48	0.47
1:A:67:SER:HA	1:A:70:SER:HB2	1.97	0.47
1:D:37:ASN:OD1	1:D:38:ILE:N	2.48	0.47
1:F:180:LYS:HG2	1:F:181:ASN:N	2.29	0.47
1:B:158:ASN:ND2	1:B:176:VAL:H	2.13	0.47
2:D:302:6GK:C03	1:E:55:GLN:HG2	2.44	0.47
1:I:139:LYS:NZ	1:I:196:GLU:HB2	2.30	0.47
1:A:51:VAL:HG22	1:A:118:ARG:HB2	1.96	0.47
1:A:147:SER:OG	1:A:191:ALA:O	2.29	0.47
1:C:15:ARG:NH1	1:D:1:LEU:HD11	2.29	0.47
1:A:102:LEU:HB2	1:E:144:THR:HG21	1.97	0.47
1:E:68:SER:CB	1:E:69:HIS:HD2	2.19	0.47
1:I:124:ASP:HB3	1:I:135:THR:O	2.15	0.47
1:C:3:ARG:HG2	1:C:71:PRO:HG2	1.96	0.47
1:D:187:CYS:SG	1:D:188:CYS:N	2.88	0.47
1:I:25:ARG:HB3	1:I:26:PRO:HD2	1.97	0.47
1:A:34:LYS:HE2	1:A:55:GLN:NE2	2.30	0.46
1:B:73:GLN:HB2	1:B:104:ARG:NH2	2.31	0.46
1:H:30:SER:HB2	1:H:57:THR:HG22	1.96	0.46
1:B:146:HIS:CD2	1:B:190:GLU:HG3	2.50	0.46
1:C:39:LEU:HD12	1:C:118:ARG:HE	1.80	0.46
1:J:139:LYS:HE2	1:J:194:ASP:CG	2.36	0.46
1:J:186:SER:OG	1:J:186:SER:O	2.33	0.46
1:B:66:ASN:OD1	1:B:68:SER:HB2	2.15	0.46
1:F:175:ASP:OD1	1:F:176:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ALA:HB3	1:H:91:ALA:HB2	1.97	0.46
1:A:162:SER:HA	1:A:165:PHE:H	1.80	0.46
1:B:24:ASP:C	1:B:24:ASP:OD1	2.54	0.46
1:E:148:ARG:NH1	1:E:190:GLU:OE2	2.47	0.46
1:I:-3:ASP:O	1:I:3:ARG:NH1	2.48	0.46
1:A:162:SER:OG	1:A:165:PHE:HB3	2.15	0.46
1:G:24:ASP:HA	1:H:-2:ASP:HB2	1.96	0.46
1:H:38:ILE:HD11	1:H:199:LEU:HD21	1.97	0.46
1:D:25:ARG:HB3	1:D:26:PRO:HD2	1.96	0.46
1:F:158:ASN:ND2	1:F:176:VAL:O	2.37	0.46
1:G:100:PRO:O	5:G:403:HOH:O	2.20	0.46
1:J:36:ILE:HG13	1:J:53:TRP:CD1	2.51	0.46
1:G:41:VAL:HG22	1:G:48:VAL:HG12	1.98	0.46
1:I:23:ARG:NH2	1:I:26:PRO:O	2.43	0.46
1:C:32:SER:O	1:C:55:GLN:HB2	2.16	0.46
1:E:88:ALA:HB1	1:E:121:PHE:HE2	1.81	0.46
1:D:94:LYS:HE3	1:E:96:GLU:HG3	1.98	0.46
1:H:187:CYS:SG	1:H:188:CYS:N	2.88	0.46
1:B:34:LYS:NZ	1:B:157:GLU:O	2.41	0.46
1:E:-3:ASP:O	1:E:3:ARG:NH1	2.49	0.46
1:J:148:ARG:HH22	1:J:190:GLU:CD	2.18	0.46
1:D:54:GLN:HB3	1:D:115:PRO:HD2	1.97	0.45
1:F:148:ARG:HH12	1:G:-6:TYR:HB3	1.82	0.45
1:I:123:CYS:O	1:I:125:VAL:HG23	2.16	0.45
1:C:22:GLN:HG2	1:C:25:ARG:HB2	1.98	0.45
1:F:94:LYS:HE2	1:F:94:LYS:HB3	1.61	0.45
1:G:88:ALA:HB1	1:G:121:PHE:HE2	1.82	0.45
1:I:23:ARG:HG3	1:I:25:ARG:HG2	1.95	0.45
1:A:127:GLY:O	1:A:130:THR:HB	2.17	0.45
1:E:97:VAL:HG11	1:E:101:GLN:CD	2.37	0.45
1:G:147:SER:HB3	1:G:193:GLU:HG3	1.98	0.45
1:D:13:THR:HG21	1:D:62:THR:O	2.17	0.45
1:F:15:ARG:HA	1:F:16:PRO:HD3	1.75	0.45
1:G:160:ASP:HB2	1:G:163:GLU:HG2	1.99	0.45
1:G:85:ASP:N	1:G:85:ASP:OD1	2.47	0.45
1:I:85:ASP:OD2	1:I:144:THR:OG1	2.31	0.45
1:I:39:LEU:HD11	1:I:51:VAL:HG23	1.99	0.45
1:A:167:GLN:HG3	1:A:168:TYR:CE1	2.52	0.44
1:A:134:ALA:O	1:A:200:ASN:ND2	2.50	0.44
1:A:49:ASP:HB2	1:A:120[B]:ARG:NH1	2.32	0.44
1:A:85:ASP:N	1:A:85:ASP:OD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:VAL:HG13	1:E:125:VAL:HG11	1.98	0.44
1:F:73:GLN:HB2	1:F:104:ARG:HH21	1.82	0.44
1:A:46:ASN:OD1	1:A:124:ASP:HA	2.16	0.44
1:F:148:ARG:NH1	1:G:-6:TYR:HB3	2.32	0.44
1:B:148:ARG:HD3	1:B:148:ARG:HA	1.85	0.44
1:C:180:LYS:HD3	1:C:193:GLU:OE1	2.17	0.44
1:F:31:VAL:HG23	1:F:152:VAL:HG13	2.00	0.44
1:B:41:VAL:HG13	1:B:125:VAL:HG11	1.99	0.44
1:B:15:ARG:NH1	1:J:12:GLN:OE1	2.49	0.44
1:F:65:TRP:CZ3	1:F:107:SER:HA	2.52	0.44
1:F:24:ASP:HA	1:G:-2:ASP:HB2	2.00	0.44
1:J:30:SER:HB3	1:J:57:THR:HG23	1.97	0.44
1:C:153:ASP:HA	1:C:180:LYS:HE2	2.00	0.44
1:A:128:VAL:HB	1:A:134:ALA:HB2	2.00	0.44
1:C:30:SER:O	1:C:56:THR:HA	2.18	0.44
1:D:147:SER:HB3	1:D:193:GLU:HG3	2.00	0.44
1:A:36:ILE:HG13	1:A:53:TRP:CD1	2.52	0.44
1:B:20:PRO:HA	1:C:0:LYS:HD2	2.00	0.44
1:C:57:THR:HG23	1:C:112:LEU:HD23	2.00	0.44
1:E:22:GLN:HG2	1:E:25:ARG:NE	2.32	0.44
1:J:25:ARG:HB3	1:J:26:PRO:HD2	2.00	0.44
1:C:22:GLN:HG3	1:C:25:ARG:HE	1.83	0.43
1:D:130:THR:C	1:D:131:GLU:HG2	2.38	0.43
1:F:146:HIS:CE1	1:F:148:ARG:HB3	2.53	0.43
1:J:-1:ASP:O	1:J:3:ARG:HG3	2.18	0.43
1:J:49:ASP:HB2	1:J:120[B]:ARG:HH11	1.84	0.43
1:H:23:ARG:CG	1:H:24:ASP:N	2.81	0.43
1:I:152:VAL:HG12	1:I:195:VAL:HG23	2.00	0.43
1:J:30:SER:HB3	1:J:57:THR:CG2	2.48	0.43
1:B:182:SER:OG	1:B:191:ALA:HB1	2.19	0.43
1:A:167:GLN:NE2	1:A:168:TYR:OH	2.48	0.43
1:A:24:ASP:HA	1:B:-2:ASP:CB	2.47	0.43
1:I:21:THR:O	1:I:22:GLN:O	2.36	0.43
1:D:30:SER:HB2	1:D:57:THR:HG23	1.99	0.43
1:G:94:LYS:HG3	1:G:95:PRO:HD2	2.01	0.43
1:H:172:GLU:OE2	1:H:202:ARG:NH2	2.52	0.43
1:H:89:TYR:N	1:H:89:TYR:CD2	2.87	0.43
1:B:23:ARG:HH11	1:B:23:ARG:HD2	1.46	0.43
1:F:24:ASP:HA	1:G:-2:ASP:HB3	2.00	0.43
1:H:20:PRO:HA	1:I:0:LYS:HE3	2.00	0.43
1:I:-3:ASP:OD1	1:I:71:PRO:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ARG:NH2	1:J:45:THR:HG22	2.34	0.42
1:C:183:VAL:HG23	1:C:194:ASP:OD1	2.19	0.42
1:J:93:SER:HB3	1:J:120[A]:ARG:HD2	2.01	0.42
1:B:15:ARG:HA	1:B:16:PRO:HD3	1.82	0.42
1:J:1:LEU:HD23	1:J:1:LEU:HA	1.76	0.42
1:J:85:ASP:OD1	1:J:85:ASP:N	2.52	0.42
1:F:1:LEU:HD12	1:F:1:LEU:HA	1.92	0.42
1:C:22:GLN:NE2	1:C:25:ARG:O	2.53	0.42
1:E:125:VAL:HA	1:E:134:ALA:HB1	2.02	0.42
1:G:-7:ASP:OD2	1:G:-4:ASP:N	2.30	0.42
1:D:99:THR:HG23	1:D:116:SER:HB3	2.02	0.42
1:A:-2:ASP:HB2	1:E:24:ASP:HA	2.01	0.42
1:F:32:SER:HA	1:F:178:GLN:HE22	1.85	0.42
1:F:177:THR:HB	1:F:198:SER:HB2	2.01	0.42
1:H:99:THR:HG23	1:H:116:SER:HB3	2.01	0.42
1:D:14:SER:O	1:D:16:PRO:HD3	2.19	0.42
1:E:181:ASN:OD1	1:E:182:SER:N	2.53	0.42
1:E:34:LYS:HB3	1:E:164:TYR:HD1	1.84	0.42
1:B:23:ARG:HD2	1:B:24:ASP:HB3	2.02	0.41
1:E:38:ILE:HD11	1:E:199:LEU:HD21	2.01	0.41
1:G:161:ASP:OD1	1:G:161:ASP:N	2.49	0.41
1:I:76:VAL:HG12	1:I:77:PRO:O	2.20	0.41
1:H:23:ARG:HG3	1:H:24:ASP:H	1.85	0.41
1:H:185:TYR:HE1	1:I:164:TYR:CE1	2.38	0.41
1:A:36:ILE:HD13	1:A:164:TYR:HB3	2.02	0.41
1:A:19:ILE:HG13	1:A:21:THR:HG23	2.02	0.41
1:I:153:ASP:OD1	1:I:180:LYS:NZ	2.53	0.41
1:C:44:ILE:O	1:D:170:ARG:NH1	2.53	0.41
1:D:185:TYR:HE1	1:E:164:TYR:CE2	2.39	0.41
1:E:105:VAL:HG22	1:E:111:VAL:HG22	2.02	0.41
1:A:92:ILE:HD11	1:A:120[B]:ARG:HG2	2.03	0.41
1:D:34:LYS:NZ	1:D:160:ASP:OD1	2.52	0.41
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.56	0.41
1:E:137:ARG:HD3	1:E:196:GLU:OE2	2.20	0.41
1:E:69:HIS:ND1	1:H:69:HIS:CD2	2.89	0.41
1:G:22:GLN:HG2	1:G:25:ARG:HB2	2.02	0.41
1:H:94:LYS:HG2	1:H:95:PRO:HD2	2.03	0.41
1:B:1:LEU:HA	1:B:1:LEU:HD12	1.89	0.41
1:C:22:GLN:HE21	1:C:25:ARG:HB2	1.86	0.41
1:E:180:LYS:HG3	1:E:181:ASN:N	2.36	0.41
1:J:22:GLN:NE2	1:J:61:ARG:NH1	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:OD1	1:A:182:SER:N	2.51	0.41
1:D:46:ASN:HA	1:D:125:VAL:HG12	2.01	0.41
1:F:145:HIS:CE1	1:G:75:SER:HB2	2.56	0.41
1:F:158:ASN:HD21	1:F:176:VAL:C	2.21	0.41
1:F:179:LYS:HE3	1:F:179:LYS:HB2	1.73	0.41
1:G:22:GLN:HG2	1:G:22:GLN:O	2.21	0.41
1:A:101:GLN:OE1	1:A:113:TYR:OH	2.33	0.41
1:C:167:GLN:HG3	1:C:167:GLN:H	1.71	0.41
1:E:-1:ASP:O	1:E:2:ASP:HB2	2.20	0.41
1:A:15:ARG:NH2	1:F:12:GLN:OE1	2.53	0.41
1:F:40:GLU:HG2	1:F:49:ASP:CB	2.51	0.41
1:I:39:LEU:HD13	1:I:118:ARG:NH1	2.36	0.41
1:J:153:ASP:HA	1:J:154:PRO:HD3	1.88	0.41
1:D:156:THR:HG21	1:D:178:GLN:HG3	2.03	0.41
1:G:37:ASN:HB2	1:G:51:VAL:HB	2.03	0.41
1:C:164:TYR:OH	2:C:301:6GK:N02	2.54	0.40
1:F:21:THR:OG1	1:G:-2:ASP:HB3	2.21	0.40
1:H:89:TYR:HD2	1:H:89:TYR:H	1.69	0.40
1:J:134:ALA:O	1:J:200:ASN:HA	2.22	0.40
1:A:15:ARG:NH1	1:B:4:ALA:HB1	2.35	0.40
1:C:100:PRO:O	5:C:402:HOH:O	2.22	0.40
1:H:184:THR:HG23	1:H:191:ALA:HB2	2.02	0.40
1:D:89:TYR:HD2	1:D:89:TYR:H	1.69	0.40
1:H:33:LEU:HD11	1:H:140:ILE:HD11	2.04	0.40
1:D:46:ASN:OD1	1:D:125:VAL:HG12	2.20	0.40
1:I:33:LEU:H	1:I:178:GLN:HE22	1.69	0.40
1:J:86:LEU:HA	1:J:86:LEU:HD23	1.81	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	202/218 (93%)	194 (96%)	6 (3%)	2 (1%)	15	37
1	B	209/218 (96%)	198 (95%)	8 (4%)	3 (1%)	11	28
1	C	199/218 (91%)	194 (98%)	3 (2%)	2 (1%)	15	37
1	D	206/218 (94%)	197 (96%)	7 (3%)	2 (1%)	15	37
1	E	204/218 (94%)	187 (92%)	10 (5%)	7 (3%)	3	8
1	F	210/218 (96%)	204 (97%)	4 (2%)	2 (1%)	15	37
1	G	210/218 (96%)	196 (93%)	12 (6%)	2 (1%)	15	37
1	H	208/218 (95%)	197 (95%)	10 (5%)	1 (0%)	29	54
1	I	198/218 (91%)	186 (94%)	10 (5%)	2 (1%)	15	37
1	J	202/218 (93%)	190 (94%)	11 (5%)	1 (0%)	29	54
All	All	2048/2180 (94%)	1943 (95%)	81 (4%)	24 (1%)	13	32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	D	-1	ASP
1	E	162	SER
1	G	-3	ASP
1	I	22	GLN
1	E	183	VAL
1	E	189	PRO
1	E	190	GLU
1	G	189	PRO
1	B	-5	LYS
1	B	24	ASP
1	C	190	GLU
1	E	187	CYS
1	A	187	CYS
1	C	155	THR
1	D	187	CYS
1	E	66	ASN
1	J	189	PRO
1	F	154	PRO
1	H	190	GLU
1	I	25	ARG
1	F	189	PRO
1	B	154	PRO
1	E	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	192/204 (94%)	183 (95%)	9 (5%)	26	54
1	B	198/204 (97%)	189 (96%)	9 (4%)	27	55
1	C	190/204 (93%)	187 (98%)	3 (2%)	62	85
1	D	195/204 (96%)	188 (96%)	7 (4%)	35	64
1	E	194/204 (95%)	184 (95%)	10 (5%)	23	49
1	F	199/204 (98%)	192 (96%)	7 (4%)	36	65
1	G	199/204 (98%)	193 (97%)	6 (3%)	41	70
1	H	197/204 (97%)	192 (98%)	5 (2%)	47	76
1	I	188/204 (92%)	181 (96%)	7 (4%)	34	63
1	J	192/204 (94%)	184 (96%)	8 (4%)	30	58
All	All	1944/2040 (95%)	1873 (96%)	71 (4%)	36	63

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	A	120[A]	ARG
1	A	120[B]	ARG
1	A	137	ARG
1	A	147	SER
1	A	148	ARG
1	A	153	ASP
1	A	161	ASP
1	A	187	CYS
1	B	13	THR
1	B	14	SER
1	B	21	THR
1	B	22	GLN
1	B	23	ARG
1	B	24	ASP
1	B	83	VAL

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Mol	Chain	Res	Type
1	B	110	GLU
1	B	148	ARG
1	C	148	ARG
1	C	162	SER
1	C	203	LYS
1	D	1	LEU
1	D	14	SER
1	D	43	GLU
1	D	131	GLU
1	D	146	HIS
1	D	184	THR
1	D	187	CYS
1	E	22	GLN
1	E	23	ARG
1	E	32	SER
1	E	39	LEU
1	E	61	ARG
1	E	120[A]	ARG
1	E	120[B]	ARG
1	E	155	THR
1	E	187	CYS
1	E	188	CYS
1	F	21	THR
1	F	24	ASP
1	F	83	VAL
1	F	132	SER
1	F	184	THR
1	F	186	SER
1	F	188	CYS
1	G	-4	ASP
1	G	159	SER
1	G	162	SER
1	G	186	SER
1	G	187	CYS
1	G	190	GLU
1	H	25	ARG
1	H	131	GLU
1	H	181	ASN
1	H	184	THR
1	H	187	CYS
1	I	22	GLN
1	I	39	LEU

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Mol	Chain	Res	Type
1	I	153	ASP
1	I	183	VAL
1	I	187	CYS
1	I	188	CYS
1	I	196	GLU
1	J	72	ASP
1	J	79	SER
1	J	110	GLU
1	J	120[A]	ARG
1	J	120[B]	ARG
1	J	147	SER
1	J	186	SER
1	J	206	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	200	ASN
1	C	22	GLN
1	D	9	ASN
1	E	69	HIS
1	F	181	ASN
1	F	200	ASN
1	G	22	GLN
1	G	55	GLN
1	H	69	HIS
1	I	200	ASN
1	J	22	GLN
1	J	167	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

31 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	B	302	1	14,14,15	0.22	0	17,19,21	0.44	0
4	PO4	H	302	-	4,4,4	0.91	0	6,6,6	0.39	0
2	6GK	B	301	-	33,33,33	2.03	6 (18%)	44,44,44	2.47	16 (36%)
2	6GK	C	301	-	33,33,33	1.97	5 (15%)	44,44,44	2.27	14 (31%)
3	NAG	I	302	1	14,14,15	0.58	0	17,19,21	0.55	0
3	NAG	H	301	1	14,14,15	0.75	1 (7%)	17,19,21	0.77	1 (5%)
4	PO4	F	304	-	4,4,4	1.16	0	6,6,6	0.41	0
4	PO4	C	303	-	4,4,4	0.95	0	6,6,6	0.48	0
3	NAG	J	302	1	14,14,15	0.37	0	17,19,21	0.71	1 (5%)
2	6GK	I	301	-	33,33,33	1.86	5 (15%)	44,44,44	2.46	13 (29%)
4	PO4	J	303	-	4,4,4	0.77	0	6,6,6	0.73	0
3	NAG	D	303	1	14,14,15	0.87	1 (7%)	17,19,21	0.95	1 (5%)
2	6GK	A	301	-	33,33,33	1.96	6 (18%)	44,44,44	2.14	13 (29%)
3	NAG	C	302	1	14,14,15	0.39	0	17,19,21	0.53	0
2	6GK	D	302	-	33,33,33	1.81	5 (15%)	44,44,44	2.38	11 (25%)
3	NAG	E	301	1	14,14,15	0.54	0	17,19,21	0.61	0
3	NAG	A	302	1	14,14,15	0.40	0	17,19,21	0.71	0
4	PO4	C	304	-	4,4,4	0.94	0	6,6,6	0.59	0
2	6GK	J	301	-	33,33,33	1.96	7 (21%)	44,44,44	2.23	10 (22%)
2	6GK	F	301	-	33,33,33	2.00	6 (18%)	44,44,44	2.39	16 (36%)
3	NAG	G	303	1	14,14,15	0.29	0	17,19,21	0.39	0
2	6GK	G	302	-	33,33,33	2.06	5 (15%)	44,44,44	2.26	16 (36%)
4	PO4	F	303	-	4,4,4	0.77	0	6,6,6	0.49	0
4	PO4	A	303	-	4,4,4	0.90	0	6,6,6	0.67	0
4	PO4	D	304	-	4,4,4	0.79	0	6,6,6	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	F	302	1	14,14,15	0.33	0	17,19,21	0.67	1 (5%)
4	PO4	I	303	-	4,4,4	0.86	0	6,6,6	0.45	0
4	PO4	F	305	-	4,4,4	0.76	0	6,6,6	0.63	0
2	6GK	G	301	-	33,33,33	1.98	5 (15%)	44,44,44	2.21	14 (31%)
2	6GK	D	301	-	33,33,33	1.94	5 (15%)	44,44,44	2.15	16 (36%)
4	PO4	A	304	-	4,4,4	0.79	0	6,6,6	0.56	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	F	302	1	-	2/6/23/26	0/1/1/1
2	6GK	I	301	-	-	0/18/18/18	0/4/4/4
2	6GK	J	301	-	-	0/18/18/18	0/4/4/4
3	NAG	B	302	1	-	2/6/23/26	0/1/1/1
2	6GK	F	301	-	-	2/18/18/18	0/4/4/4
3	NAG	G	303	1	-	4/6/23/26	0/1/1/1
3	NAG	D	303	1	-	3/6/23/26	0/1/1/1
2	6GK	A	301	-	-	0/18/18/18	0/4/4/4
2	6GK	B	301	-	-	2/18/18/18	0/4/4/4
2	6GK	C	301	-	-	0/18/18/18	0/4/4/4
2	6GK	G	302	-	-	0/18/18/18	0/4/4/4
3	NAG	I	302	1	-	1/6/23/26	0/1/1/1
2	6GK	D	302	-	-	0/18/18/18	0/4/4/4
2	6GK	G	301	-	-	1/18/18/18	0/4/4/4
3	NAG	A	302	1	-	3/6/23/26	0/1/1/1
3	NAG	E	301	1	-	3/6/23/26	0/1/1/1
3	NAG	H	301	1	-	3/6/23/26	0/1/1/1
3	NAG	J	302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	302	1	-	2/6/23/26	0/1/1/1
2	6GK	D	301	-	-	0/18/18/18	0/4/4/4

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	6GK	C18-C19	-7.16	1.39	1.51
2	F	301	6GK	C18-C19	-7.02	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	302	6GK	C18-C19	-7.00	1.39	1.51
2	D	301	6GK	C18-C19	-6.65	1.40	1.51
2	G	302	6GK	C12-C13	-6.64	1.40	1.51
2	G	301	6GK	C18-C19	-6.52	1.40	1.51
2	G	301	6GK	C12-C13	-6.45	1.40	1.51
2	C	301	6GK	C18-C19	-6.39	1.40	1.51
2	D	301	6GK	C12-C13	-6.37	1.40	1.51
2	I	301	6GK	C12-C13	-6.34	1.40	1.51
2	C	301	6GK	C12-C13	-6.33	1.40	1.51
2	A	301	6GK	C12-C13	-6.31	1.40	1.51
2	B	301	6GK	C12-C13	-6.30	1.40	1.51
2	F	301	6GK	C12-C13	-6.21	1.41	1.51
2	J	301	6GK	C12-C13	-6.17	1.41	1.51
2	D	302	6GK	C18-C19	-6.13	1.41	1.51
2	D	302	6GK	C12-C13	-6.11	1.41	1.51
2	I	301	6GK	C18-C19	-6.05	1.41	1.51
2	J	301	6GK	C18-C19	-5.96	1.41	1.51
2	A	301	6GK	C18-C19	-5.93	1.41	1.51
2	C	301	6GK	C03-C08	-3.87	1.38	1.48
2	D	301	6GK	C03-C08	-3.78	1.38	1.48
2	G	301	6GK	C03-C08	-3.62	1.39	1.48
2	G	302	6GK	C03-C08	-3.61	1.39	1.48
2	A	301	6GK	C03-C08	-3.61	1.39	1.48
2	J	301	6GK	C03-C08	-3.56	1.39	1.48
2	F	301	6GK	C03-C08	-3.48	1.39	1.48
2	I	301	6GK	C03-C08	-3.47	1.39	1.48
2	A	301	6GK	C17-N05	3.47	1.41	1.34
2	D	302	6GK	C03-C08	-3.35	1.40	1.48
2	J	301	6GK	C20-N06	3.33	1.41	1.34
2	J	301	6GK	C17-N05	3.33	1.41	1.34
2	B	301	6GK	C03-C08	-3.32	1.40	1.48
2	B	301	6GK	C20-N06	3.27	1.41	1.34
2	G	301	6GK	C20-N06	3.18	1.41	1.34
2	G	302	6GK	C17-N05	3.14	1.41	1.34
2	G	302	6GK	C20-N06	3.10	1.41	1.34
2	C	301	6GK	C20-N06	3.01	1.41	1.34
2	F	301	6GK	C20-N06	3.00	1.40	1.34
2	D	301	6GK	C20-N06	3.00	1.40	1.34
2	F	301	6GK	C17-N05	2.88	1.40	1.34
2	I	301	6GK	C17-N05	2.84	1.40	1.34
2	B	301	6GK	C17-N05	2.78	1.40	1.34
2	B	301	6GK	C12-N04	2.77	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	6GK	C17-N05	2.74	1.40	1.34
2	A	301	6GK	C20-N06	2.73	1.40	1.34
2	D	302	6GK	C20-N06	2.69	1.40	1.34
2	G	301	6GK	C17-N05	2.68	1.40	1.34
2	C	301	6GK	C17-N05	2.62	1.40	1.34
2	A	301	6GK	C10-N04	-2.51	1.32	1.37
2	I	301	6GK	C20-N06	2.44	1.39	1.34
2	D	302	6GK	C17-N05	2.39	1.39	1.34
3	H	301	NAG	O5-C1	2.22	1.47	1.43
2	J	301	6GK	C10-N04	-2.13	1.33	1.37
2	J	301	6GK	C18-N04	2.05	1.49	1.46
2	F	301	6GK	C12-N04	2.05	1.49	1.46
3	D	303	NAG	C1-C2	2.00	1.55	1.52

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	301	6GK	C09-N03-C10	8.95	123.07	116.73
2	B	301	6GK	C08-N01-C09	8.89	121.41	116.34
2	D	302	6GK	C08-N01-C09	8.76	121.34	116.34
2	F	301	6GK	C08-N01-C09	8.59	121.24	116.34
2	J	301	6GK	C08-N01-C09	8.18	121.00	116.34
2	I	301	6GK	C08-N01-C09	7.77	120.77	116.34
2	A	301	6GK	C08-N01-C09	7.62	120.68	116.34
2	G	301	6GK	C08-N01-C09	7.43	120.57	116.34
2	G	302	6GK	C08-N01-C09	7.34	120.53	116.34
2	D	302	6GK	C09-N03-C10	7.16	121.80	116.73
2	B	301	6GK	C09-N03-C10	6.93	121.64	116.73
2	F	301	6GK	C09-N03-C10	6.86	121.59	116.73
2	C	301	6GK	C08-N01-C09	6.53	120.06	116.34
2	C	301	6GK	C09-N03-C10	6.26	121.16	116.73
2	J	301	6GK	C09-N03-C10	6.00	120.98	116.73
2	G	302	6GK	C09-N03-C10	5.91	120.92	116.73
2	D	301	6GK	C09-N03-C10	5.89	120.90	116.73
2	A	301	6GK	C09-N03-C10	5.70	120.77	116.73
2	G	301	6GK	C09-N03-C10	5.47	120.60	116.73
2	D	301	6GK	C08-N01-C09	5.36	119.40	116.34
2	G	301	6GK	C01-O01-C02	-5.34	109.46	117.53
2	D	302	6GK	C01-O01-C02	-5.02	109.95	117.53
2	D	301	6GK	C01-O01-C02	-4.84	110.23	117.53
2	J	301	6GK	C01-O01-C02	-4.77	110.33	117.53
2	C	301	6GK	C01-O01-C02	-4.73	110.39	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	6GK	C01-O01-C02	-4.64	110.52	117.53
2	F	301	6GK	C01-O01-C02	-4.49	110.76	117.53
2	I	301	6GK	C01-O01-C02	-4.23	111.14	117.53
2	A	301	6GK	C01-O01-C02	-4.17	111.23	117.53
2	G	302	6GK	C01-O01-C02	-4.04	111.43	117.53
2	C	301	6GK	C20-N06-C19	3.94	122.82	117.42
2	D	301	6GK	C17-N05-C13	3.90	122.76	117.42
2	I	301	6GK	N03-C09-N01	-3.87	119.35	125.42
2	D	302	6GK	N03-C09-N01	-3.78	119.49	125.42
2	G	302	6GK	N03-C10-N04	3.72	120.72	116.55
2	D	301	6GK	C20-N06-C19	3.64	122.40	117.42
2	G	302	6GK	C17-N05-C13	3.36	122.02	117.42
2	J	301	6GK	N03-C09-N01	-3.31	120.23	125.42
2	F	301	6GK	N03-C09-N01	-3.26	120.30	125.42
2	B	301	6GK	N03-C09-N01	-3.26	120.31	125.42
2	F	301	6GK	C17-N05-C13	3.25	121.88	117.42
2	G	302	6GK	C11-C08-C03	-3.20	117.95	122.25
2	C	301	6GK	C21-C20-N06	-3.20	118.20	123.43
2	B	301	6GK	C17-N05-C13	3.12	121.69	117.42
2	D	301	6GK	N03-C10-N04	3.08	120.00	116.55
2	A	301	6GK	N03-C09-N01	-3.06	120.61	125.42
2	B	301	6GK	C08-C11-C10	3.03	119.02	117.03
2	B	301	6GK	C11-C08-N01	-2.94	118.85	122.35
2	I	301	6GK	C21-C20-N06	-2.93	118.64	123.43
2	G	302	6GK	N03-C09-N01	-2.93	120.83	125.42
2	B	301	6GK	O01-C02-C07	-2.84	119.50	124.37
2	C	301	6GK	C15-C14-C13	2.83	122.46	118.93
2	G	302	6GK	C20-N06-C19	2.82	121.28	117.42
2	C	301	6GK	N03-C09-N01	-2.77	121.08	125.42
2	I	301	6GK	C20-N06-C19	2.75	121.19	117.42
2	G	302	6GK	C16-C17-N05	-2.74	118.95	123.43
2	D	301	6GK	C16-C17-N05	-2.67	119.07	123.43
2	F	301	6GK	N03-C10-N04	2.65	119.52	116.55
2	G	301	6GK	C12-C13-N05	2.63	122.40	116.28
3	D	303	NAG	C1-O5-C5	2.63	115.76	112.19
2	F	301	6GK	C11-C08-N01	-2.62	119.24	122.35
2	F	301	6GK	C11-C08-C03	-2.61	118.75	122.25
3	H	301	NAG	C1-O5-C5	2.61	115.72	112.19
2	G	301	6GK	N03-C09-N01	-2.58	121.37	125.42
2	G	302	6GK	C03-C08-N01	2.57	122.38	116.45
2	D	302	6GK	C12-C13-N05	2.57	122.25	116.28
2	I	301	6GK	C13-C12-N04	-2.55	110.96	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	301	6GK	C18-N04-C10	2.54	124.37	120.97
2	J	301	6GK	C18-C19-N06	2.53	122.16	116.28
2	D	301	6GK	C11-C08-C03	-2.53	118.86	122.25
2	D	301	6GK	C08-C11-C10	2.52	118.69	117.03
2	A	301	6GK	C20-N06-C19	2.48	120.82	117.42
2	C	301	6GK	C11-C08-C03	-2.47	118.93	122.25
2	J	301	6GK	C17-N05-C13	2.47	120.81	117.42
2	B	301	6GK	C12-C13-N05	2.47	122.01	116.28
2	G	301	6GK	C11-C08-N01	-2.46	119.42	122.35
2	C	301	6GK	C18-N04-C10	2.46	124.27	120.97
2	G	301	6GK	C15-C14-C13	2.46	122.00	118.93
2	D	301	6GK	C14-C13-N05	-2.46	118.63	122.17
2	B	301	6GK	C14-C13-N05	-2.46	118.63	122.17
2	F	301	6GK	C12-C13-N05	2.45	121.98	116.28
2	C	301	6GK	C12-C13-N05	2.44	121.96	116.28
2	G	301	6GK	C17-N05-C13	2.44	120.76	117.42
2	J	301	6GK	C22-C23-C19	2.42	121.94	118.93
2	J	301	6GK	C12-C13-N05	2.41	121.88	116.28
2	I	301	6GK	C17-N05-C13	2.41	120.72	117.42
2	A	301	6GK	C17-N05-C13	2.40	120.70	117.42
2	F	301	6GK	C03-C08-N01	2.39	121.97	116.45
2	D	301	6GK	N03-C09-N01	-2.39	121.67	125.42
2	D	302	6GK	C17-N05-C13	2.39	120.69	117.42
2	D	302	6GK	C21-C20-N06	-2.38	119.53	123.43
2	F	301	6GK	C20-N06-C19	2.36	120.65	117.42
2	A	301	6GK	C11-C08-C03	-2.35	119.09	122.25
2	I	301	6GK	C11-C10-N03	-2.35	118.58	123.15
2	A	301	6GK	C12-C13-N05	2.34	121.72	116.28
2	D	301	6GK	C12-C13-N05	2.34	121.72	116.28
2	D	301	6GK	C18-C19-N06	2.32	121.68	116.28
2	D	301	6GK	C23-C19-N06	-2.32	118.83	122.17
2	D	302	6GK	N02-C09-N01	2.31	120.85	117.25
2	A	301	6GK	C18-C19-N06	2.30	121.63	116.28
2	B	301	6GK	C20-N06-C19	2.29	120.55	117.42
2	A	301	6GK	N02-C09-N01	2.28	120.80	117.25
2	G	302	6GK	C11-C08-N01	-2.28	119.64	122.35
3	F	302	NAG	C1-O5-C5	2.27	115.27	112.19
2	B	301	6GK	C03-C08-N01	2.27	121.69	116.45
2	B	301	6GK	C11-C10-N03	-2.26	118.75	123.15
2	D	301	6GK	C21-C20-N06	-2.26	119.74	123.43
2	G	302	6GK	C11-C10-N04	-2.26	119.61	122.29
2	A	301	6GK	C11-C08-N01	-2.25	119.67	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	302	6GK	C19-C18-N04	-2.25	111.35	114.27
2	D	302	6GK	C11-C08-N01	-2.23	119.70	122.35
2	C	301	6GK	C18-C19-N06	2.23	121.45	116.28
2	F	301	6GK	C14-C13-N05	-2.22	118.98	122.17
2	J	301	6GK	C11-C08-N01	-2.21	119.72	122.35
2	D	301	6GK	C11-C10-N03	-2.21	118.85	123.15
2	G	302	6GK	C18-C19-N06	2.20	121.38	116.28
2	G	301	6GK	C20-N06-C19	2.18	120.40	117.42
2	G	301	6GK	C08-C11-C10	2.17	118.46	117.03
2	B	301	6GK	N02-C09-N01	2.16	120.62	117.25
2	I	301	6GK	N02-C09-N01	2.16	120.61	117.25
2	G	301	6GK	C16-C17-N05	-2.16	119.90	123.43
2	B	301	6GK	O01-C02-C03	2.12	119.43	116.26
2	G	302	6GK	C08-C11-C10	2.12	118.42	117.03
2	D	302	6GK	C14-C13-N05	-2.11	119.13	122.17
2	B	301	6GK	C11-C08-C03	-2.11	119.42	122.25
2	F	301	6GK	C08-C11-C10	2.11	118.42	117.03
2	G	301	6GK	C18-C19-N06	2.11	121.18	116.28
2	G	302	6GK	C12-C13-N05	2.11	121.18	116.28
2	I	301	6GK	C19-C18-N04	-2.11	111.53	114.27
2	G	301	6GK	C14-C13-N05	-2.10	119.14	122.17
2	A	301	6GK	C21-C20-N06	-2.09	120.02	123.43
3	J	302	NAG	C1-O5-C5	2.06	114.98	112.19
2	C	301	6GK	C11-C10-N03	-2.06	119.14	123.15
2	A	301	6GK	C03-C08-N01	2.06	121.19	116.45
2	J	301	6GK	C23-C19-N06	-2.06	119.21	122.17
2	F	301	6GK	C18-C19-N06	2.05	121.04	116.28
2	F	301	6GK	C16-C17-N05	-2.05	120.08	123.43
2	C	301	6GK	C08-C11-C10	2.04	118.38	117.03
2	C	301	6GK	O01-C02-C07	-2.03	120.88	124.37
2	I	301	6GK	N03-C10-N04	2.03	118.83	116.55
2	F	301	6GK	C11-C10-N03	-2.03	119.19	123.15
2	I	301	6GK	C18-N04-C10	2.02	123.67	120.97
2	G	302	6GK	C14-C13-N05	-2.01	119.28	122.17

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	302	NAG	O5-C5-C6-O6
3	A	302	NAG	O5-C5-C6-O6
3	G	303	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	E	301	NAG	O5-C5-C6-O6
3	A	302	NAG	C4-C5-C6-O6
3	F	302	NAG	O5-C5-C6-O6
3	J	302	NAG	C4-C5-C6-O6
3	G	303	NAG	C4-C5-C6-O6
2	B	301	6GK	C07-C02-O01-C01
3	B	302	NAG	O5-C5-C6-O6
3	H	301	NAG	O5-C5-C6-O6
3	E	301	NAG	C4-C5-C6-O6
3	J	302	NAG	C8-C7-N2-C2
3	J	302	NAG	O7-C7-N2-C2
3	G	303	NAG	C8-C7-N2-C2
3	G	303	NAG	O7-C7-N2-C2
3	D	303	NAG	O5-C5-C6-O6
3	H	301	NAG	C4-C5-C6-O6
2	B	301	6GK	C03-C02-O01-C01
3	D	303	NAG	C4-C5-C6-O6
3	F	302	NAG	C4-C5-C6-O6
2	F	301	6GK	C07-C02-O01-C01
3	B	302	NAG	C4-C5-C6-O6
2	F	301	6GK	C03-C02-O01-C01
3	C	302	NAG	O5-C5-C6-O6
3	I	302	NAG	C3-C2-N2-C7
3	D	303	NAG	C3-C2-N2-C7
3	C	302	NAG	C3-C2-N2-C7
3	E	301	NAG	C3-C2-N2-C7
3	A	302	NAG	C3-C2-N2-C7
3	H	301	NAG	C1-C2-N2-C7
2	G	301	6GK	N04-C12-C13-N05

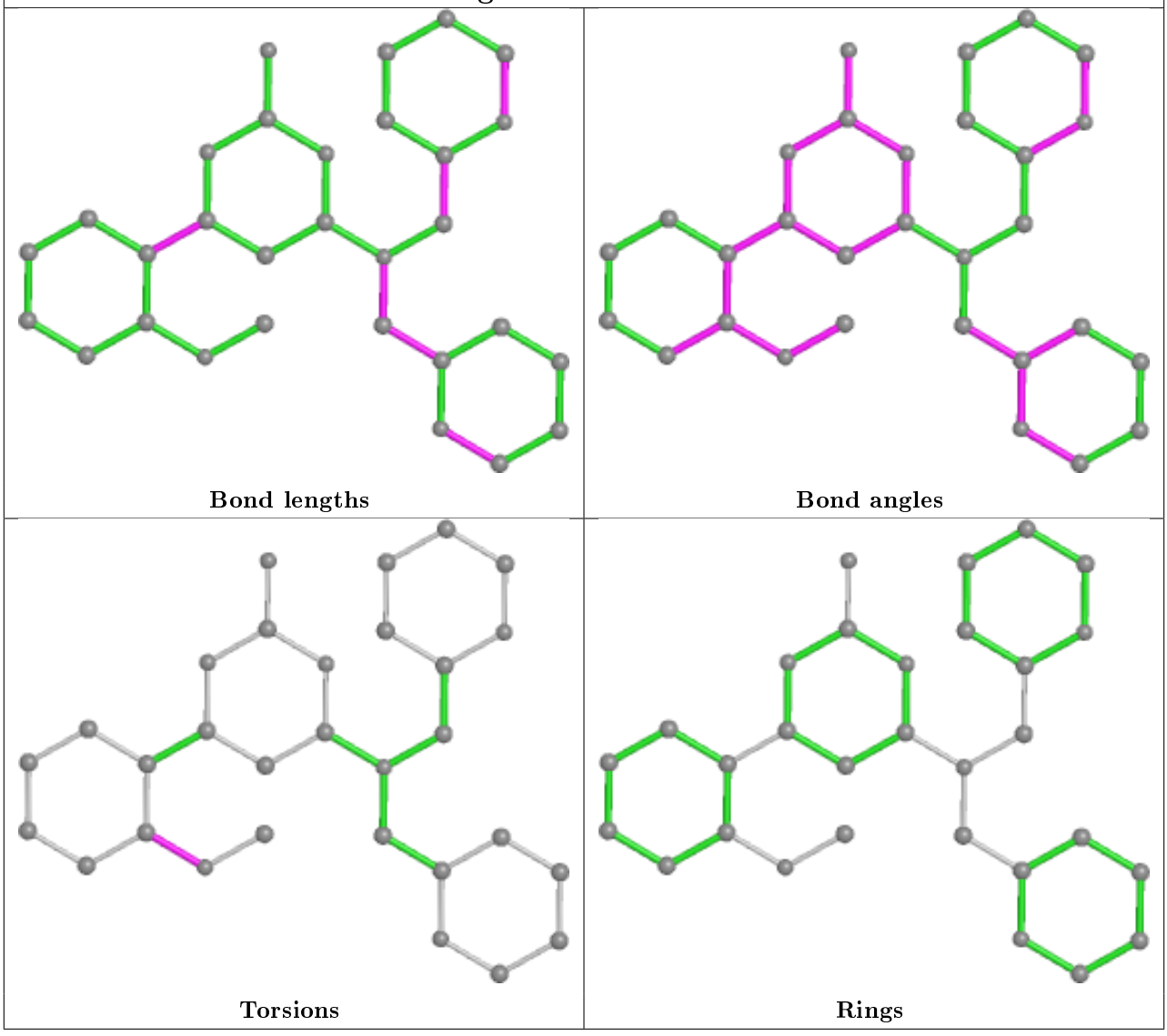
There are no ring outliers.

8 monomers are involved in 10 short contacts:

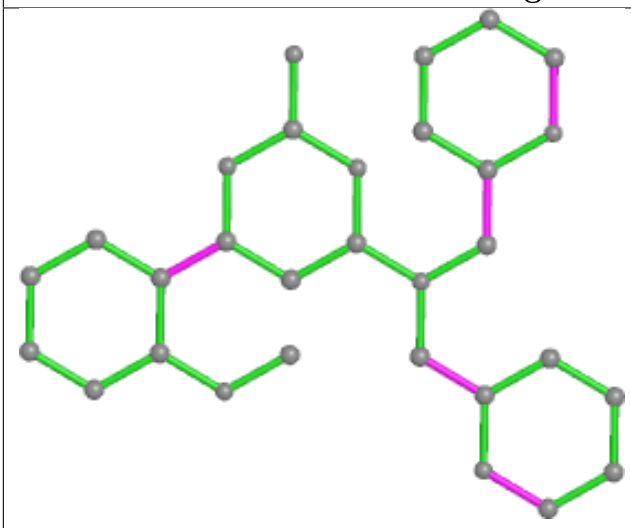
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	PO4	1	0
2	B	301	6GK	1	0
2	C	301	6GK	3	0
2	D	302	6GK	1	0
4	C	304	PO4	1	0
2	G	301	6GK	1	0
2	D	301	6GK	1	0
4	A	304	PO4	1	0

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

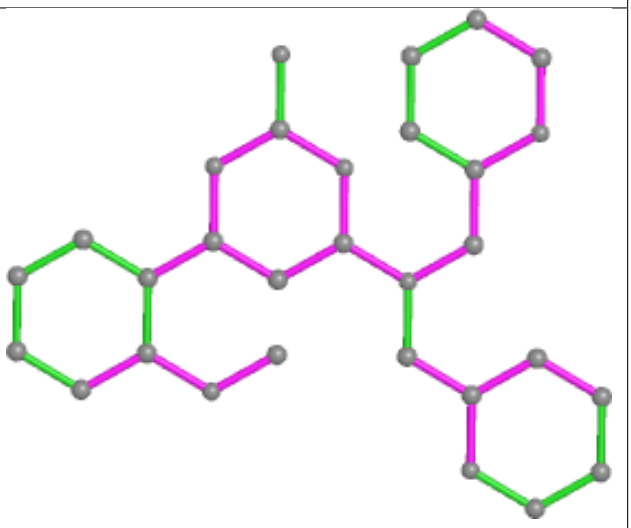
Ligand 6GK B 301



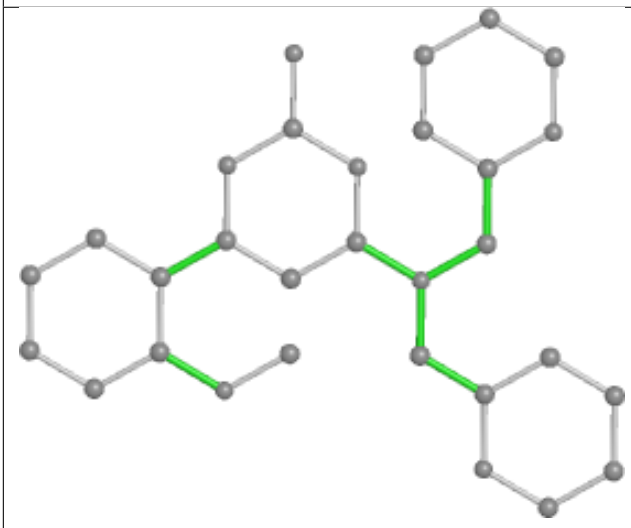
Ligand 6GK C 301



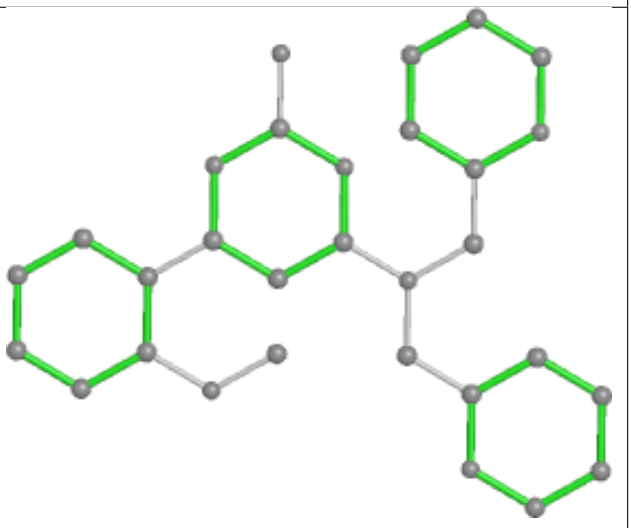
Bond lengths



Bond angles

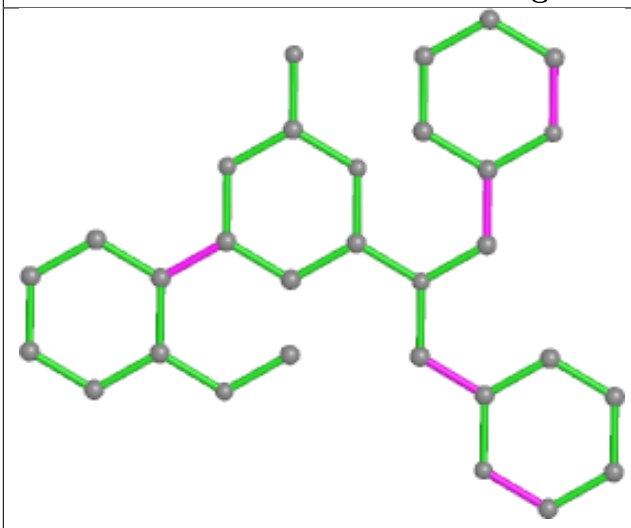


Torsions

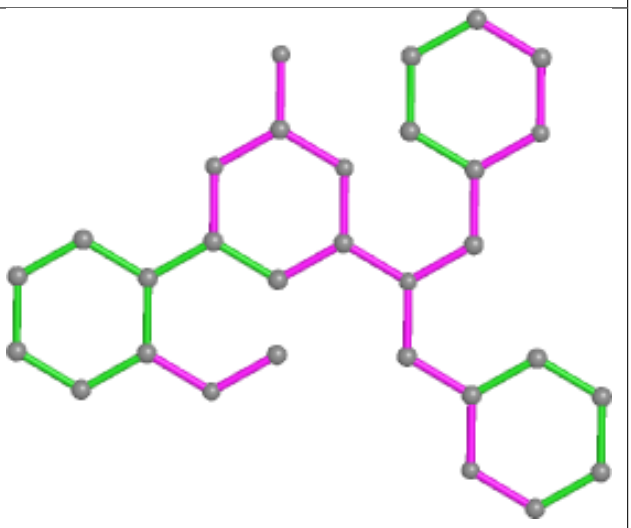


Rings

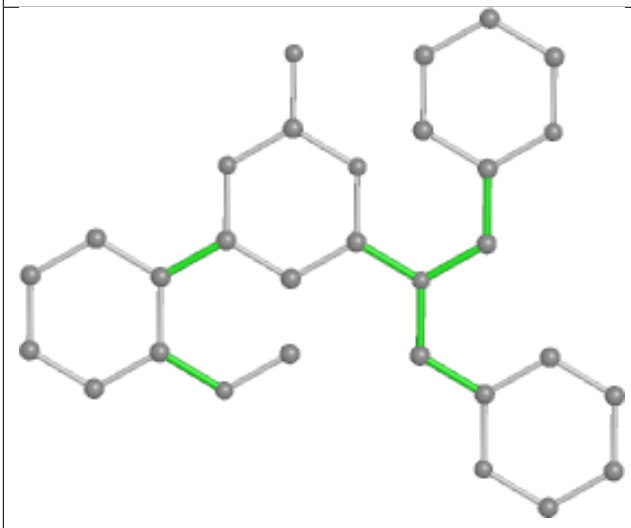
Ligand 6GK I 301



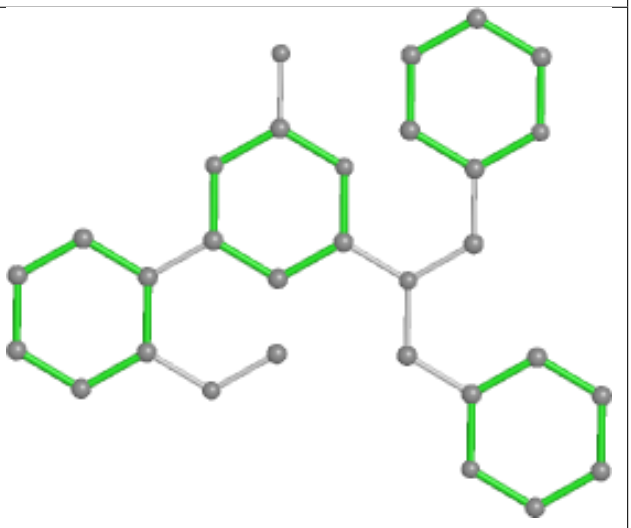
Bond lengths



Bond angles

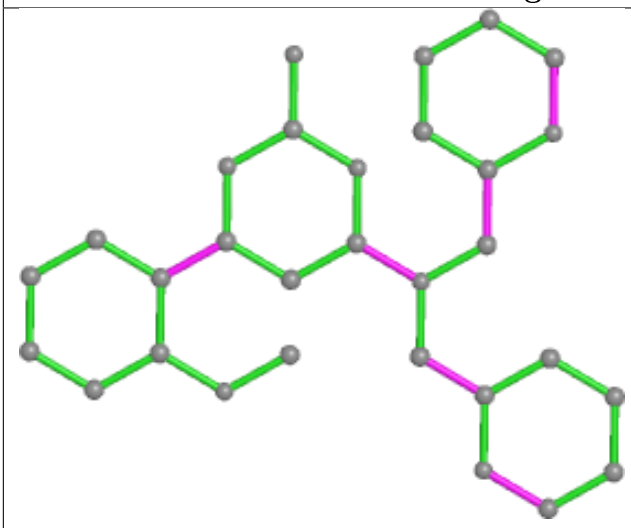


Torsions

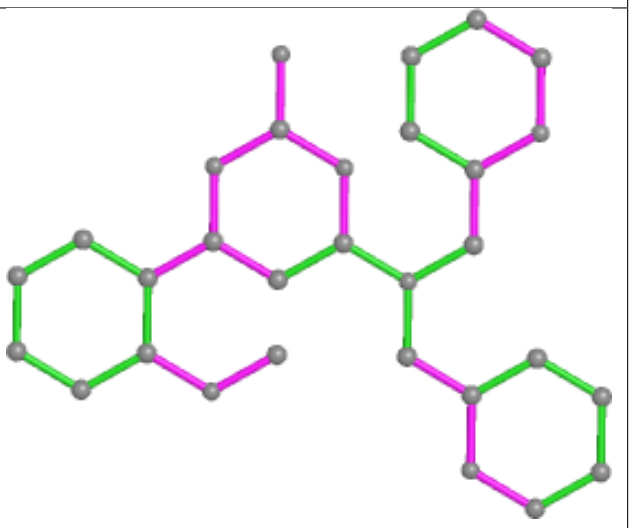


Rings

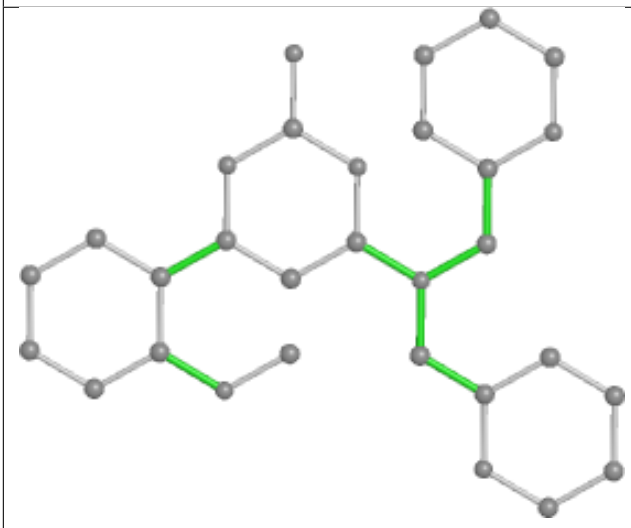
Ligand 6GK A 301



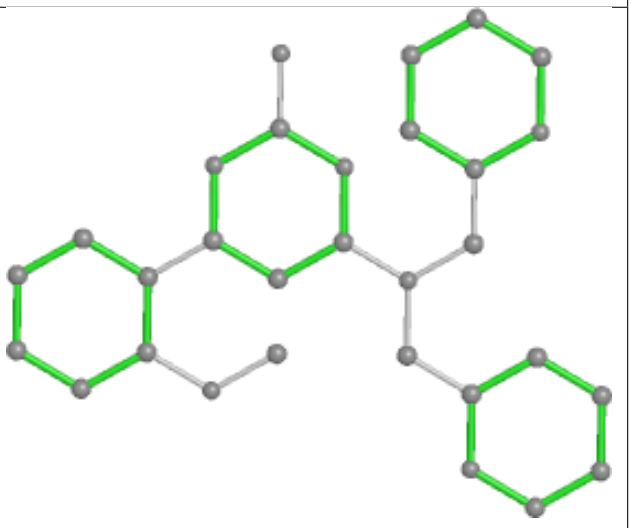
Bond lengths



Bond angles

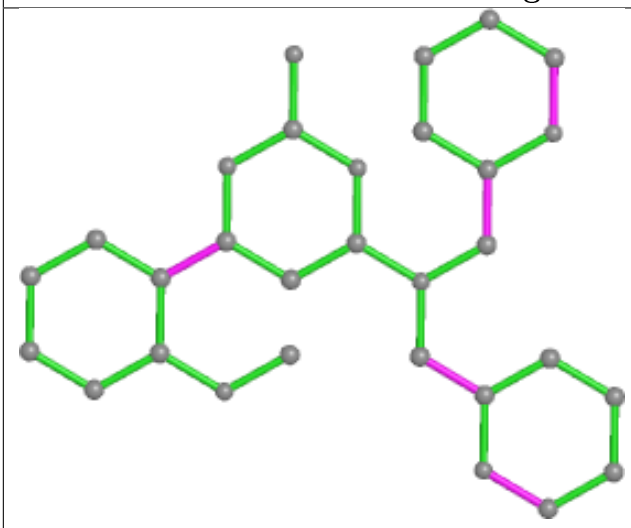


Torsions

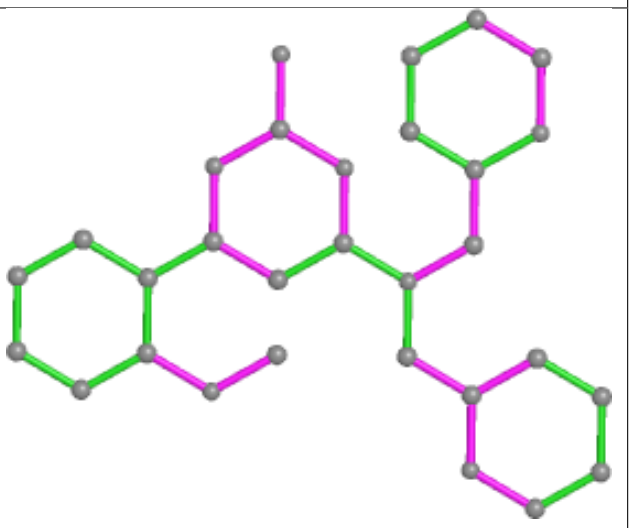


Rings

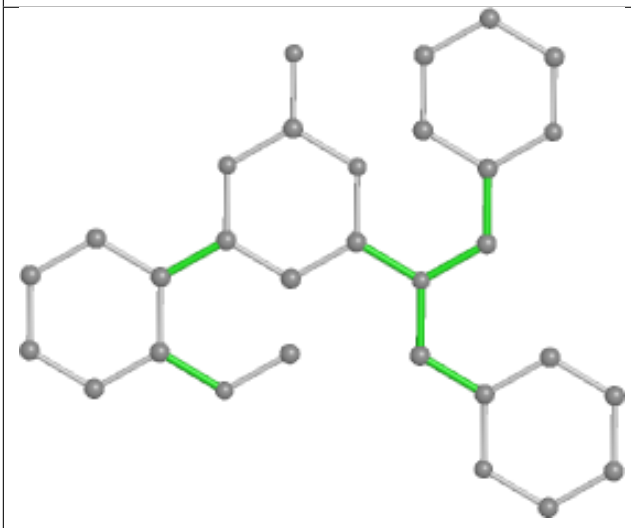
Ligand 6GK D 302



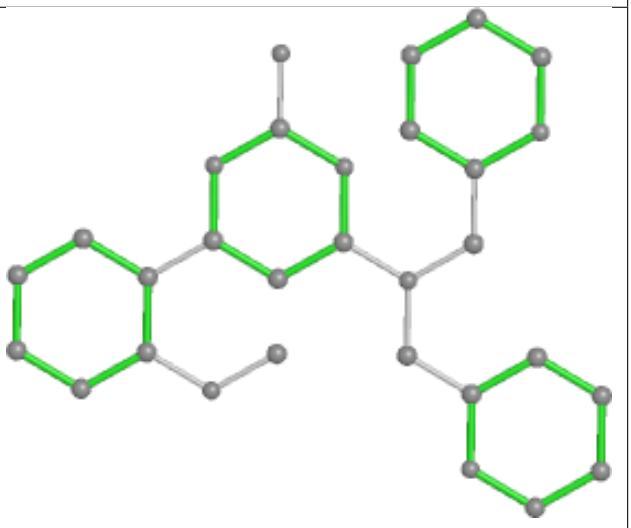
Bond lengths



Bond angles

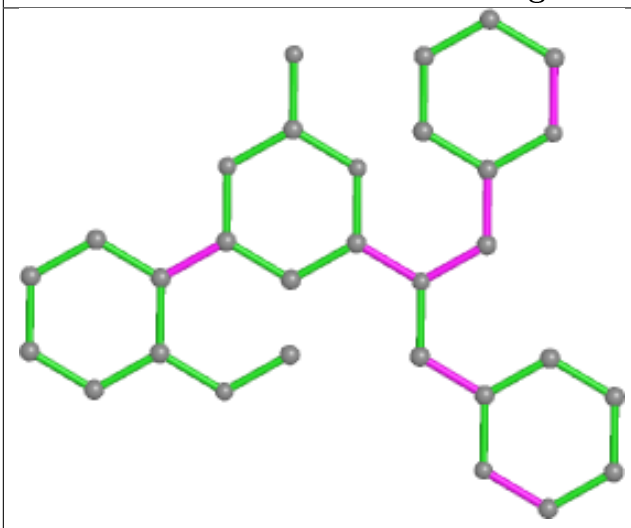


Torsions

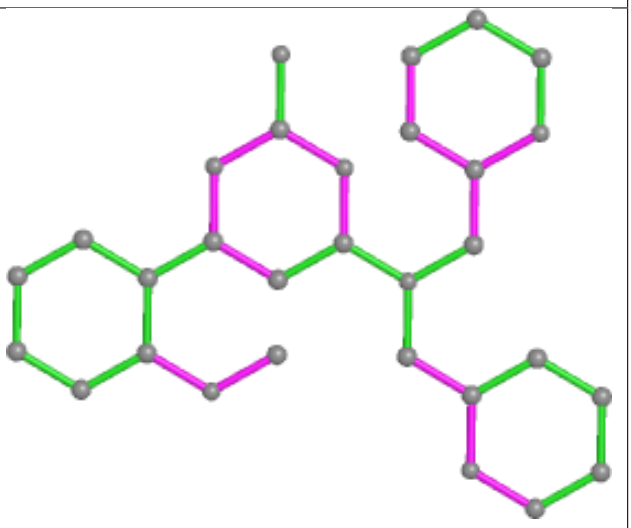


Rings

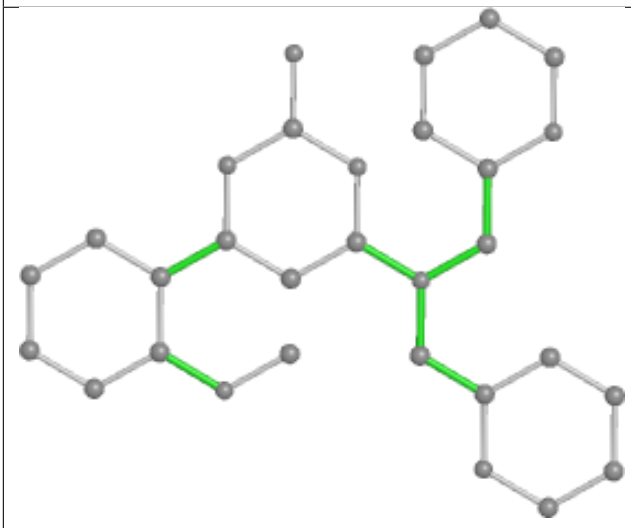
Ligand 6GK J 301



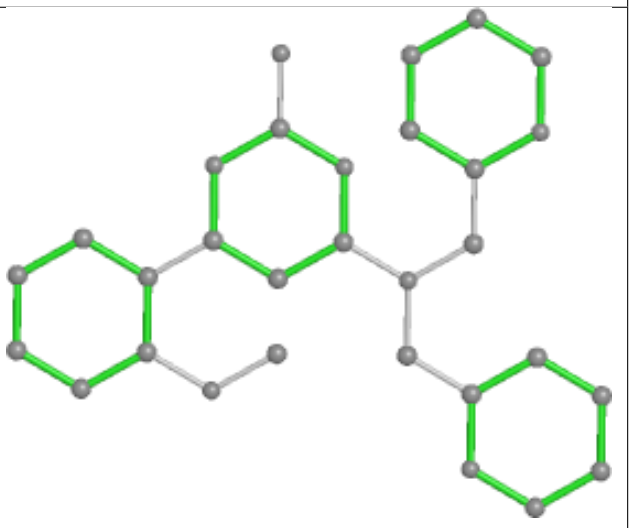
Bond lengths



Bond angles

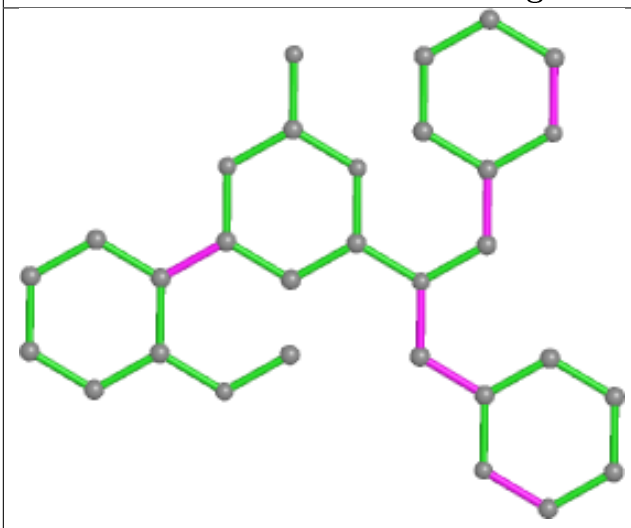


Torsions

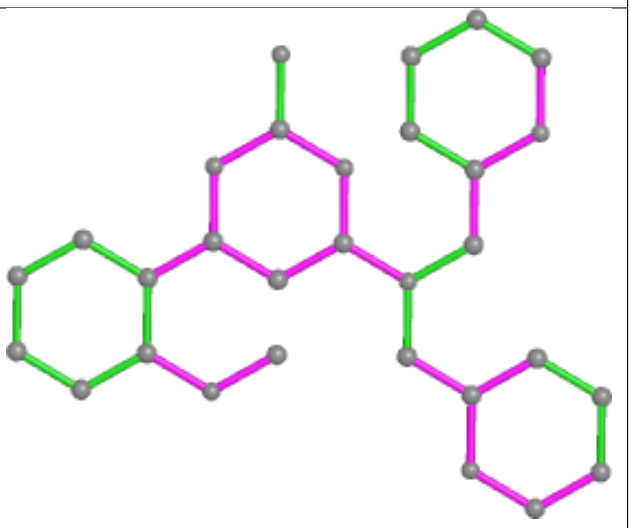


Rings

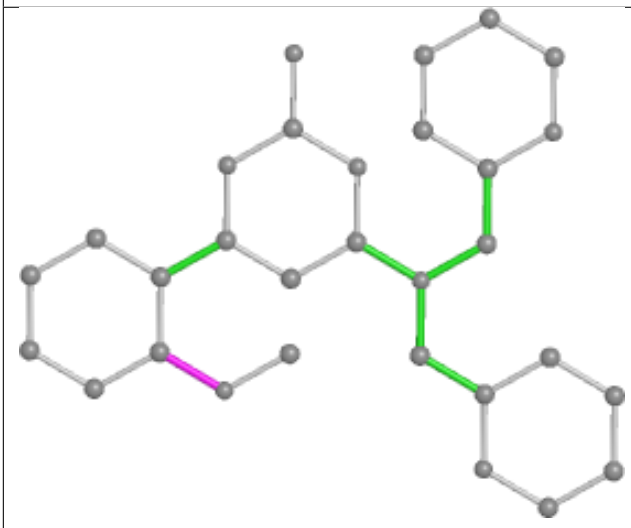
Ligand 6GK F 301



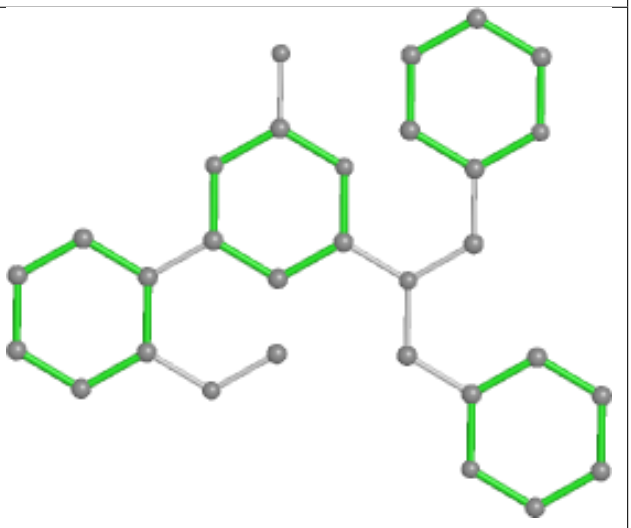
Bond lengths



Bond angles

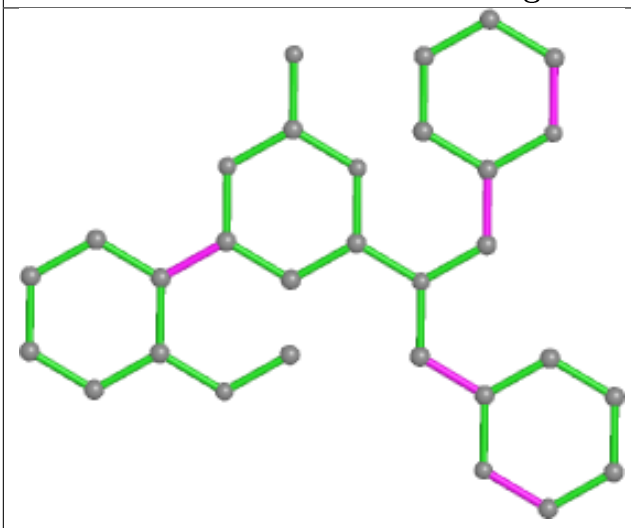


Torsions

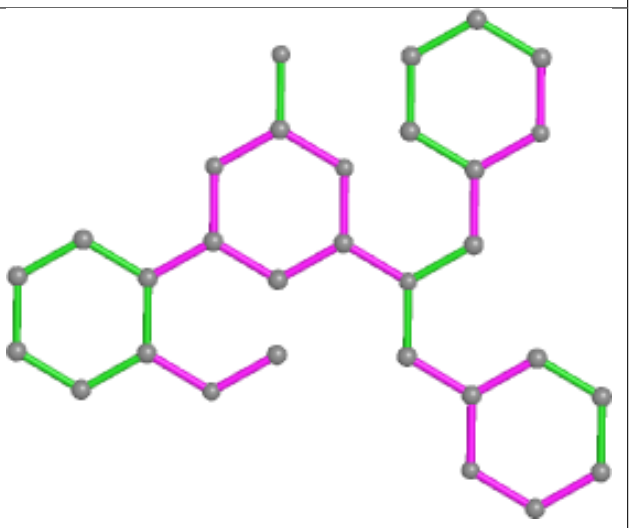


Rings

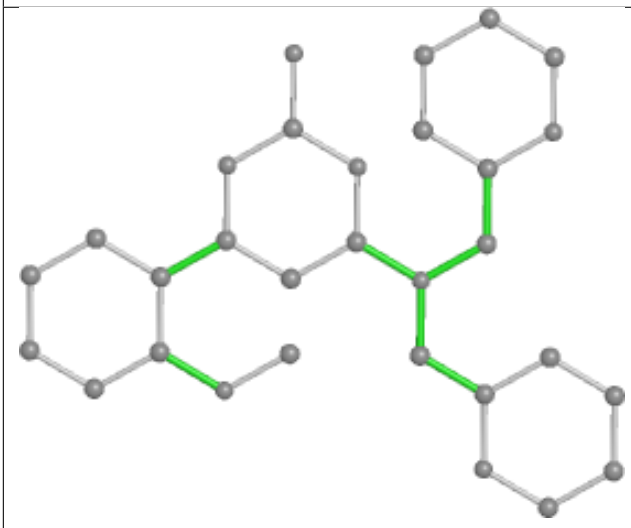
Ligand 6GK G 302



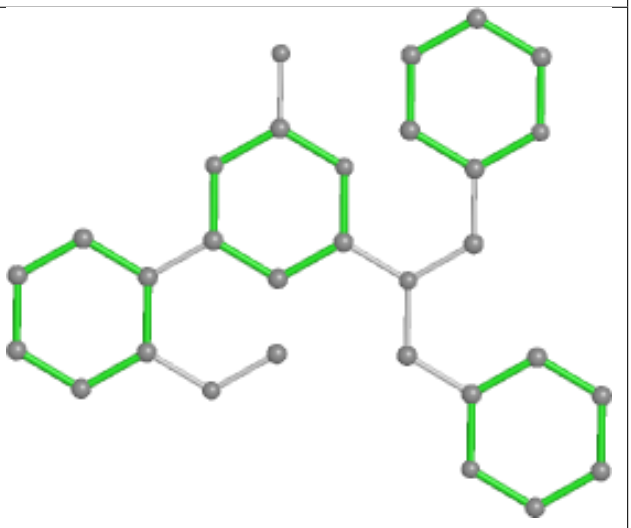
Bond lengths



Bond angles

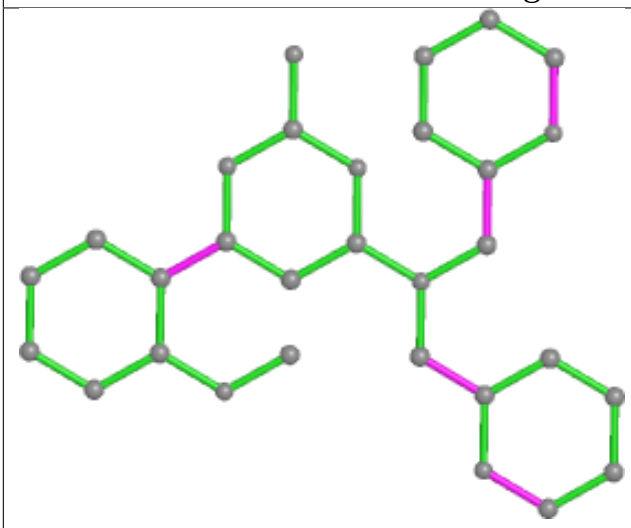


Torsions

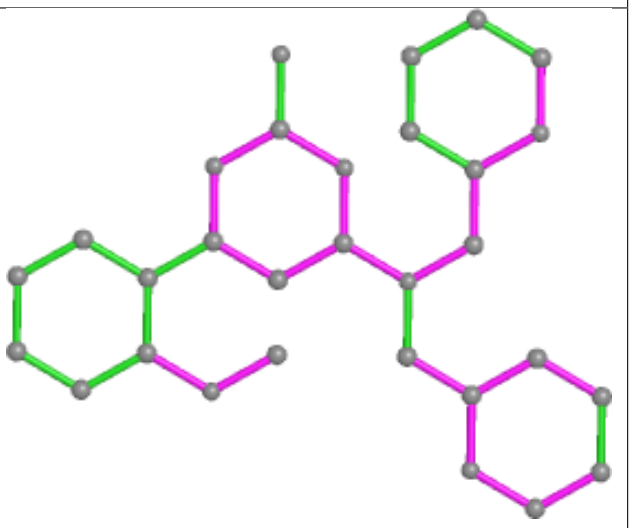


Rings

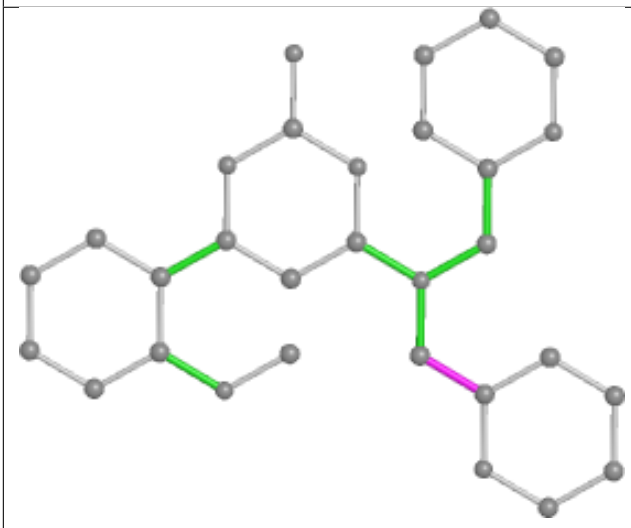
Ligand 6GK G 301



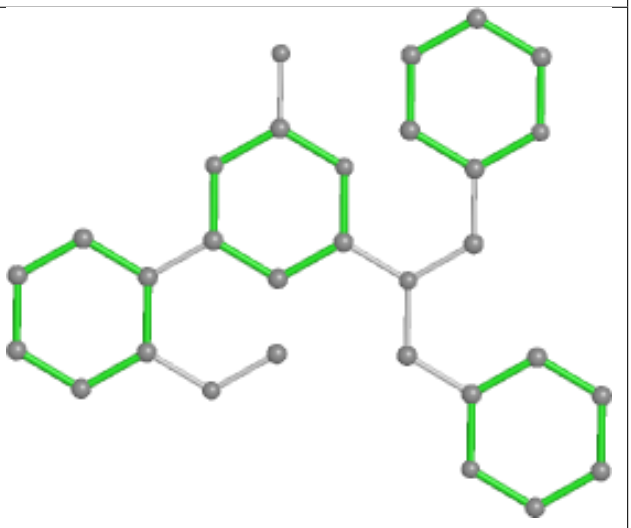
Bond lengths



Bond angles

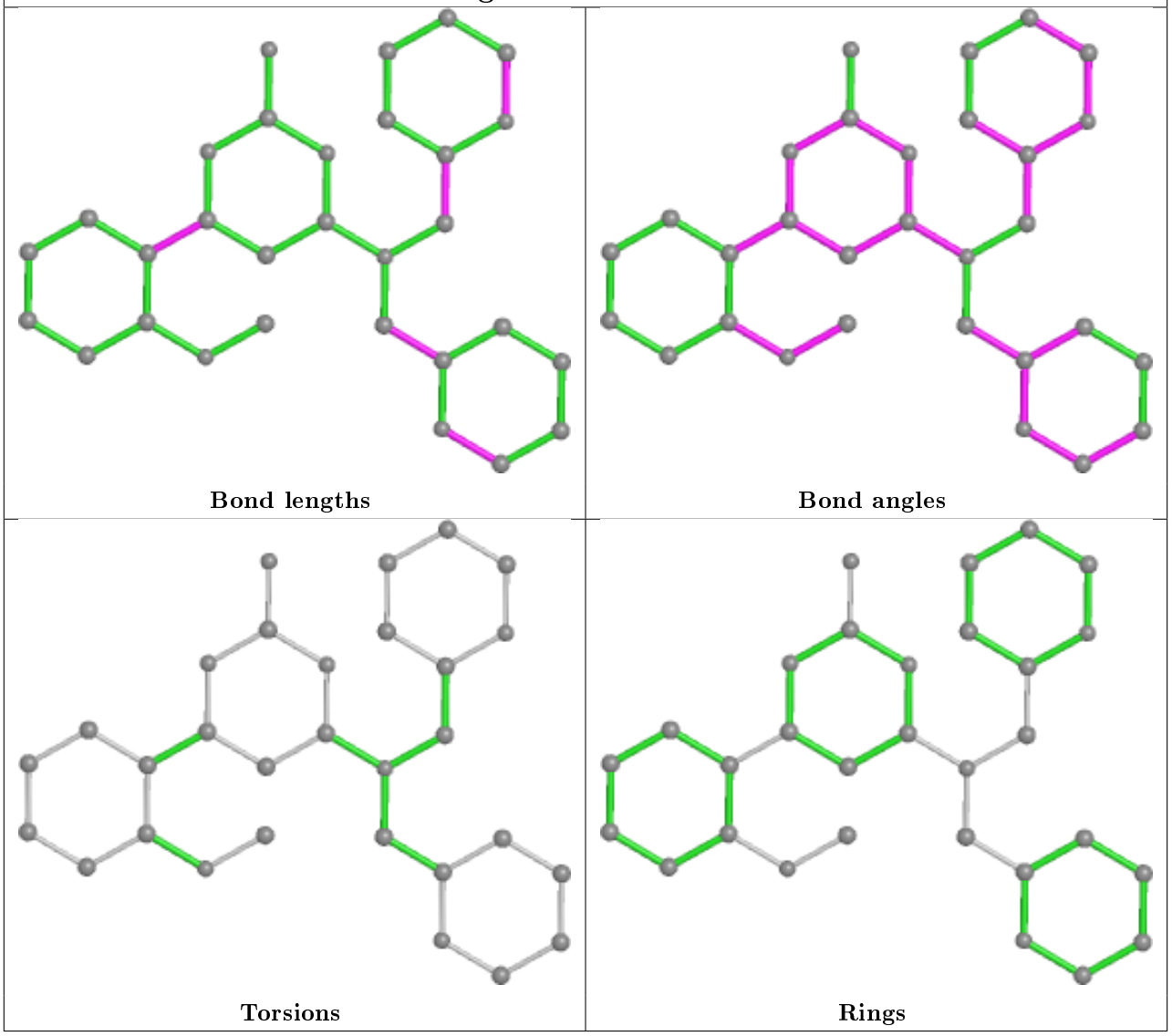


Torsions



Rings

Ligand 6GK D 301



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	204/218 (93%)	0.02	2 (0%)	82	83	30, 55, 82, 99	0
1	B	211/218 (96%)	0.03	4 (1%)	66	69	34, 53, 84, 109	0
1	C	203/218 (93%)	-0.13	1 (0%)	91	92	31, 53, 79, 93	0
1	D	207/218 (94%)	-0.06	2 (0%)	82	83	31, 50, 78, 93	0
1	E	206/218 (94%)	-0.01	2 (0%)	82	83	33, 52, 84, 96	0
1	F	212/218 (97%)	0.12	6 (2%)	53	54	33, 53, 85, 106	0
1	G	212/218 (97%)	-0.11	2 (0%)	84	85	31, 54, 86, 104	0
1	H	210/218 (96%)	-0.02	5 (2%)	59	60	27, 49, 78, 102	0
1	I	202/218 (92%)	-0.03	1 (0%)	91	92	32, 53, 85, 96	0
1	J	205/218 (94%)	-0.03	1 (0%)	91	92	24, 55, 80, 97	0
All	All	2072/2180 (95%)	-0.02	26 (1%)	77	78	24, 53, 82, 109	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ASP	3.4
1	B	68	SER	3.1
1	H	184	THR	3.0
1	I	-2	ASP	2.9
1	E	43	GLU	2.9
1	F	173	ILE	2.8
1	H	159	SER	2.7
1	J	164	TYR	2.7
1	H	69	HIS	2.6
1	B	167	GLN	2.5
1	F	157	GLU	2.5
1	D	184	THR	2.5
1	F	156	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	61	ARG	2.4
1	G	23	ARG	2.3
1	H	187	CYS	2.3
1	B	202	ARG	2.3
1	D	185	TYR	2.2
1	A	1	LEU	2.2
1	H	68	SER	2.2
1	B	183	VAL	2.2
1	C	199	LEU	2.2
1	E	69	HIS	2.1
1	F	1	LEU	2.0
1	G	-7	ASP	2.0
1	F	159	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	302	14/15	0.52	0.34	95,102,106,106	0
3	NAG	B	302	14/15	0.56	0.28	81,94,100,101	0
3	NAG	H	301	14/15	0.72	0.23	85,90,95,96	0
3	NAG	D	303	14/15	0.77	0.25	87,98,106,107	0
3	NAG	I	302	14/15	0.77	0.26	87,93,98,99	0
3	NAG	F	302	14/15	0.78	0.16	86,95,103,103	0
3	NAG	G	303	14/15	0.80	0.18	83,94,101,111	0
3	NAG	J	302	14/15	0.82	0.24	77,93,98,104	0
3	NAG	E	301	14/15	0.83	0.21	79,87,90,91	0
3	NAG	C	302	14/15	0.83	0.22	86,92,97,105	0

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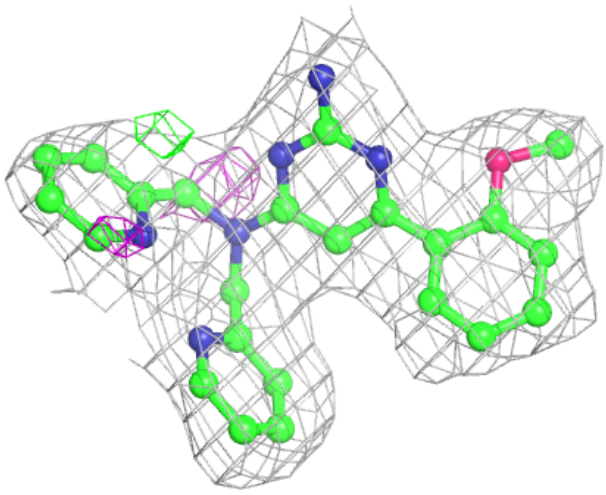
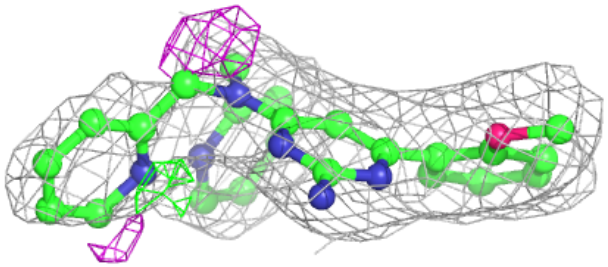
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	H	302	5/5	0.89	0.16	38,47,56,57	0
2	6GK	C	301	30/30	0.90	0.16	33,43,52,55	0
2	6GK	G	301	30/30	0.90	0.19	37,44,53,60	0
2	6GK	A	301	30/30	0.91	0.16	44,55,63,65	0
2	6GK	G	302	30/30	0.91	0.20	36,44,52,56	0
2	6GK	B	301	30/30	0.92	0.21	43,49,58,59	0
2	6GK	D	302	30/30	0.92	0.19	38,51,59,63	0
2	6GK	J	301	30/30	0.92	0.20	42,53,58,63	0
4	PO4	F	305	5/5	0.92	0.15	51,55,66,76	0
2	6GK	F	301	30/30	0.92	0.17	39,50,58,64	0
2	6GK	D	301	30/30	0.92	0.14	33,42,49,50	0
2	6GK	I	301	30/30	0.93	0.15	38,47,52,57	0
4	PO4	J	303	5/5	0.93	0.12	50,51,56,61	0
4	PO4	A	304	5/5	0.93	0.12	45,51,56,61	0
4	PO4	A	303	5/5	0.95	0.12	52,54,57,62	0
4	PO4	C	304	5/5	0.97	0.10	41,46,49,55	0
4	PO4	I	303	5/5	0.98	0.11	44,47,51,57	0
4	PO4	F	303	5/5	0.98	0.14	49,50,55,57	0
4	PO4	F	304	5/5	0.98	0.14	44,44,49,53	0
4	PO4	D	304	5/5	0.98	0.12	40,48,52,54	0
4	PO4	C	303	5/5	0.98	0.12	45,46,53,54	0

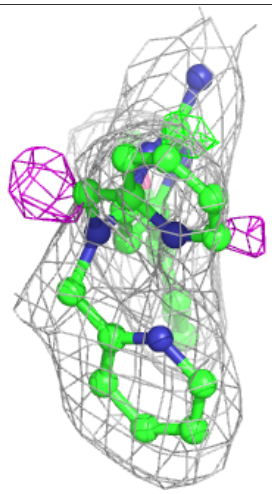
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6GK 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)

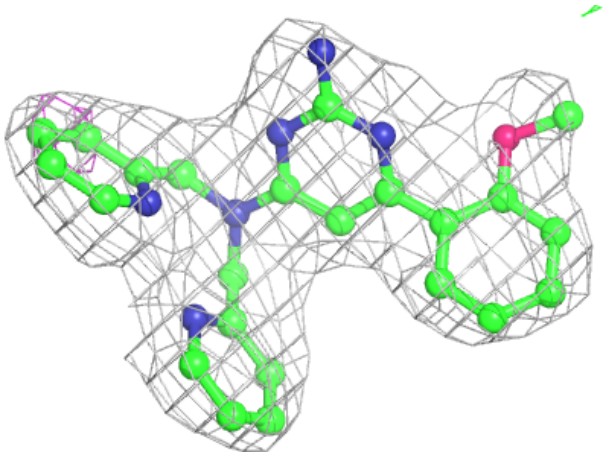


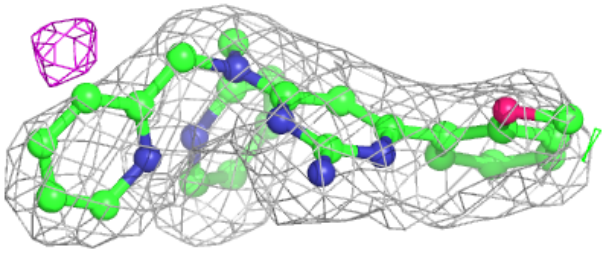


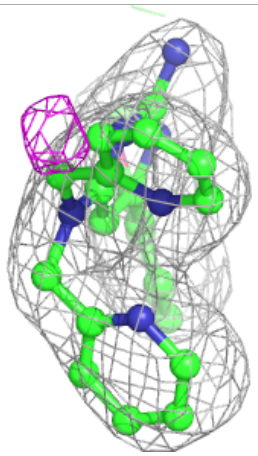


Electron density around 6GK G 301:

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

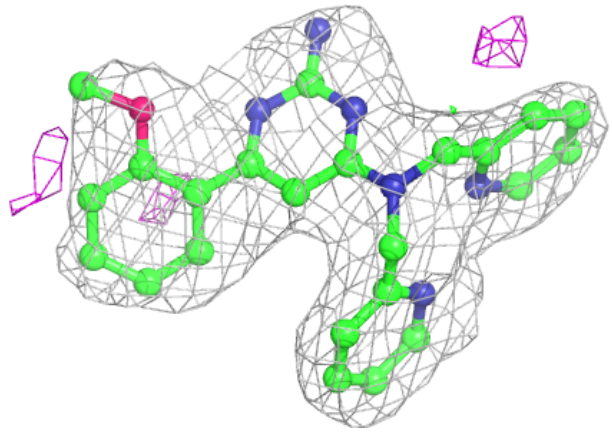


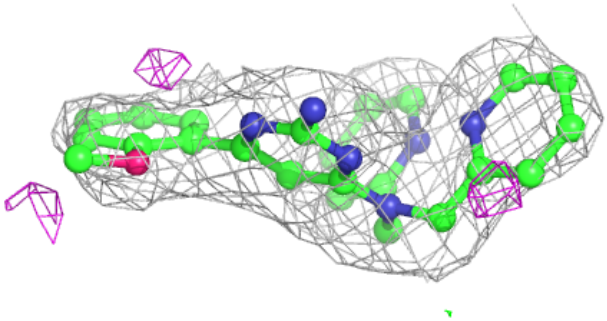


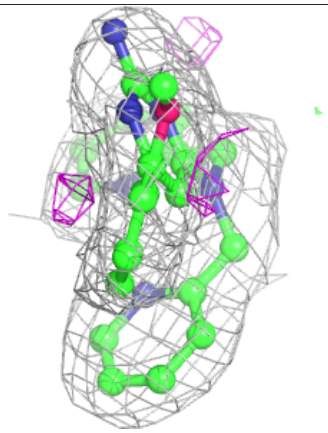


Electron density around 6GK A 301:

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

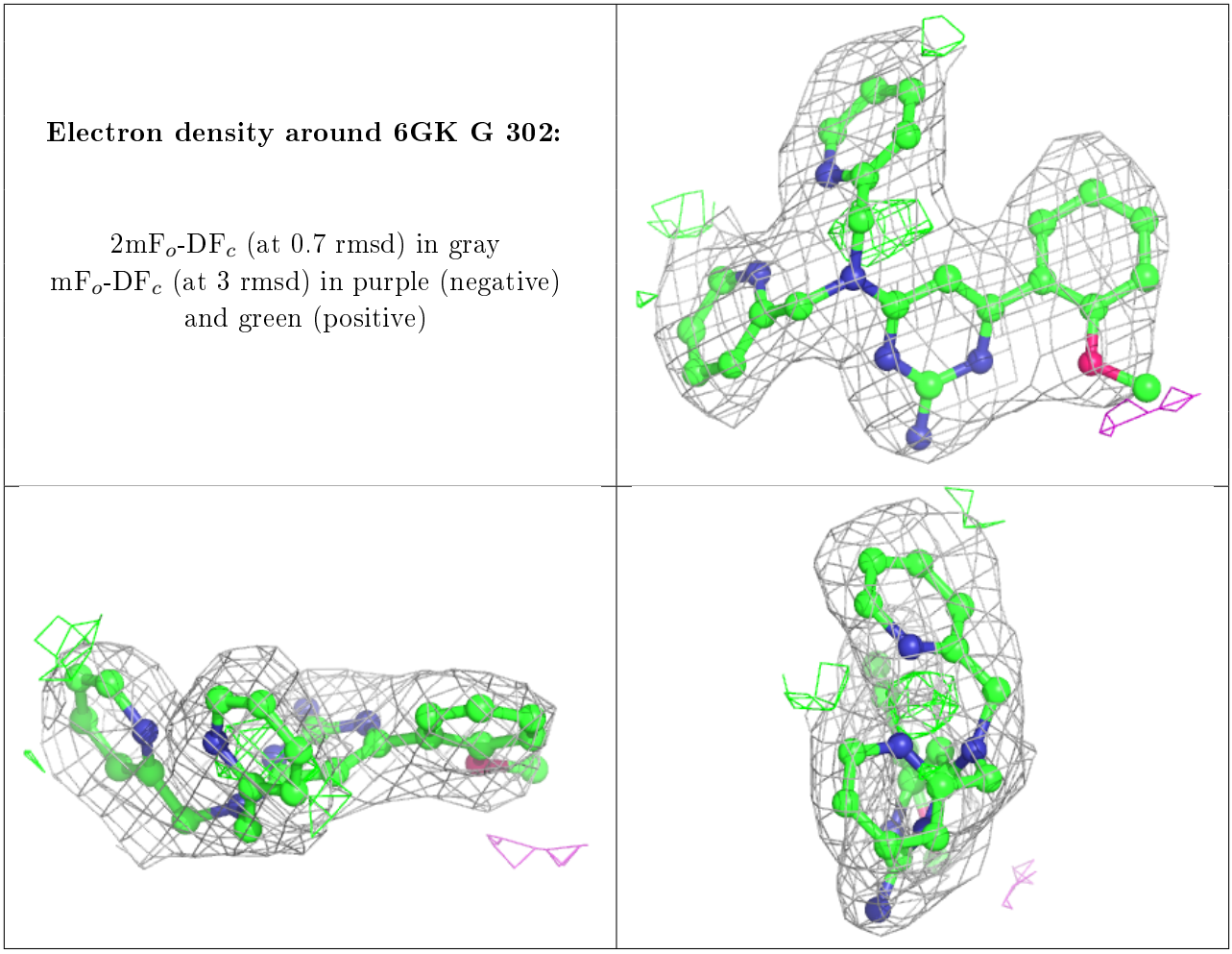






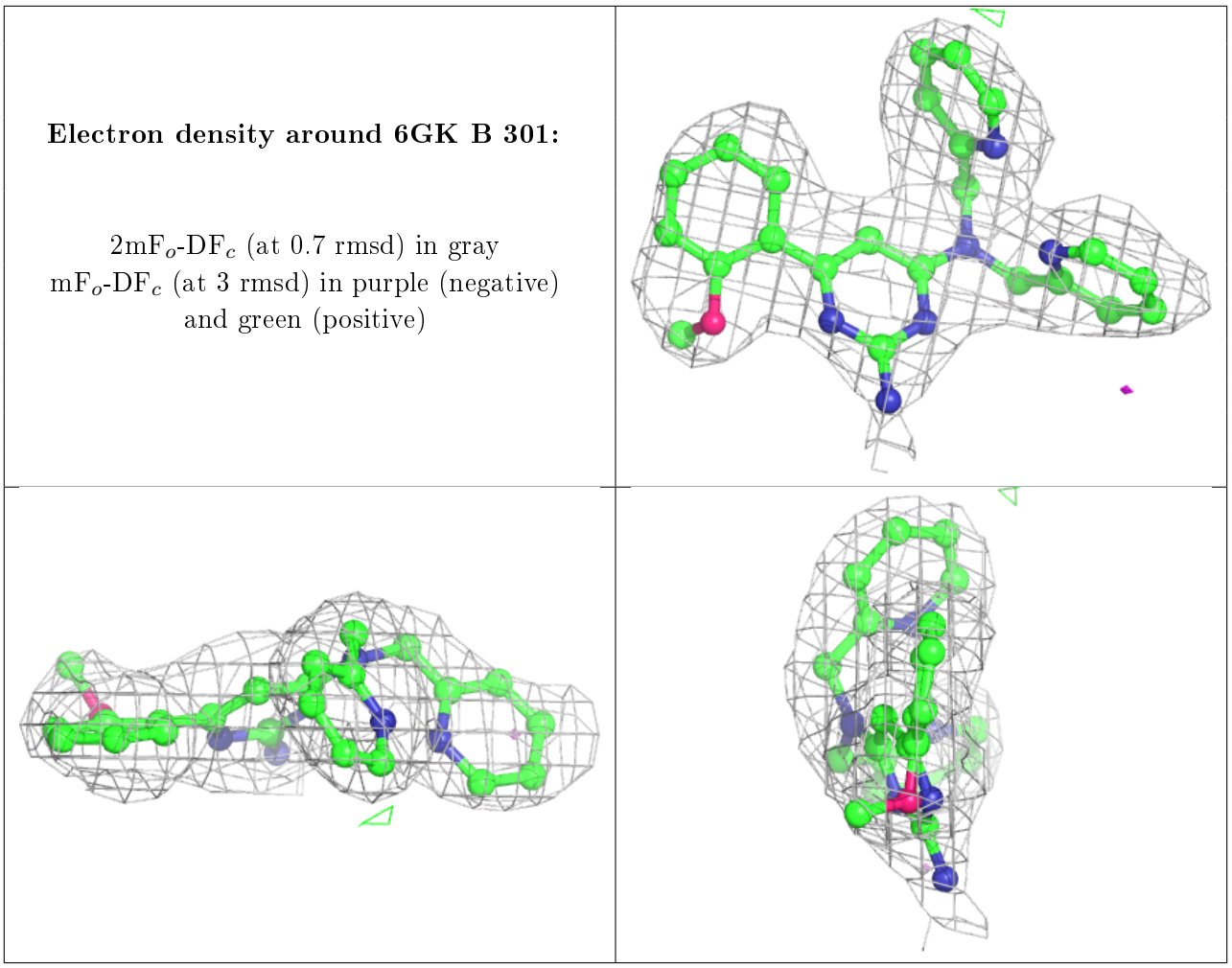
Electron density around 6GK G 302:

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



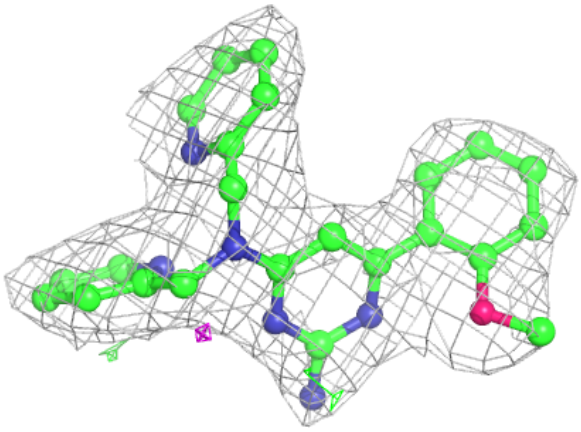
Electron density around 6GK B 301:

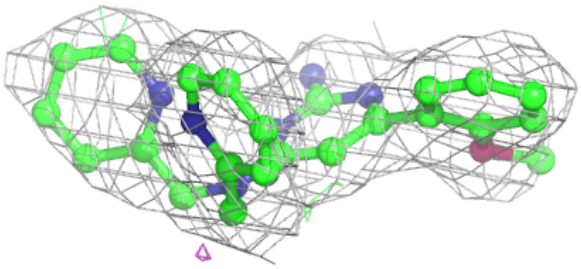
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

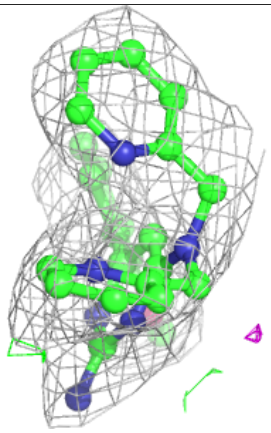


Electron density around 6GK D 302:

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

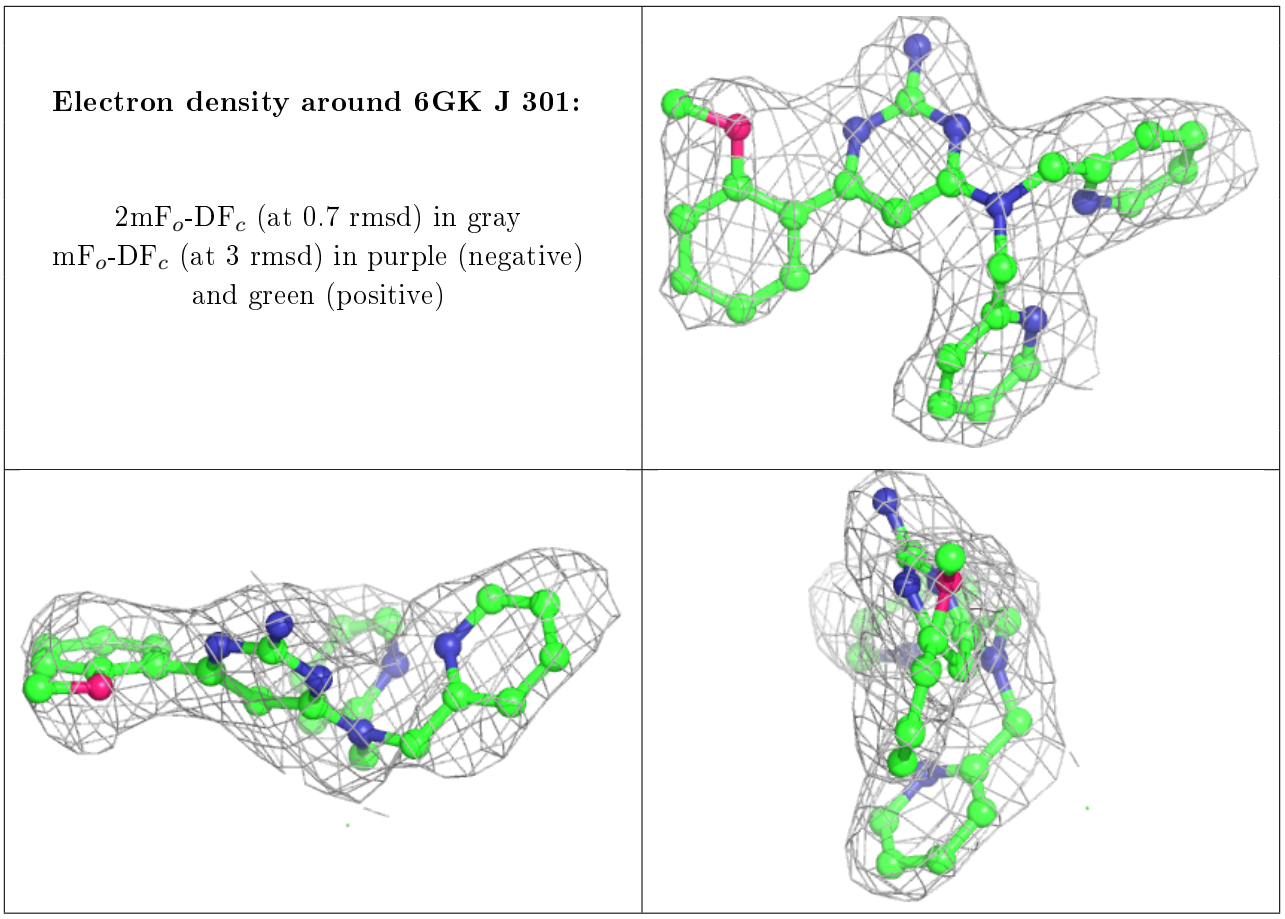






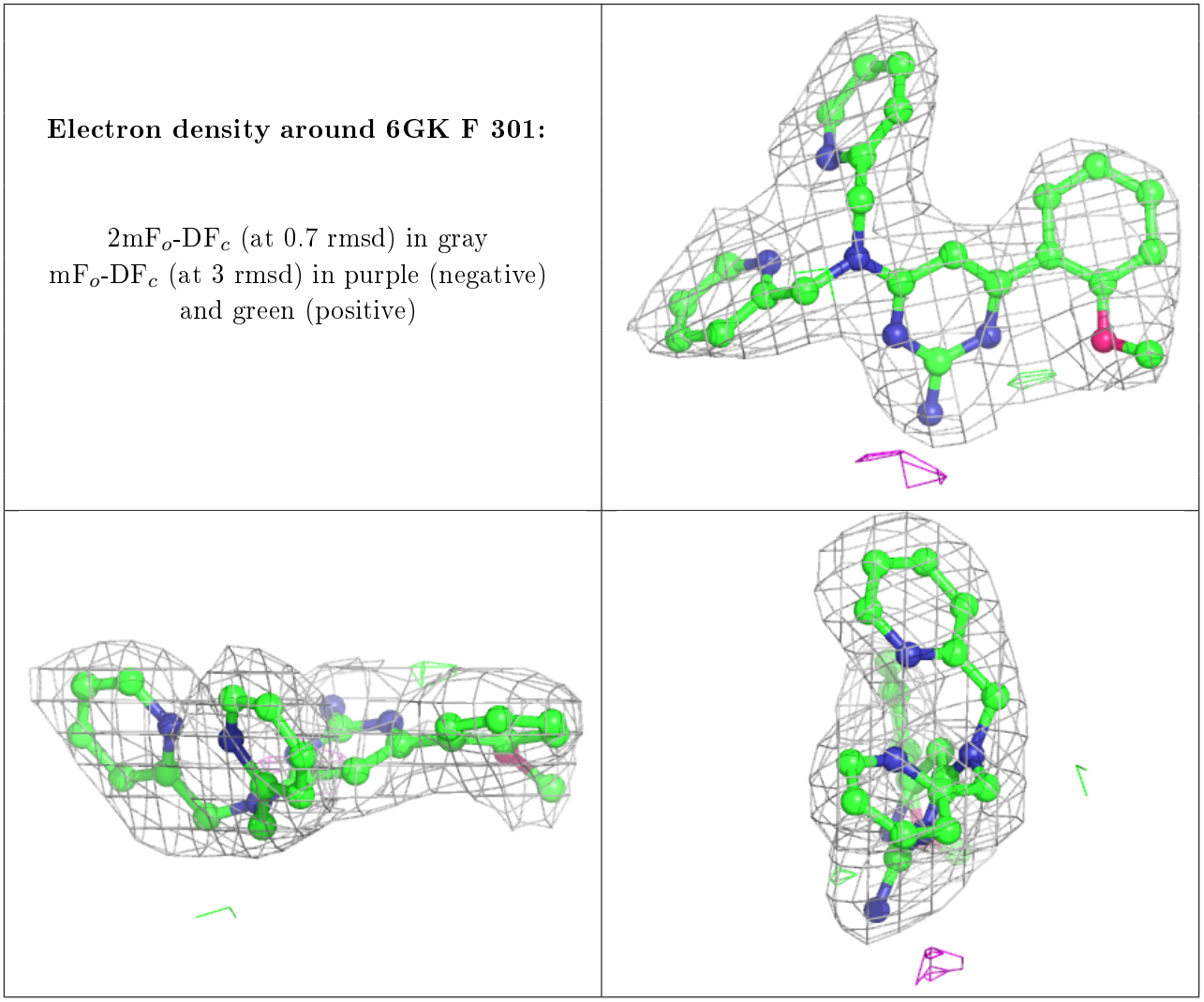
Electron density around 6GK J 301:

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



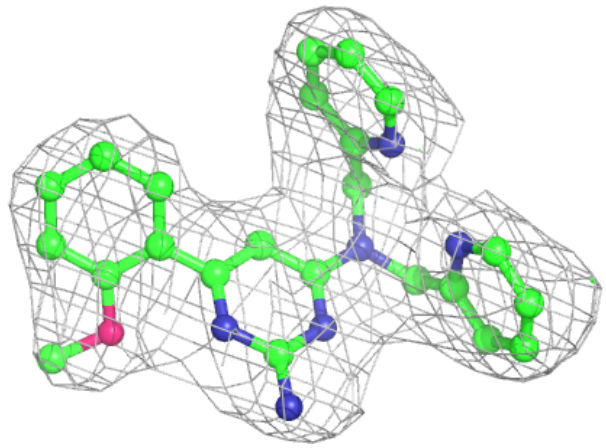
Electron density around 6GK F 301:

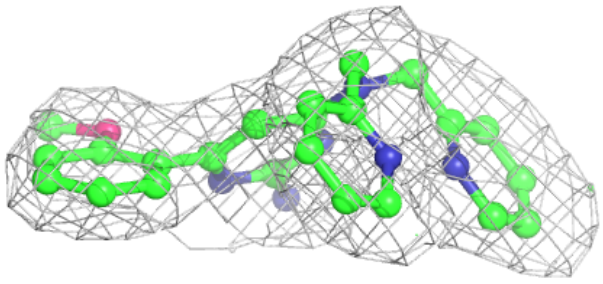
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

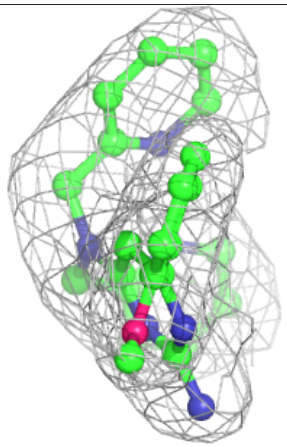


Electron density around 6GK D 301:

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

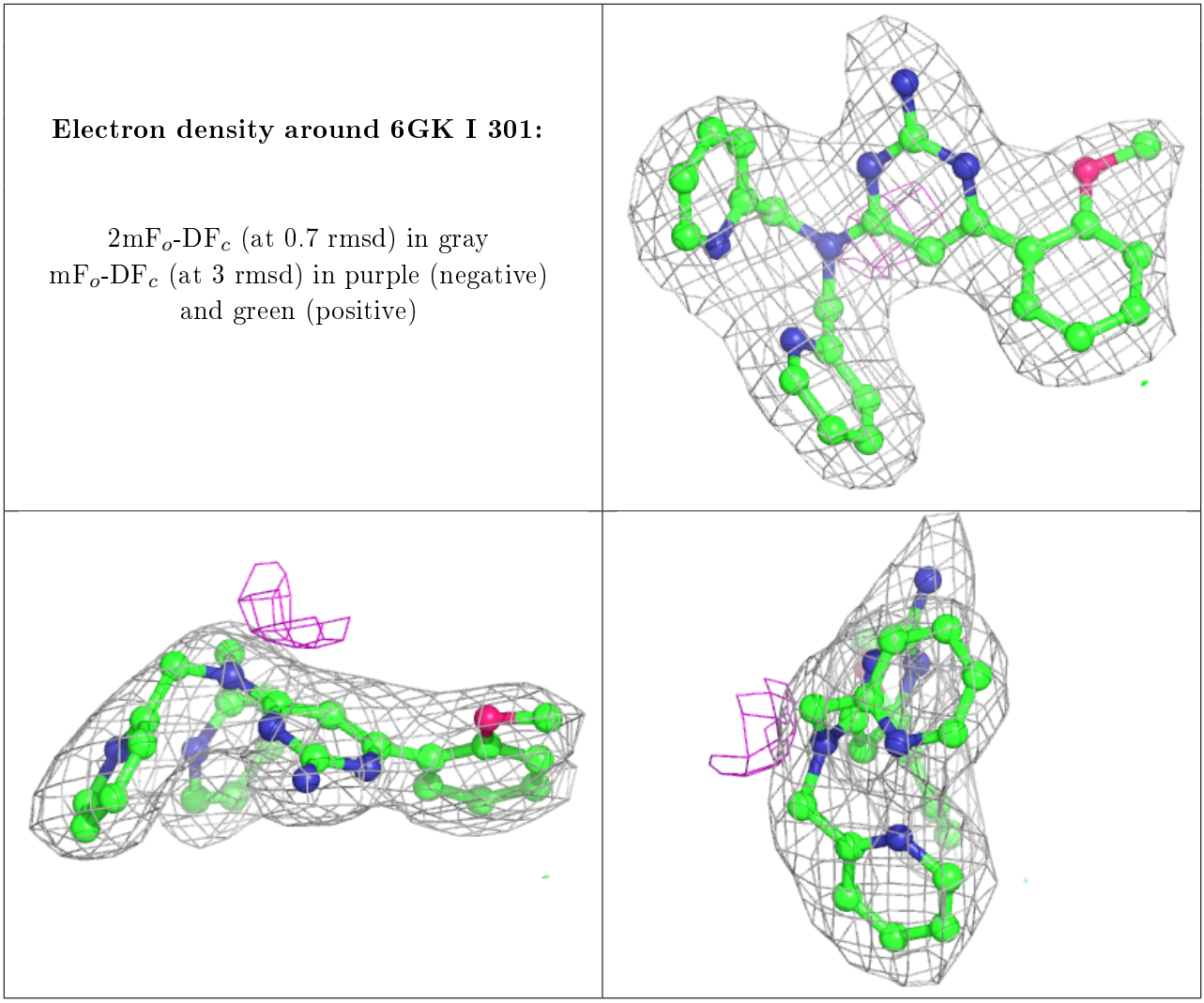






Electron density around 6GK I 301:

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



6.5 Other polymers

There are no such residues in this entry.