Full wwPDB X-ray Structure Validation Report

Jun 23, 2024 – 12:36 AM EDT

PDB ID	:	4QAC
Title	:	X-RAY STRUCTURE OF ACETYLCHOLINE BINDING PROTEIN (ACHBP) IN COMPLEX WITH 4-(4-methylpiperidin-1-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	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

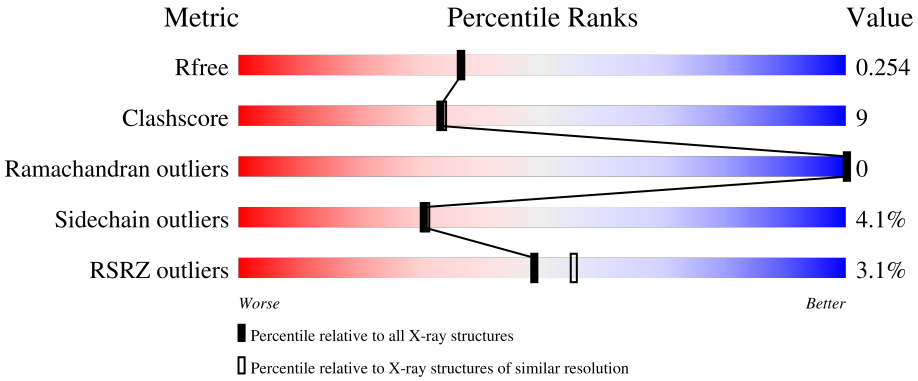
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	2% 86% 10% ·
1	B	217	5% 79% 13% · 6%
1	C	217	2% 83% 11% · ·
1	D	217	2% 83% 13% · ·
1	E	217	4% 79% 17% · ·

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Mol	Chain	Length	Quality of chain
1	F	217	5% 80% 15%
1	G	217	3% 82% 12%
1	H	217	2% 86% 10%
1	I	217	% 87% 9%
1	J	217	4% 80% 12% 6%

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	301	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17777 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	209	Total	C	N	O	S	0	0	0
			1676	1048	285	338	5			
1	B	205	Total	C	N	O	S	0	0	0
			1636	1024	280	327	5			
1	C	208	Total	C	N	O	S	0	0	0
			1668	1044	284	335	5			
1	D	213	Total	C	N	O	S	0	0	0
			1710	1068	292	345	5			
1	E	211	Total	C	N	O	S	0	0	0
			1691	1056	288	342	5			
1	F	213	Total	C	N	O	S	0	0	0
			1706	1064	290	347	5			
1	G	209	Total	C	N	O	S	0	1	0
			1679	1050	285	339	5			
1	H	210	Total	C	N	O	S	0	0	0
			1681	1051	286	339	5			
1	I	208	Total	C	N	O	S	0	0	0
			1668	1044	284	335	5			
1	J	205	Total	C	N	O	S	0	0	0
			1639	1025	280	329	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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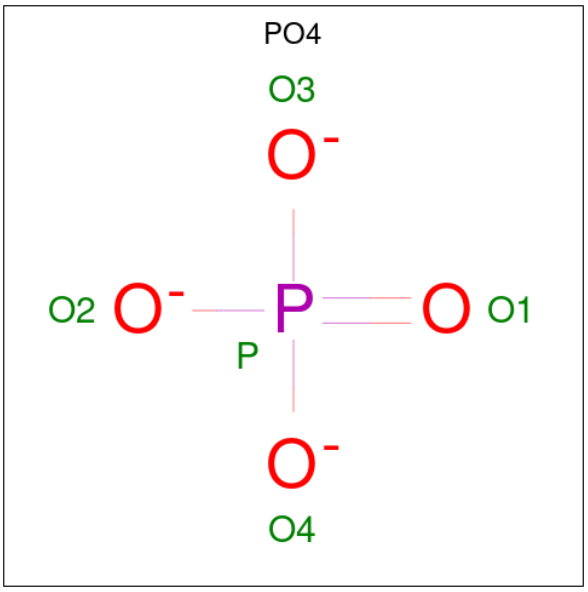
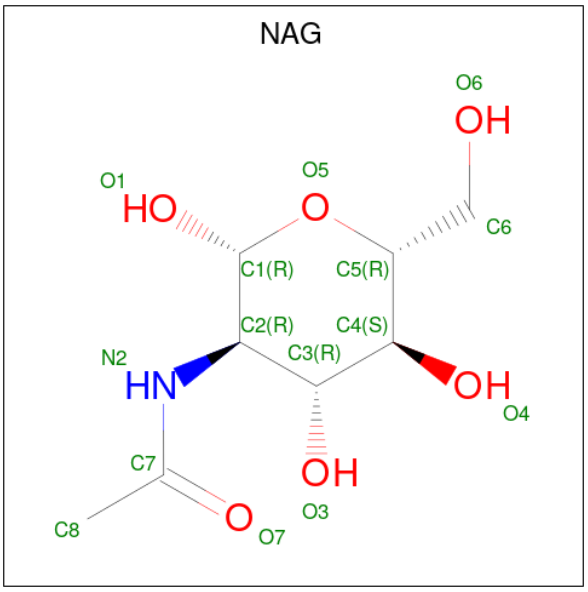
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP P58154
G	-3	ASP	-	expression tag	UNP P58154
G	-2	ASP	-	expression tag	UNP P58154
G	-1	ASP	-	expression tag	UNP P58154
G	0	LYS	-	expression tag	UNP P58154
H	-7	ASP	-	expression tag	UNP P58154
H	-6	TYR	-	expression tag	UNP P58154
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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



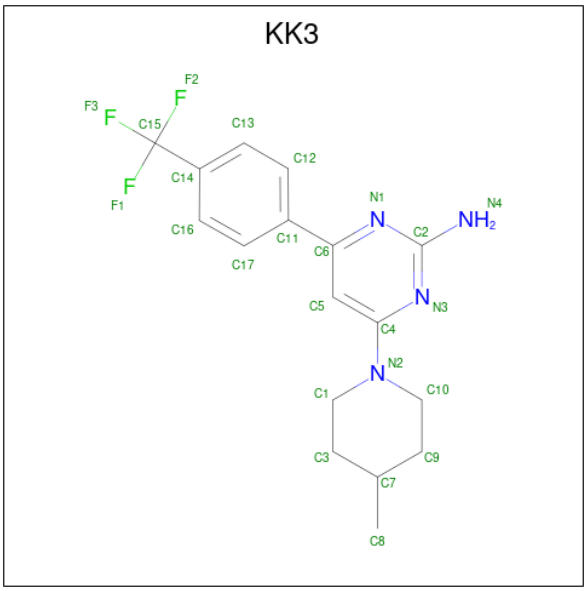
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0

- 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	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 4-(4-methylpiperidin-1-yl)-6-[4-(trifluoromethyl)phenyl]pyrimidin-2-amine (three-letter code: KK3) (formula: $C_{17}H_{19}F_3N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N 24 17 3 4	0	0
4	B	1	Total C F N 24 17 3 4	0	0
4	C	1	Total C F N 24 17 3 4	0	0
4	D	1	Total C F N 24 17 3 4	0	0
4	E	1	Total C F N 24 17 3 4	0	0
4	F	1	Total C F N 24 17 3 4	0	0
4	G	1	Total C F N 24 17 3 4	0	0
4	H	1	Total C F N 24 17 3 4	0	0
4	I	1	Total C F N 24 17 3 4	0	0
4	J	1	Total C F N 24 17 3 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	50	Total O 50 50	0	0

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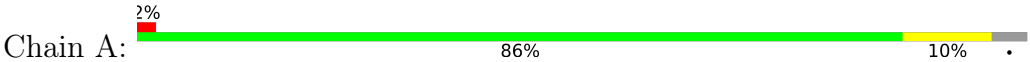
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	59	Total O 59 59	0	0
5	D	71	Total O 71 71	0	0
5	E	57	Total O 57 57	0	0
5	F	61	Total O 61 61	0	0
5	G	59	Total O 59 59	0	0
5	H	79	Total O 79 79	0	0
5	I	71	Total O 71 71	0	0
5	J	52	Total O 52 52	0	0

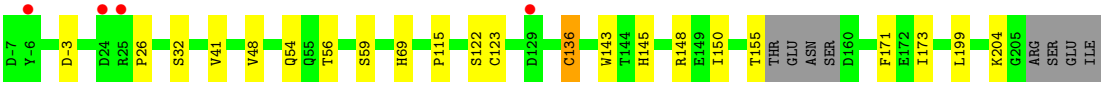
3 Residue-property plots (i)

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

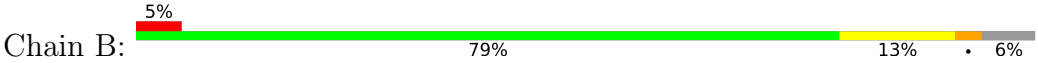
Chain A:

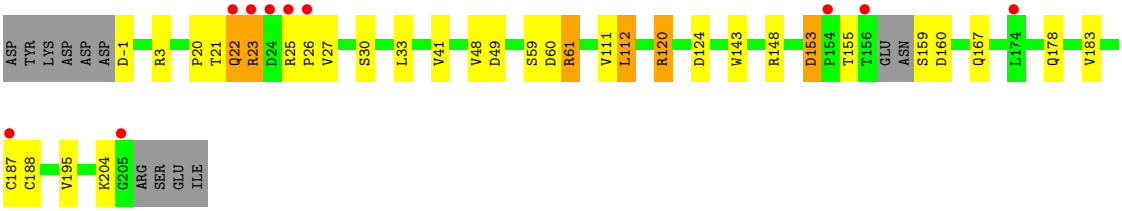




• Molecule 1: Acetylcholine-binding protein

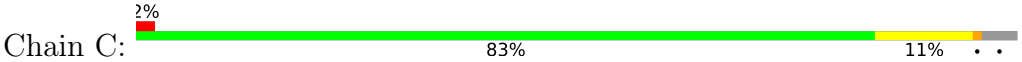
Chain B:

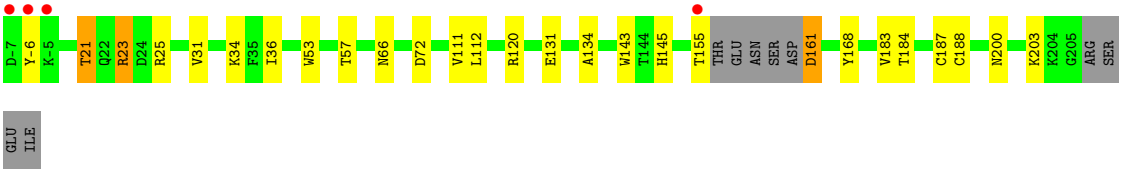




• Molecule 1: Acetylcholine-binding protein

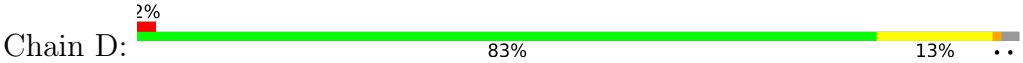
Chain C:

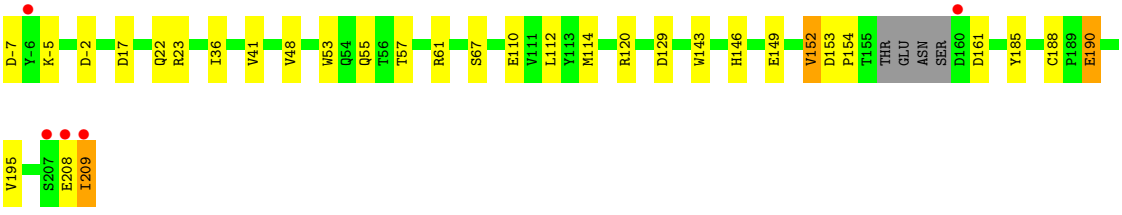




• Molecule 1: Acetylcholine-binding protein

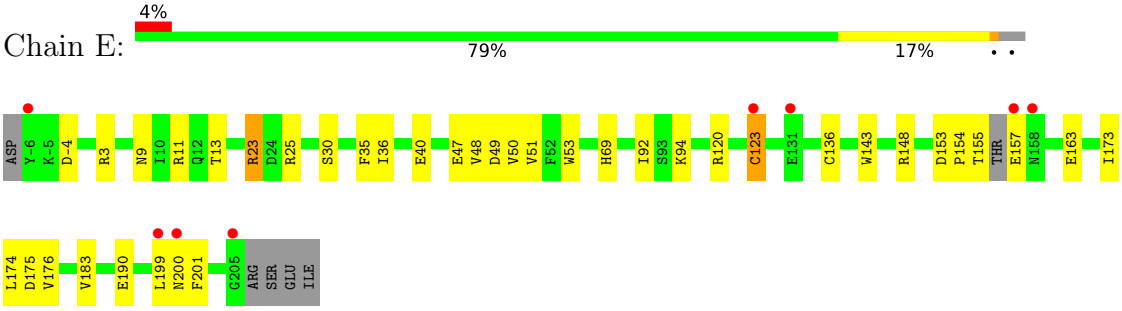
Chain D:





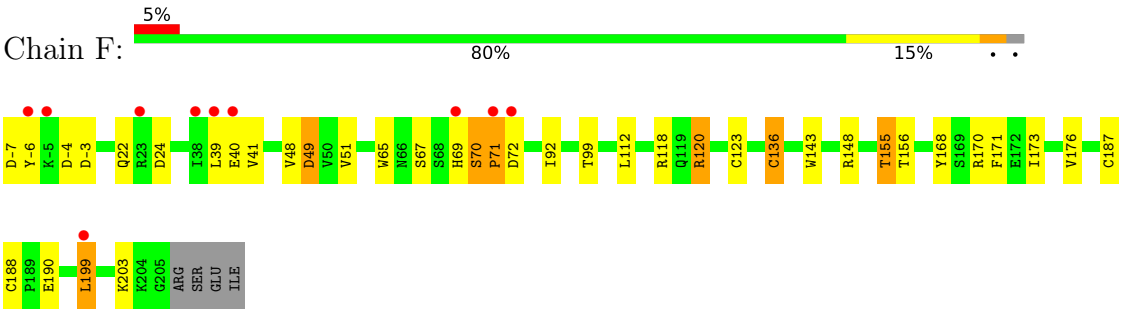
• Molecule 1: Acetylcholine-binding protein

Chain E:



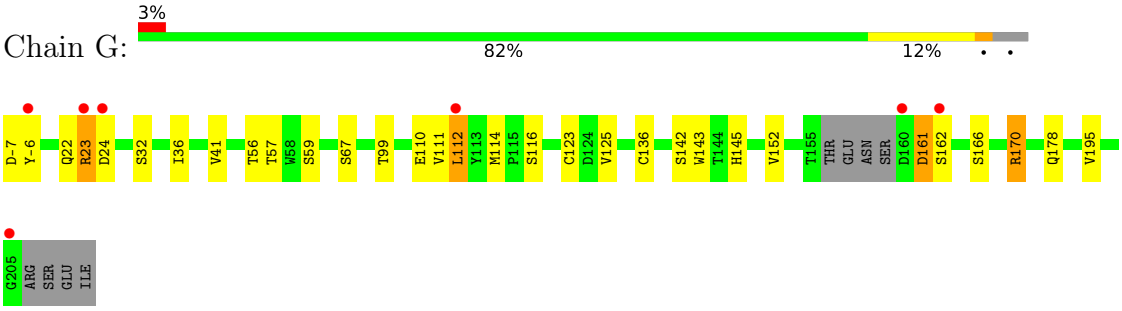
• Molecule 1: Acetylcholine-binding protein

Chain F:



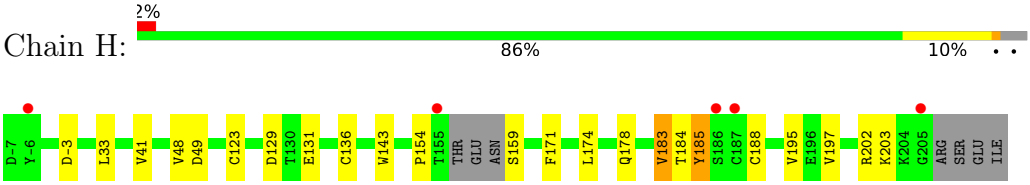
• Molecule 1: Acetylcholine-binding protein

Chain G:



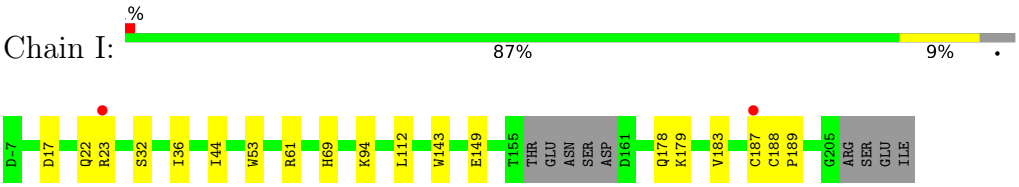
• Molecule 1: Acetylcholine-binding protein

Chain H:



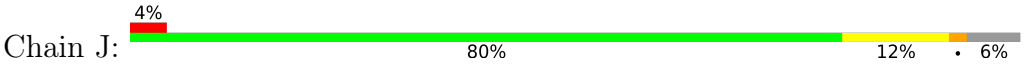
• Molecule 1: Acetylcholine-binding protein

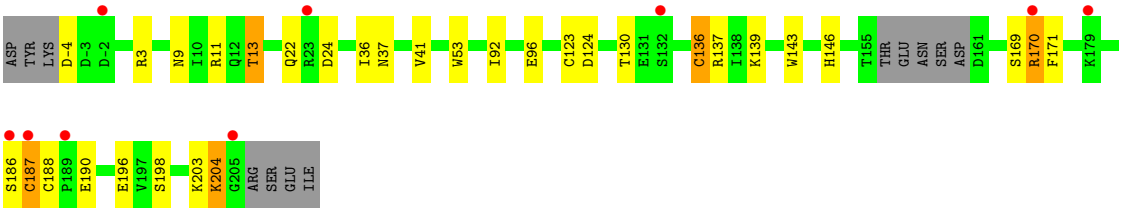
Chain I:



• Molecule 1: Acetylcholine-binding protein

Chain J:


4%
80%
12%
6%


ASP
TYR
LYS
D-4
D-3
D-2
R3
N9
I10
R11
Q12
T13
Q22
R23
D24
I36
N37
V41
W53
I92
E96
C123
D124
T130
E131
S132
C136
R137
I138
K139
W143
H146
T155
THR
GLU
ASN
SER
ASP
D161
S169
R170
F171
K179

S186
C187
C188
P189
E190
E196
V197
S198
K203
K204
G205
ARG
SER
GLU
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	240.06Å 75.50Å 149.76Å 90.00° 117.96° 90.00°	Depositor
Resolution (Å)	49.83 – 2.10 49.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.83-2.10) 91.5 (49.83-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.200 , 0.247 0.208 , 0.254	Depositor DCC
R_{free} test set	6836 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17777	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: KK3, PO4, NAG

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	0.42	0/1712	0.54	0/2333
1	B	0.42	0/1671	0.58	1/2278 (0.0%)
1	C	0.44	0/1704	0.58	0/2322
1	D	0.44	0/1746	0.56	0/2378
1	E	0.43	0/1727	0.60	0/2353
1	F	0.44	1/1743 (0.1%)	0.59	1/2377 (0.0%)
1	G	0.42	0/1718	0.57	0/2341
1	H	0.53	3/1717 (0.2%)	0.60	0/2340
1	I	0.44	0/1704	0.58	0/2322
1	J	0.41	0/1674	0.59	0/2282
All	All	0.44	4/17116 (0.0%)	0.58	2/23326 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	185	TYR	CE1-CZ	-5.68	1.31	1.38
1	H	185	TYR	CG-CD1	-5.55	1.31	1.39
1	H	185	TYR	C-O	-5.40	1.13	1.23
1	F	71	PRO	N-CD	5.09	1.54	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	70	SER	C-N-CD	5.74	140.45	128.40
1	B	153	ASP	C-N-CD	5.58	140.12	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	1676	0	1612	13	0
1	B	1636	0	1583	25	0
1	C	1668	0	1607	19	0
1	D	1710	0	1645	23	0
1	E	1691	0	1625	39	0
1	F	1706	0	1637	80	0
1	G	1679	0	1617	38	0
1	H	1681	0	1614	13	0
1	I	1668	0	1605	11	0
1	J	1639	0	1582	28	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	D	10	0	0	1	0
2	F	10	0	0	0	0
2	H	5	0	0	0	0
2	I	10	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	5	0
3	D	14	0	13	1	0
3	E	14	0	13	0	0
3	F	14	0	13	2	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	1	0
3	J	14	0	13	1	0
4	A	24	0	19	1	0
4	B	24	0	19	2	0
4	C	24	0	19	1	0
4	D	24	0	19	3	0
4	E	24	0	19	1	0
4	F	24	0	19	2	0
4	G	24	0	19	1	0
4	H	24	0	19	3	0
4	I	24	0	19	2	0
4	J	24	0	19	2	0
5	A	48	0	0	0	0
5	B	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	59	0	0	3	0
5	D	71	0	0	1	0
5	E	57	0	0	2	0
5	F	61	0	0	2	0
5	G	59	0	0	1	0
5	H	79	0	0	1	0
5	I	71	0	0	0	0
5	J	52	0	0	1	0
All	All	17777	0	16434	282	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 (282) 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:G:57:THR:HG22	1:G:112:LEU:CD1	1.57	1.34
1:G:57:THR:CG2	1:G:112:LEU:HD13	1.60	1.30
1:F:-4:ASP:O	1:F:71:PRO:HG3	1.50	1.11
1:F:176:VAL:HG22	1:F:199:LEU:HD12	1.33	1.10
1:B:21:THR:HG22	1:B:27:VAL:HG23	1.29	1.09
1:F:39:LEU:HB2	1:F:49:ASP:HB3	1.13	1.08
1:G:161:ASP:HA	1:G:162:SER:HB3	1.11	1.08
1:G:57:THR:CG2	1:G:112:LEU:CD1	2.26	1.05
1:F:41:VAL:HG21	1:F:171:PHE:CZ	1.95	1.02
1:F:39:LEU:HD23	1:F:51:VAL:HG23	1.36	1.00
1:F:176:VAL:CG2	1:F:199:LEU:HD12	1.91	1.00
1:F:39:LEU:HD12	1:F:118:ARG:CZ	1.91	1.00
1:G:161:ASP:HA	1:G:162:SER:CB	1.92	0.99
1:F:39:LEU:CB	1:F:49:ASP:HB3	1.94	0.97
1:B:21:THR:HG22	1:B:27:VAL:CG2	1.94	0.96
1:B:21:THR:CG2	1:B:27:VAL:HG23	1.96	0.95
1:E:176:VAL:HG22	1:E:199:LEU:HG	1.51	0.93
1:F:40:GLU:N	1:F:49:ASP:HB2	1.85	0.91
1:F:-3:ASP:HA	1:F:71:PRO:HB3	1.53	0.90
1:F:39:LEU:HD12	1:F:118:ARG:NH1	1.87	0.89
1:F:39:LEU:CD2	1:F:51:VAL:HG23	2.01	0.89
1:E:123:CYS:SG	1:E:136:CYS:HB2	2.13	0.88
1:C:-6:TYR:CE1	1:C:72:ASP:OD2	2.26	0.88
1:H:123:CYS:CB	1:H:136:CYS:SG	2.62	0.87
1:E:123:CYS:SG	1:E:136:CYS:CB	2.62	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:GLU:CB	1:F:120:ARG:HH12	1.89	0.86
1:F:39:LEU:CD1	1:F:118:ARG:NH1	2.39	0.85
1:F:39:LEU:CD1	1:F:118:ARG:CZ	2.55	0.85
1:B:26:PRO:HG3	1:B:148:ARG:O	1.78	0.83
1:F:40:GLU:HB2	1:F:120:ARG:HH12	1.41	0.82
1:F:39:LEU:HB2	1:F:49:ASP:CB	2.05	0.82
1:F:-3:ASP:HA	1:F:71:PRO:CB	2.09	0.81
1:D:57:THR:HG22	1:D:112:LEU:HG	1.63	0.80
1:H:33:LEU:H	1:H:178:GLN:HE22	1.30	0.80
3:F:303:NAG:H83	3:F:303:NAG:O3	1.83	0.79
1:F:39:LEU:HG	1:F:118:ARG:NE	1.98	0.77
1:F:40:GLU:O	1:F:48:VAL:HA	1.84	0.77
1:F:176:VAL:HG22	1:F:199:LEU:CD1	2.13	0.77
1:F:-4:ASP:O	1:F:71:PRO:CG	2.30	0.77
1:E:199:LEU:HD23	1:E:200:ASN:N	1.99	0.76
1:F:41:VAL:HG21	1:F:171:PHE:CE1	2.20	0.76
1:D:146:HIS:CD2	1:D:190:GLU:HG3	2.22	0.75
1:C:23:ARG:HD2	1:C:25:ARG:HH21	1.51	0.75
1:F:39:LEU:CD2	1:F:51:VAL:CG2	2.65	0.74
1:G:161:ASP:CA	1:G:162:SER:HB3	2.06	0.74
1:F:39:LEU:HD12	1:F:118:ARG:NH2	2.04	0.72
1:E:123:CYS:CB	1:E:136:CYS:SG	2.78	0.72
1:E:123:CYS:HG	1:E:136:CYS:CB	2.01	0.71
1:F:-3:ASP:HA	1:F:71:PRO:CG	2.21	0.71
1:F:-3:ASP:CA	1:F:71:PRO:HG3	2.21	0.71
1:F:49:ASP:OD2	1:F:120:ARG:HG2	1.91	0.71
1:E:173:ILE:HG23	1:E:199:LEU:HD21	1.73	0.70
1:G:123:CYS:HG	1:G:136:CYS:HG	0.79	0.70
1:G:123:CYS:SG	1:G:136:CYS:CB	2.80	0.70
1:C:-6:TYR:HE1	1:C:72:ASP:OD2	1.70	0.70
1:F:-4:ASP:C	1:F:71:PRO:HG3	2.11	0.70
5:F:426:HOH:O	1:J:187:CYS:HB3	1.92	0.70
1:F:92:ILE:HD11	1:F:120:ARG:HD2	1.74	0.69
1:F:40:GLU:HB2	1:F:120:ARG:NH1	2.07	0.69
1:G:57:THR:HG21	1:G:112:LEU:CD1	2.20	0.68
1:E:123:CYS:CB	1:E:136:CYS:HG	2.06	0.68
1:H:159:SER:N	5:H:478:HOH:O	2.26	0.68
1:B:112:LEU:HD23	1:B:112:LEU:N	2.08	0.68
1:G:-7:ASP:N	1:G:67:SER:O	2.27	0.67
1:F:39:LEU:CG	1:F:118:ARG:CZ	2.73	0.67
1:G:112:LEU:HD12	1:G:114:MET:CE	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:CYS:CB	1:F:136:CYS:SG	2.83	0.67
1:F:39:LEU:CB	1:F:49:ASP:CB	2.70	0.66
3:B:302:NAG:H83	3:B:302:NAG:O3	1.94	0.66
1:C:66:ASN:ND2	5:C:408:HOH:O	2.22	0.66
1:D:209:ILE:C	1:D:209:ILE:HD13	2.16	0.66
1:F:40:GLU:H	1:F:49:ASP:HB2	1.60	0.66
1:F:39:LEU:HG	1:F:118:ARG:CZ	2.25	0.66
1:F:-3:ASP:HA	1:F:71:PRO:HG3	1.77	0.66
1:D:152:VAL:HG23	1:D:195:VAL:HG23	1.78	0.65
1:E:176:VAL:HG22	1:E:199:LEU:CG	2.24	0.65
1:G:111:VAL:C	1:G:112:LEU:HD22	2.15	0.65
1:F:39:LEU:HD21	1:F:51:VAL:CG2	2.27	0.65
3:B:302:NAG:H83	3:B:302:NAG:C3	2.26	0.65
1:G:123:CYS:SG	1:G:136:CYS:HB2	2.37	0.64
4:D:304:KK3:H6	1:E:36:ILE:HD12	1.78	0.64
1:I:32:SER:HB2	1:I:178:GLN:HE22	1.63	0.64
1:I:149:GLU:OE2	1:J:3:ARG:NH2	2.30	0.64
1:G:152:VAL:HG12	1:G:195:VAL:HG23	1.79	0.63
1:G:143:TRP:CE2	4:G:302:KK3:H19	2.33	0.63
1:J:143:TRP:CE2	4:J:302:KK3:H19	2.34	0.63
1:E:30:SER:HB3	1:E:155:THR:HG22	1.82	0.62
1:D:149:GLU:OE2	1:E:3:ARG:NH2	2.26	0.62
1:E:123:CYS:HG	1:E:136:CYS:HG	0.90	0.62
1:G:57:THR:HG21	1:G:112:LEU:HD11	1.81	0.62
1:F:39:LEU:HD11	1:J:92:ILE:HB	1.81	0.61
1:G:123:CYS:HG	1:G:136:CYS:CB	2.10	0.61
1:J:123:CYS:CB	1:J:136:CYS:SG	2.88	0.61
1:D:41:VAL:HG22	1:D:48:VAL:HG12	1.83	0.60
3:B:302:NAG:H83	3:B:302:NAG:H3	1.83	0.60
1:H:143:TRP:CE2	4:H:303:KK3:H19	2.36	0.60
1:C:23:ARG:HD2	1:C:25:ARG:NH2	2.15	0.60
4:B:303:KK3:H6	1:C:36:ILE:HD12	1.84	0.60
1:G:-7:ASP:OD1	1:G:-6:TYR:N	2.35	0.60
4:F:304:KK3:H6	1:G:36:ILE:HD12	1.84	0.59
1:E:143:TRP:CE2	4:E:302:KK3:H19	2.37	0.59
1:F:40:GLU:HB3	1:F:120:ARG:HH12	1.65	0.59
1:C:-6:TYR:CD1	1:C:72:ASP:OD2	2.54	0.59
1:E:174:LEU:HD12	1:E:200:ASN:OD1	2.03	0.59
1:E:155:THR:O	1:E:157:GLU:N	2.35	0.59
1:B:41:VAL:HG22	1:B:48:VAL:HG12	1.83	0.58
1:H:123:CYS:HB2	1:H:136:CYS:SG	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:VAL:CG2	1:E:199:LEU:HG	2.30	0.58
1:D:110:GLU:CD	1:D:112:LEU:HD11	2.25	0.57
1:B:111:VAL:C	1:B:112:LEU:HD23	2.24	0.57
1:F:173:ILE:HD13	1:F:199:LEU:HD11	1.85	0.57
1:G:123:CYS:CB	1:G:136:CYS:HG	2.16	0.57
1:D:120:ARG:NH1	5:D:433:HOH:O	2.36	0.57
1:D:146:HIS:CG	1:D:190:GLU:HG3	2.40	0.57
1:F:39:LEU:HD23	1:F:51:VAL:CG2	2.21	0.57
1:G:112:LEU:HD12	1:G:114:MET:HE3	1.87	0.57
1:F:39:LEU:HG	1:F:118:ARG:CD	2.35	0.56
1:G:123:CYS:CB	1:G:136:CYS:SG	2.93	0.56
1:E:148:ARG:NH1	1:E:190:GLU:OE2	2.38	0.56
1:F:41:VAL:CG2	1:F:171:PHE:CZ	2.82	0.56
1:G:110:GLU:OE2	1:G:112:LEU:HD21	2.05	0.56
1:J:146:HIS:CD2	1:J:190:GLU:HG3	2.40	0.56
1:D:17:ASP:OD2	1:E:11:ARG:NH2	2.31	0.56
1:C:36:ILE:HD11	1:C:53:TRP:HB2	1.88	0.56
1:A:-3:ASP:OD2	1:E:148:ARG:NH2	2.39	0.56
1:H:129:ASP:OD1	1:H:203:LYS:HE2	2.07	0.55
1:G:112:LEU:HD12	1:G:114:MET:HE1	1.87	0.55
1:A:143:TRP:CE2	4:A:304:KK3:H19	2.41	0.55
1:F:-4:ASP:OD2	1:F:69:HIS:O	2.24	0.55
1:G:57:THR:HG22	1:G:112:LEU:HD13	0.70	0.55
1:I:143:TRP:CE2	4:I:304:KK3:H19	2.42	0.55
1:C:203:LYS:NZ	5:C:406:HOH:O	2.22	0.55
1:E:36:ILE:HD11	1:E:53:TRP:HB2	1.88	0.54
1:B:21:THR:CG2	1:B:27:VAL:CG2	2.70	0.54
1:J:186:SER:O	1:J:187:CYS:SG	2.66	0.54
1:E:199:LEU:HD23	1:E:199:LEU:C	2.28	0.54
1:H:131:GLU:O	1:H:202:ARG:NH1	2.40	0.54
1:J:137:ARG:NH1	1:J:198:SER:OG	2.41	0.54
1:J:123:CYS:HB2	1:J:136:CYS:SG	2.48	0.54
1:C:143:TRP:CE2	4:C:301:KK3:H19	2.43	0.54
1:F:40:GLU:HA	1:F:40:GLU:OE1	2.08	0.54
1:G:57:THR:CG2	1:G:112:LEU:HD11	2.25	0.54
1:D:154:PRO:HG3	1:D:195:VAL:HG22	1.90	0.53
4:H:303:KK3:H6	1:I:36:ILE:HD12	1.90	0.53
1:A:26:PRO:HB3	1:A:148:ARG:C	2.29	0.53
1:B:30:SER:HB3	1:B:155:THR:HG22	1.91	0.53
1:D:57:THR:CG2	1:D:112:LEU:HG	2.38	0.53
1:D:143:TRP:CE2	4:D:304:KK3:H19	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:GLU:CB	1:F:120:ARG:NH1	2.65	0.53
1:B:167:GLN:O	1:B:204:LYS:NZ	2.41	0.53
1:F:39:LEU:HD11	1:F:118:ARG:NH1	2.23	0.53
1:F:123:CYS:HG	1:F:136:CYS:HG	0.53	0.52
1:F:173:ILE:HD13	1:F:199:LEU:CD1	2.40	0.52
1:G:111:VAL:O	1:G:112:LEU:HD22	2.09	0.52
1:G:112:LEU:N	1:G:112:LEU:CD2	2.73	0.52
1:I:94:LYS:HZ2	1:J:96:GLU:HG3	1.75	0.52
1:G:170:ARG:HB2	5:G:449:HOH:O	2.09	0.52
1:F:143:TRP:CE2	4:F:304:KK3:H19	2.45	0.52
1:C:21:THR:OG1	1:D:-2:ASP:HB3	2.08	0.52
1:B:49:ASP:OD2	1:B:120:ARG:NH1	2.43	0.51
1:E:199:LEU:HD22	1:E:201:PHE:HB3	1.92	0.51
1:F:187:CYS:SG	1:F:188:CYS:N	2.83	0.51
1:A:41:VAL:HG22	1:A:48:VAL:HG23	1.91	0.51
1:E:174:LEU:HD12	1:E:200:ASN:CG	2.31	0.51
3:J:301:NAG:O7	3:J:301:NAG:H3	2.10	0.51
1:F:-3:ASP:CA	1:F:71:PRO:CG	2.87	0.51
1:J:9:ASN:O	1:J:13:THR:HG23	2.11	0.51
1:F:39:LEU:HD21	1:F:51:VAL:HG21	1.93	0.50
1:D:110:GLU:OE2	1:D:112:LEU:HD11	2.11	0.50
1:E:174:LEU:HB2	1:E:200:ASN:O	2.12	0.50
1:F:173:ILE:CG1	1:F:199:LEU:HD11	2.41	0.50
1:B:26:PRO:HG3	1:B:148:ARG:C	2.31	0.50
1:F:173:ILE:CD1	1:F:199:LEU:HD11	2.40	0.50
1:G:41:VAL:HG13	1:G:125:VAL:HG11	1.94	0.50
1:J:170:ARG:O	1:J:204:LYS:HB2	2.10	0.50
1:C:187:CYS:SG	1:C:188:CYS:N	2.84	0.49
1:G:32:SER:HA	1:G:178:GLN:HE22	1.76	0.49
1:B:60:ASP:OD2	5:B:428:HOH:O	2.20	0.49
1:F:155:THR:HG22	1:F:156:THR:H	1.77	0.49
1:B:20:PRO:HD2	1:B:27:VAL:HG21	1.95	0.49
1:B:21:THR:HG22	1:B:27:VAL:HG22	1.91	0.49
1:E:47:GLU:OE1	1:E:120:ARG:NH2	2.46	0.49
1:A:26:PRO:HB3	1:A:148:ARG:O	2.12	0.49
1:B:22:GLN:HA	1:B:23:ARG:C	2.33	0.49
1:F:65:TRP:CZ2	1:F:72:ASP:O	2.66	0.49
1:J:41:VAL:HB	1:J:171:PHE:CZ	2.47	0.49
1:A:69:HIS:HB3	1:F:69:HIS:CD2	2.48	0.49
3:D:303:NAG:O7	3:D:303:NAG:H3	2.12	0.48
1:J:37:ASN:OD1	1:J:169:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:VAL:HG22	1:F:199:LEU:HB2	1.95	0.48
1:B:187:CYS:SG	1:B:188:CYS:N	2.87	0.48
3:B:302:NAG:H3	3:B:302:NAG:C8	2.43	0.48
3:B:302:NAG:C3	3:B:302:NAG:C8	2.90	0.48
1:I:187:CYS:SG	1:I:188:CYS:N	2.87	0.48
1:F:67:SER:HA	1:F:70:SER:OG	2.14	0.47
1:J:203:LYS:NZ	5:J:445:HOH:O	2.29	0.47
1:A:69:HIS:CG	1:F:69:HIS:CD2	3.03	0.47
1:A:32:SER:HB2	1:A:155:THR:HB	1.97	0.47
1:G:23:ARG:HA	1:G:24:ASP:HA	1.62	0.47
1:E:48:VAL:HG13	1:E:50:VAL:HG13	1.96	0.47
1:F:40:GLU:O	1:F:48:VAL:HG23	2.15	0.46
1:J:187:CYS:C	1:J:188:CYS:SG	2.94	0.46
1:F:-6:TYR:HA	1:F:-3:ASP:OD1	2.15	0.46
1:F:173:ILE:HG23	1:F:199:LEU:CD1	2.46	0.46
1:E:92:ILE:HD11	1:E:120:ARG:HG2	1.98	0.46
1:B:-1:ASP:O	1:B:3:ARG:HG3	2.16	0.46
1:B:143:TRP:CE2	4:B:303:KK3:H19	2.51	0.46
1:E:23:ARG:HB2	1:E:25:ARG:HE	1.81	0.46
1:F:170:ARG:NH1	5:F:455:HOH:O	2.47	0.46
1:B:33:LEU:H	1:B:178:GLN:HE22	1.63	0.46
1:C:161:ASP:N	5:C:451:HOH:O	2.49	0.45
1:J:203:LYS:HE3	1:J:203:LYS:HB2	1.61	0.45
1:F:40:GLU:HB2	1:F:49:ASP:HB2	1.98	0.45
1:B:61:ARG:HE	1:B:61:ARG:HB2	1.49	0.45
1:E:199:LEU:C	1:E:199:LEU:CD2	2.86	0.45
1:E:94:LYS:HE2	5:E:423:HOH:O	2.16	0.44
4:H:303:KK3:H13	1:I:53:TRP:CZ2	2.53	0.44
1:D:112:LEU:HD23	1:D:114:MET:HE1	1.99	0.44
1:E:-4:ASP:OD2	1:E:69:HIS:O	2.35	0.44
1:H:178:GLN:HG2	1:H:197:VAL:HG13	1.99	0.44
4:I:304:KK3:H6	1:J:36:ILE:HD12	2.00	0.44
1:F:173:ILE:HG12	1:F:199:LEU:HD11	1.98	0.44
1:G:161:ASP:CA	1:G:162:SER:CB	2.75	0.44
1:H:154:PRO:HG3	1:H:195:VAL:HG22	2.00	0.44
1:I:69:HIS:HD2	3:I:303:NAG:H82	1.82	0.44
1:J:187:CYS:C	1:J:188:CYS:HG	2.21	0.44
1:J:139:LYS:HE3	1:J:196:GLU:OE1	2.18	0.44
1:E:153:ASP:HA	1:E:154:PRO:HD2	1.82	0.43
1:F:99:THR:HG21	1:J:143:TRP:CE2	2.53	0.43
1:B:148:ARG:HH12	1:C:-6:TYR:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:THR:HG22	1:C:112:LEU:HD22	2.00	0.43
1:F:-7:ASP:N	1:F:67:SER:O	2.50	0.43
1:G:110:GLU:CD	1:G:112:LEU:HD21	2.38	0.43
1:D:209:ILE:C	1:D:209:ILE:CD1	2.86	0.43
1:F:41:VAL:CG2	1:F:171:PHE:CE1	2.96	0.43
1:F:48:VAL:HG12	1:F:123:CYS:SG	2.58	0.43
3:F:303:NAG:H83	3:F:303:NAG:C3	2.48	0.43
1:H:41:VAL:HG22	1:H:48:VAL:HG12	2.00	0.43
1:F:123:CYS:HB2	1:F:136:CYS:SG	2.59	0.43
1:F:173:ILE:CG2	1:F:199:LEU:HD11	2.48	0.43
1:A:54:GLN:O	1:A:115:PRO:HD2	2.19	0.43
1:A:123:CYS:CB	1:A:136:CYS:SG	3.06	0.43
1:D:36:ILE:HD11	1:D:53:TRP:HB2	2.00	0.43
1:J:36:ILE:HD11	1:J:53:TRP:HB2	2.01	0.43
1:D:-7:ASP:N	1:D:67:SER:O	2.37	0.42
1:F:39:LEU:CD1	1:J:92:ILE:HD12	2.49	0.42
1:I:36:ILE:HD11	1:I:53:TRP:HB2	2.00	0.42
1:E:-4:ASP:OD2	1:E:69:HIS:C	2.57	0.42
1:A:145:HIS:HB2	1:A:150:ILE:HD12	2.01	0.42
1:F:168:TYR:CE1	1:J:124:ASP:HB2	2.54	0.42
1:G:142:SER:OG	1:G:145:HIS:HB2	2.19	0.42
1:A:173:ILE:HG12	1:A:199:LEU:HD11	2.00	0.42
1:B:124:ASP:HB2	1:C:168:TYR:CZ	2.54	0.42
1:D:22:GLN:HE22	1:D:61:ARG:CZ	2.32	0.42
1:E:9:ASN:ND2	5:E:405:HOH:O	2.43	0.42
1:B:159:SER:OG	1:B:160:ASP:N	2.48	0.42
1:G:111:VAL:C	1:G:112:LEU:CD2	2.85	0.42
1:G:112:LEU:HD22	1:G:112:LEU:N	2.34	0.42
1:J:143:TRP:NE1	4:J:302:KK3:H19	2.34	0.42
1:F:203:LYS:HE3	1:F:203:LYS:HB2	1.94	0.42
1:H:174:LEU:HD11	1:H:202:ARG:HD3	2.01	0.42
1:E:36:ILE:HG13	1:E:51:VAL:HG12	2.02	0.42
1:C:134:ALA:O	1:C:200:ASN:HA	2.20	0.42
1:G:99:THR:HG23	1:G:116:SER:HB3	2.01	0.42
1:D:185:TYR:CZ	4:D:304:KK3:H1	2.54	0.41
1:J:187:CYS:O	1:J:188:CYS:SG	2.77	0.41
1:F:173:ILE:HG23	1:F:199:LEU:HD11	2.02	0.41
1:C:111:VAL:C	1:C:112:LEU:HD23	2.41	0.41
1:E:35:PHE:CD1	1:E:199:LEU:HD12	2.55	0.41
1:F:39:LEU:HD11	1:J:92:ILE:HD12	2.02	0.41
1:E:174:LEU:CD1	1:E:200:ASN:OD1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:PHE:CE2	1:H:203:LYS:HD3	2.56	0.41
1:H:183:VAL:HG22	1:H:185:TYR:CZ	2.56	0.41
1:B:20:PRO:O	1:B:22:GLN:NE2	2.54	0.41
1:C:145:HIS:HE1	2:D:301:PO4:O4	2.04	0.41
1:A:171:PHE:O	1:A:204:LYS:HE3	2.20	0.41
1:D:55:GLN:HB3	1:D:114:MET:HE2	2.03	0.41
1:E:199:LEU:HD23	1:E:200:ASN:C	2.41	0.41
1:I:17:ASP:OD2	1:J:11:ARG:NH2	2.36	0.41
1:F:-3:ASP:O	1:F:71:PRO:HG2	2.20	0.40
1:D:188:CYS:HB3	1:D:190:GLU:OE2	2.20	0.40
1:I:188:CYS:HA	1:I:189:PRO:HD3	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	205/217 (94%)	204 (100%)	1 (0%)	0	100	100
1	B	201/217 (93%)	201 (100%)	0	0	100	100
1	C	204/217 (94%)	204 (100%)	0	0	100	100
1	D	209/217 (96%)	209 (100%)	0	0	100	100
1	E	207/217 (95%)	207 (100%)	0	0	100	100
1	F	211/217 (97%)	210 (100%)	1 (0%)	0	100	100
1	G	206/217 (95%)	204 (99%)	2 (1%)	0	100	100
1	H	206/217 (95%)	203 (98%)	3 (2%)	0	100	100
1	I	204/217 (94%)	203 (100%)	1 (0%)	0	100	100
1	J	201/217 (93%)	200 (100%)	1 (0%)	0	100	100
All	All	2054/2170 (95%)	2045 (100%)	9 (0%)	0	100	100

There are no Ramachandran outliers to report.

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%)	191 (98%)	4 (2%)	53	59
1	B	191/203 (94%)	181 (95%)	10 (5%)	23	21
1	C	194/203 (96%)	184 (95%)	10 (5%)	23	21
1	D	199/203 (98%)	190 (96%)	9 (4%)	27	27
1	E	197/203 (97%)	189 (96%)	8 (4%)	30	31
1	F	199/203 (98%)	189 (95%)	10 (5%)	24	23
1	G	196/203 (97%)	188 (96%)	8 (4%)	30	31
1	H	195/203 (96%)	190 (97%)	5 (3%)	46	50
1	I	194/203 (96%)	187 (96%)	7 (4%)	35	36
1	J	191/203 (94%)	182 (95%)	9 (5%)	26	25
All	All	1951/2030 (96%)	1871 (96%)	80 (4%)	30	31

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	59	SER
1	A	122	SER
1	A	136	CYS
1	B	22	GLN
1	B	23	ARG
1	B	25	ARG
1	B	59	SER
1	B	61	ARG
1	B	112	LEU
1	B	120	ARG
1	B	153	ASP
1	B	183	VAL
1	B	195	VAL

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Mol	Chain	Res	Type
1	C	21	THR
1	C	23	ARG
1	C	31	VAL
1	C	34	LYS
1	C	120	ARG
1	C	131	GLU
1	C	155	THR
1	C	161	ASP
1	C	183	VAL
1	C	184	THR
1	D	-5	LYS
1	D	23	ARG
1	D	129	ASP
1	D	152	VAL
1	D	153	ASP
1	D	161	ASP
1	D	190	GLU
1	D	208	GLU
1	D	209	ILE
1	E	13	THR
1	E	23	ARG
1	E	40	GLU
1	E	49	ASP
1	E	123	CYS
1	E	163	GLU
1	E	175	ASP
1	E	183	VAL
1	F	22	GLN
1	F	24	ASP
1	F	49	ASP
1	F	112	LEU
1	F	120	ARG
1	F	136	CYS
1	F	148	ARG
1	F	155	THR
1	F	190	GLU
1	F	199	LEU
1	G	22	GLN
1	G	23	ARG
1	G	56	THR
1	G	59	SER
1	G	112	LEU

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Mol	Chain	Res	Type
1	G	161	ASP
1	G	166	SER
1	G	170	ARG
1	H	-3	ASP
1	H	49	ASP
1	H	183	VAL
1	H	184	THR
1	H	188	CYS
1	I	22	GLN
1	I	23	ARG
1	I	44	ILE
1	I	61	ARG
1	I	112	LEU
1	I	179	LYS
1	I	183	VAL
1	J	-4	ASP
1	J	13	THR
1	J	22	GLN
1	J	24	ASP
1	J	130	THR
1	J	136	CYS
1	J	170	ARG
1	J	187	CYS
1	J	204	LYS

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

Mol	Chain	Res	Type
1	A	69	HIS
1	A	145	HIS
1	E	9	ASN
1	F	9	ASN
1	F	69	HIS
1	H	178	GLN
1	I	9	ASN

5.3.3 RNA

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	$\#\|Z\| > 2$
2	PO4	B	301	-	4,4,4	0.84	0	6,6,6	0.58	0
2	PO4	A	301	-	4,4,4	0.79	0	6,6,6	0.79	0
3	NAG	H	302	1	14,14,15	0.59	0	17,19,21	1.68	6 (35%)
2	PO4	D	302	-	4,4,4	0.62	0	6,6,6	0.52	0
2	PO4	F	302	-	4,4,4	0.55	0	6,6,6	0.85	0
4	KK3	C	301	-	26,26,26	1.21	3 (11%)	38,38,38	1.43	2 (5%)
3	NAG	G	301	1	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
2	PO4	F	301	-	4,4,4	0.56	0	6,6,6	0.44	0
2	PO4	D	301	-	4,4,4	0.88	0	6,6,6	0.53	0
4	KK3	E	302	-	26,26,26	1.21	4 (15%)	38,38,38	1.48	3 (7%)
3	NAG	J	301	1	14,14,15	0.89	0	17,19,21	2.81	7 (41%)
3	NAG	D	303	1	14,14,15	0.37	0	17,19,21	0.78	1 (5%)
2	PO4	I	301	-	4,4,4	0.62	0	6,6,6	0.61	0
2	PO4	H	301	-	4,4,4	0.68	0	6,6,6	0.53	0
3	NAG	B	302	1	14,14,15	1.24	1 (7%)	17,19,21	2.16	5 (29%)
3	NAG	I	303	1	14,14,15	0.30	0	17,19,21	0.62	0
4	KK3	H	303	-	26,26,26	1.34	4 (15%)	38,38,38	1.49	4 (10%)
4	KK3	G	302	-	26,26,26	1.19	2 (7%)	38,38,38	1.71	5 (13%)
2	PO4	I	302	-	4,4,4	0.83	0	6,6,6	0.52	0
4	KK3	D	304	-	26,26,26	1.58	7 (26%)	38,38,38	1.50	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	KK3	B	303	-	26,26,26	1.53	4 (15%)	38,38,38	1.22	3 (7%)
2	PO4	A	302	-	4,4,4	0.64	0	6,6,6	0.68	0
4	KK3	F	304	-	26,26,26	1.34	6 (23%)	38,38,38	1.30	2 (5%)
4	KK3	I	304	-	26,26,26	1.18	3 (11%)	38,38,38	1.63	4 (10%)
3	NAG	F	303	1	14,14,15	1.02	1 (7%)	17,19,21	1.97	5 (29%)
3	NAG	E	301	1	14,14,15	0.44	0	17,19,21	1.24	1 (5%)
3	NAG	A	303	1	14,14,15	1.72	4 (28%)	17,19,21	1.61	3 (17%)
4	KK3	A	304	-	26,26,26	1.40	4 (15%)	38,38,38	1.42	4 (10%)
4	KK3	J	302	-	26,26,26	1.44	5 (19%)	38,38,38	1.42	5 (13%)

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	H	302	1	-	4/6/23/26	0/1/1/1
4	KK3	C	301	-	-	4/14/24/24	0/3/3/3
3	NAG	G	301	1	-	5/6/23/26	0/1/1/1
4	KK3	E	302	-	-	4/14/24/24	0/3/3/3
3	NAG	J	301	1	-	3/6/23/26	0/1/1/1
3	NAG	D	303	1	-	6/6/23/26	0/1/1/1
3	NAG	I	303	1	-	4/6/23/26	0/1/1/1
3	NAG	B	302	1	-	5/6/23/26	0/1/1/1
4	KK3	H	303	-	-	4/14/24/24	0/3/3/3
4	KK3	G	302	-	-	6/14/24/24	0/3/3/3
4	KK3	D	304	-	-	4/14/24/24	0/3/3/3
4	KK3	B	303	-	-	4/14/24/24	0/3/3/3
4	KK3	F	304	-	-	4/14/24/24	0/3/3/3
4	KK3	I	304	-	-	4/14/24/24	0/3/3/3
3	NAG	F	303	1	-	4/6/23/26	0/1/1/1
3	NAG	E	301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	303	1	-	3/6/23/26	0/1/1/1
4	KK3	A	304	-	-	6/14/24/24	0/3/3/3
4	KK3	J	302	-	-	4/14/24/24	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	KK3	C4-N2	3.69	1.45	1.37
4	J	302	KK3	C4-N2	3.37	1.44	1.37
4	B	303	KK3	C2-N3	3.24	1.41	1.35
4	D	304	KK3	C10-N2	3.23	1.51	1.46
4	C	301	KK3	C2-N4	3.21	1.40	1.33
3	A	303	NAG	C2-N2	-3.21	1.40	1.46
4	G	302	KK3	C5-C4	3.17	1.44	1.39
4	D	304	KK3	C4-N3	3.05	1.39	1.34
4	F	304	KK3	C4-N2	3.04	1.43	1.37
4	H	303	KK3	C2-N4	3.02	1.40	1.33
4	A	304	KK3	C2-N4	3.01	1.39	1.33
3	B	302	NAG	O5-C1	-2.92	1.39	1.43
4	H	303	KK3	C4-N2	2.92	1.43	1.37
4	F	304	KK3	C10-N2	2.91	1.51	1.46
4	D	304	KK3	C4-N2	2.90	1.43	1.37
4	I	304	KK3	C2-N4	2.89	1.39	1.33
4	G	302	KK3	C1-N2	2.78	1.51	1.46
4	E	302	KK3	C4-N2	2.76	1.43	1.37
3	F	303	NAG	C2-N2	-2.75	1.41	1.46
4	J	302	KK3	C2-N3	2.75	1.40	1.35
4	A	304	KK3	C1-N2	2.73	1.51	1.46
4	J	302	KK3	C10-N2	2.73	1.51	1.46
4	A	304	KK3	C5-C4	2.56	1.43	1.39
4	D	304	KK3	C1-N2	2.50	1.50	1.46
4	D	304	KK3	C2-N3	2.50	1.39	1.35
4	J	302	KK3	C2-N4	2.41	1.38	1.33
4	F	304	KK3	C2-N4	2.40	1.38	1.33
4	F	304	KK3	C5-C4	2.37	1.43	1.39
4	B	303	KK3	C4-N3	2.37	1.37	1.34
4	D	304	KK3	C2-N4	2.35	1.38	1.33
4	H	303	KK3	C10-N2	2.28	1.50	1.46
4	C	301	KK3	C5-C4	2.26	1.43	1.39
4	J	302	KK3	C5-C4	2.26	1.43	1.39
4	E	302	KK3	C10-N2	2.26	1.50	1.46
3	A	303	NAG	C1-C2	-2.25	1.49	1.52
3	A	303	NAG	O5-C1	-2.25	1.40	1.43
4	B	303	KK3	C2-N4	2.24	1.38	1.33
4	F	304	KK3	C2-N3	2.24	1.39	1.35
4	A	304	KK3	C2-N3	2.24	1.39	1.35
4	C	301	KK3	C4-N2	2.21	1.42	1.37
3	A	303	NAG	O7-C7	-2.19	1.18	1.23
4	H	303	KK3	C2-N3	2.18	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	302	KK3	C2-N3	2.15	1.39	1.35
4	I	304	KK3	C5-C4	2.14	1.42	1.39
4	F	304	KK3	C4-N3	2.11	1.37	1.34
4	E	302	KK3	C2-N4	2.08	1.38	1.33
4	I	304	KK3	C11-C6	-2.05	1.45	1.48
4	D	304	KK3	C5-C4	2.01	1.42	1.39

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	301	NAG	C1-O5-C5	7.05	121.75	112.19
4	G	302	KK3	N3-C4-N2	-6.41	109.36	116.55
4	I	304	KK3	N3-C4-N2	-6.04	109.78	116.55
4	I	304	KK3	C5-C4-N2	5.42	128.74	122.29
3	F	303	NAG	O3-C3-C4	-5.39	97.89	110.35
3	B	302	NAG	O4-C4-C3	-5.34	98.00	110.35
4	G	302	KK3	C5-C4-N2	5.33	128.63	122.29
4	C	301	KK3	N3-C4-N2	-5.22	110.70	116.55
4	A	304	KK3	N3-C4-N2	-4.98	110.97	116.55
4	C	301	KK3	C5-C4-N2	4.89	128.10	122.29
4	D	304	KK3	C5-C4-N2	4.70	127.88	122.29
4	D	304	KK3	N3-C4-N2	-4.67	111.31	116.55
4	E	302	KK3	C5-C4-N2	4.67	127.84	122.29
3	J	301	NAG	C4-C3-C2	-4.59	104.30	111.02
4	E	302	KK3	N3-C4-N2	-4.55	111.45	116.55
4	H	303	KK3	N3-C4-N2	-4.44	111.58	116.55
4	A	304	KK3	C5-C4-N2	4.36	127.48	122.29
4	J	302	KK3	C5-C4-N2	4.30	127.40	122.29
4	H	303	KK3	C5-C4-N2	4.28	127.39	122.29
4	F	304	KK3	N3-C4-N2	-4.18	111.86	116.55
4	J	302	KK3	N3-C4-N2	-4.18	111.86	116.55
3	J	301	NAG	O3-C3-C4	-4.16	100.73	110.35
3	B	302	NAG	C1-C2-N2	-4.14	103.41	110.49
4	F	304	KK3	C5-C4-N2	4.07	127.13	122.29
3	E	301	NAG	C1-O5-C5	3.97	117.57	112.19
3	J	301	NAG	C3-C4-C5	-3.76	103.54	110.24
3	A	303	NAG	C1-O5-C5	3.36	116.75	112.19
3	A	303	NAG	O5-C1-C2	-3.18	106.26	111.29
3	H	302	NAG	O5-C5-C6	3.11	112.08	107.20
4	B	303	KK3	C5-C4-N2	3.10	125.98	122.29
3	J	301	NAG	O3-C3-C2	3.04	115.75	109.47
3	F	303	NAG	C3-C4-C5	3.00	115.59	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	301	NAG	O5-C5-C6	3.00	111.91	107.20
3	B	302	NAG	O4-C4-C5	-2.97	101.93	109.30
3	J	301	NAG	C6-C5-C4	-2.95	106.09	113.00
4	B	303	KK3	N3-C4-N2	-2.91	113.29	116.55
4	G	302	KK3	C11-C6-N1	-2.81	112.03	116.02
3	H	302	NAG	O5-C5-C4	-2.79	104.04	110.83
4	I	304	KK3	C10-N2-C1	2.71	117.50	111.52
3	H	302	NAG	O5-C1-C2	2.68	115.52	111.29
4	G	302	KK3	C5-C6-C11	2.63	125.36	121.85
4	H	303	KK3	C10-N2-C1	2.59	117.23	111.52
4	J	302	KK3	F3-C15-C14	-2.51	107.42	112.93
4	B	303	KK3	C6-C5-C4	2.49	118.67	117.03
4	E	302	KK3	C10-N2-C1	2.45	116.92	111.52
4	A	304	KK3	C10-N2-C4	-2.42	114.76	120.39
4	D	304	KK3	C10-N2-C1	2.36	116.72	111.52
3	F	303	NAG	C6-C5-C4	-2.34	107.53	113.00
4	J	302	KK3	C6-C5-C4	2.34	118.57	117.03
3	H	302	NAG	C3-C4-C5	-2.29	106.15	110.24
3	A	303	NAG	C1-C2-N2	-2.27	106.61	110.49
3	B	302	NAG	O5-C1-C2	-2.25	107.74	111.29
4	H	303	KK3	F2-C15-C14	2.22	117.81	112.93
4	D	304	KK3	C11-C6-N1	-2.22	112.87	116.02
3	F	303	NAG	O5-C5-C6	2.20	110.65	107.20
3	B	302	NAG	C2-N2-C7	2.17	126.00	122.90
4	I	304	KK3	C8-C7-C3	-2.15	107.41	112.09
3	H	302	NAG	C1-C2-N2	-2.12	106.87	110.49
3	H	302	NAG	C4-C3-C2	2.09	114.08	111.02
3	D	303	NAG	C3-C4-C5	2.08	113.95	110.24
3	G	301	NAG	C3-C4-C5	2.07	113.94	110.24
4	J	302	KK3	F1-C15-C14	2.06	117.46	112.93
4	A	304	KK3	C5-C6-C11	2.05	124.58	121.85
3	F	303	NAG	C2-N2-C7	2.03	125.80	122.90
4	G	302	KK3	C10-N2-C4	-2.02	115.70	120.39

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	NAG	C3-C2-N2-C7
3	B	302	NAG	C8-C7-N2-C2
3	B	302	NAG	O7-C7-N2-C2
3	D	303	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	D	303	NAG	O7-C7-N2-C2
3	E	301	NAG	C8-C7-N2-C2
3	E	301	NAG	O7-C7-N2-C2
3	F	303	NAG	C8-C7-N2-C2
3	F	303	NAG	O7-C7-N2-C2
3	G	301	NAG	C8-C7-N2-C2
3	G	301	NAG	O7-C7-N2-C2
3	H	302	NAG	C8-C7-N2-C2
3	H	302	NAG	O7-C7-N2-C2
3	J	301	NAG	C3-C2-N2-C7
4	A	304	KK3	C5-C4-N2-C1
4	E	302	KK3	C17-C11-C6-N1
4	H	303	KK3	C12-C11-C6-N1
4	B	303	KK3	C17-C11-C6-N1
4	C	301	KK3	C12-C11-C6-N1
4	F	304	KK3	C17-C11-C6-N1
4	J	302	KK3	C12-C11-C6-N1
4	C	301	KK3	C12-C11-C6-C5
4	E	302	KK3	C17-C11-C6-C5
4	A	304	KK3	C12-C11-C6-N1
4	A	304	KK3	C17-C11-C6-N1
4	C	301	KK3	C17-C11-C6-N1
4	D	304	KK3	C12-C11-C6-N1
4	D	304	KK3	C17-C11-C6-N1
4	E	302	KK3	C12-C11-C6-N1
4	F	304	KK3	C12-C11-C6-N1
4	G	302	KK3	C12-C11-C6-N1
4	G	302	KK3	C17-C11-C6-N1
4	H	303	KK3	C17-C11-C6-N1
4	I	304	KK3	C12-C11-C6-N1
4	I	304	KK3	C17-C11-C6-N1
4	J	302	KK3	C17-C11-C6-N1
4	A	304	KK3	C12-C11-C6-C5
4	A	304	KK3	C17-C11-C6-C5
4	B	303	KK3	C17-C11-C6-C5
4	C	301	KK3	C17-C11-C6-C5
4	D	304	KK3	C12-C11-C6-C5
4	D	304	KK3	C17-C11-C6-C5
4	E	302	KK3	C12-C11-C6-C5
4	F	304	KK3	C12-C11-C6-C5
4	G	302	KK3	C12-C11-C6-C5
4	G	302	KK3	C17-C11-C6-C5

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Mol	Chain	Res	Type	Atoms
4	H	303	KK3	C17-C11-C6-C5
4	I	304	KK3	C12-C11-C6-C5
4	I	304	KK3	C17-C11-C6-C5
4	J	302	KK3	C12-C11-C6-C5
4	J	302	KK3	C17-C11-C6-C5
4	B	303	KK3	C12-C11-C6-N1
4	F	304	KK3	C17-C11-C6-C5
4	H	303	KK3	C12-C11-C6-C5
4	B	303	KK3	C12-C11-C6-C5
3	A	303	NAG	C8-C7-N2-C2
3	A	303	NAG	O7-C7-N2-C2
3	E	301	NAG	O5-C5-C6-O6
3	H	302	NAG	O5-C5-C6-O6
3	B	302	NAG	O5-C5-C6-O6
4	A	304	KK3	N3-C4-N2-C1
4	G	302	KK3	N3-C4-N2-C1
3	D	303	NAG	O5-C5-C6-O6
4	G	302	KK3	C5-C4-N2-C1
3	G	301	NAG	O5-C5-C6-O6
3	E	301	NAG	C4-C5-C6-O6
3	I	303	NAG	C1-C2-N2-C7
3	I	303	NAG	C4-C5-C6-O6
3	J	301	NAG	O5-C5-C6-O6
3	B	302	NAG	C4-C5-C6-O6
3	I	303	NAG	O5-C5-C6-O6
3	H	302	NAG	C4-C5-C6-O6
3	D	303	NAG	C4-C5-C6-O6
3	J	301	NAG	C4-C5-C6-O6
3	D	303	NAG	C1-C2-N2-C7
3	D	303	NAG	C3-C2-N2-C7
3	G	301	NAG	C4-C5-C6-O6
3	F	303	NAG	C1-C2-N2-C7
3	G	301	NAG	C3-C2-N2-C7
3	I	303	NAG	C3-C2-N2-C7
3	A	303	NAG	C4-C5-C6-O6
3	F	303	NAG	C3-C2-N2-C7

There are no ring outliers.

16 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	KK3	1	0

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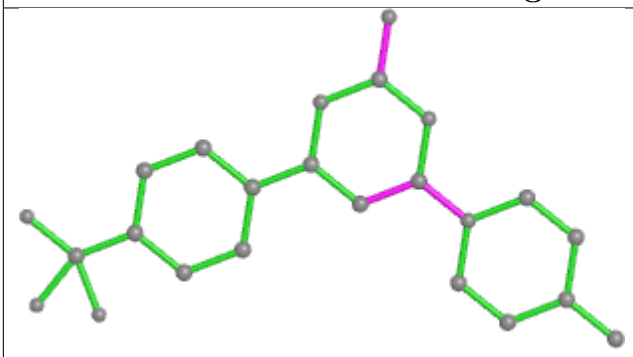
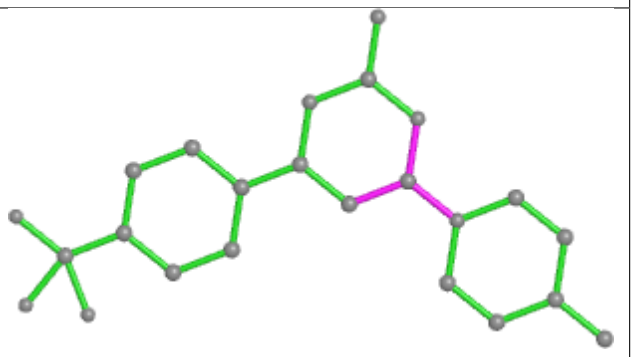
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	PO4	1	0
4	E	302	KK3	1	0
3	J	301	NAG	1	0
3	D	303	NAG	1	0
3	B	302	NAG	5	0
3	I	303	NAG	1	0
4	H	303	KK3	3	0
4	G	302	KK3	1	0
4	D	304	KK3	3	0
4	B	303	KK3	2	0
4	F	304	KK3	2	0
4	I	304	KK3	2	0
3	F	303	NAG	2	0
4	A	304	KK3	1	0
4	J	302	KK3	2	0

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

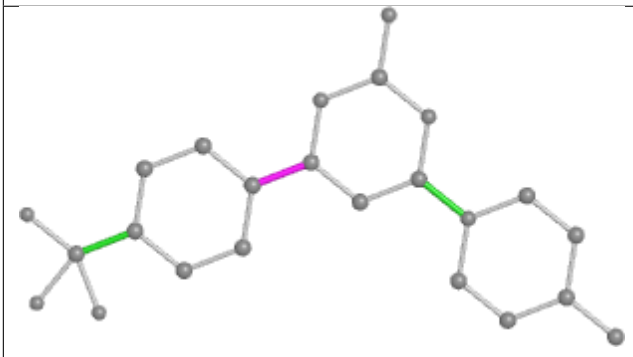
Ligand KK3 C 301



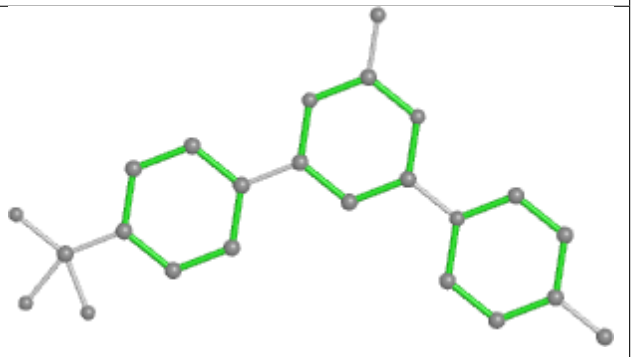
Bond lengths



Bond angles

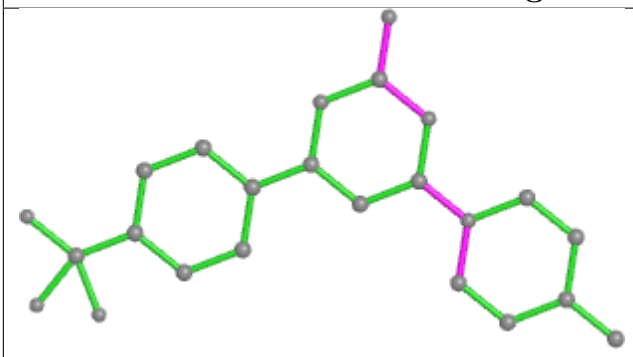


Torsions

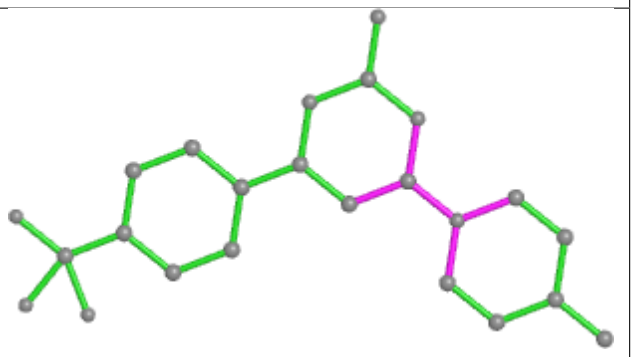


Rings

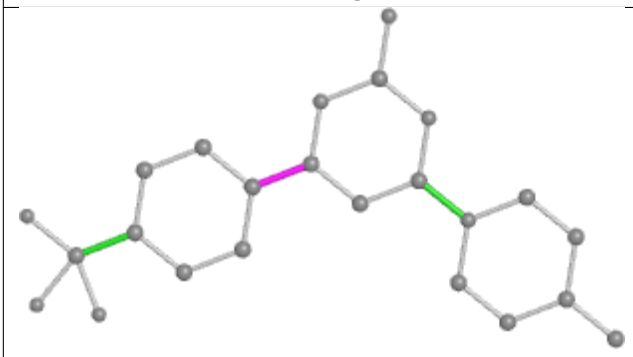
Ligand KK3 E 302



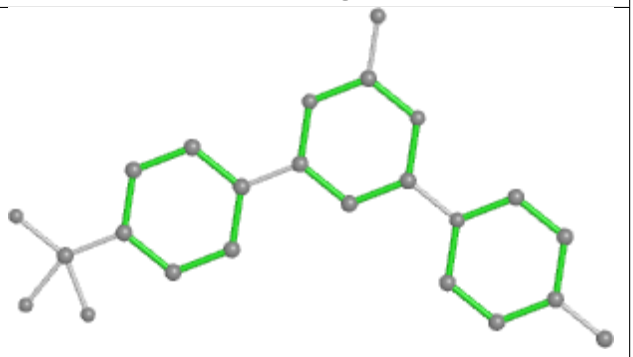
Bond lengths



Bond angles

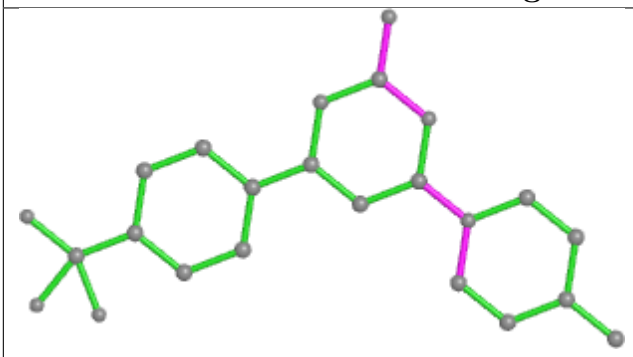


Torsions

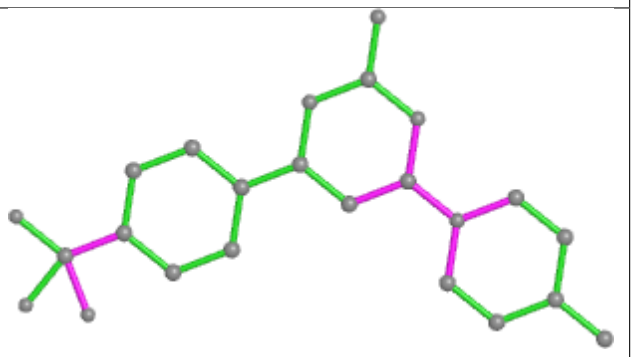


Rings

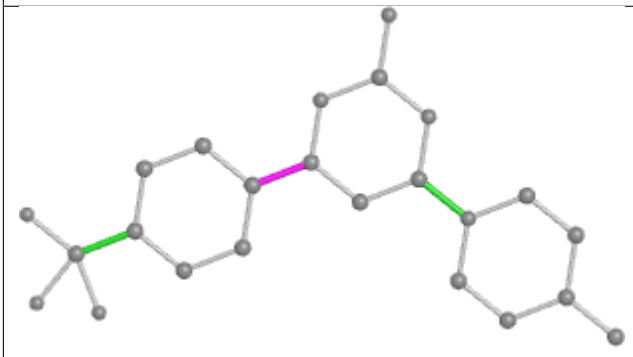
Ligand KK3 H 303



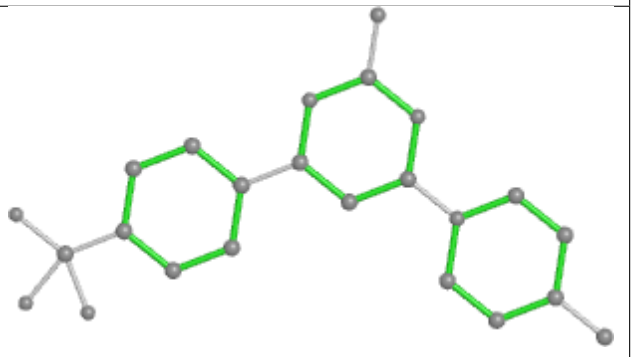
Bond lengths



Bond angles

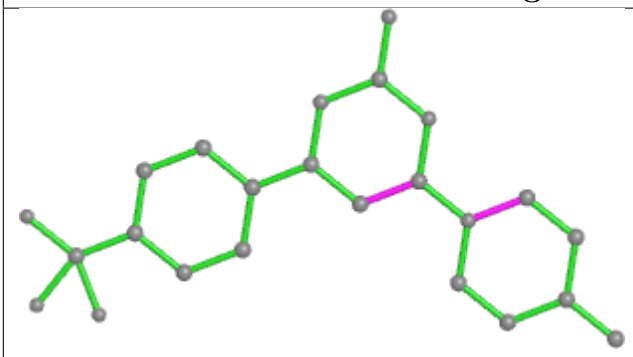


Torsions

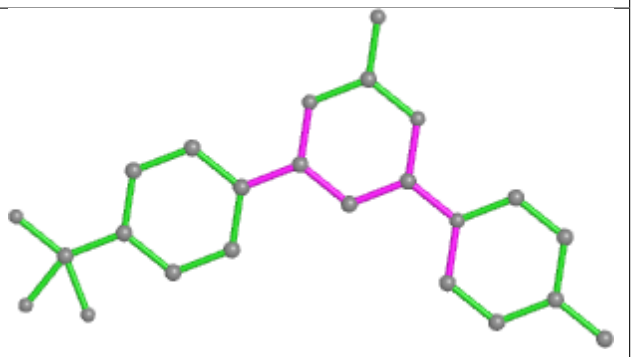


Rings

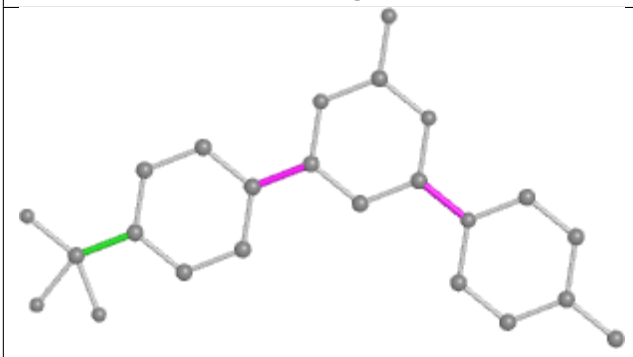
Ligand KK3 G 302



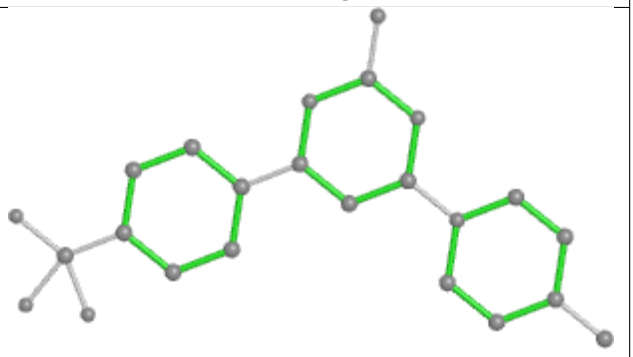
Bond lengths



Bond angles

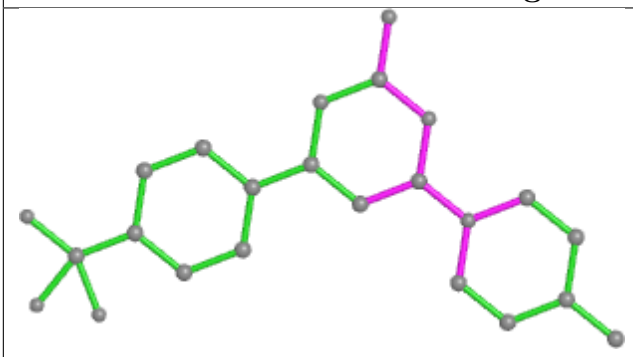


Torsions

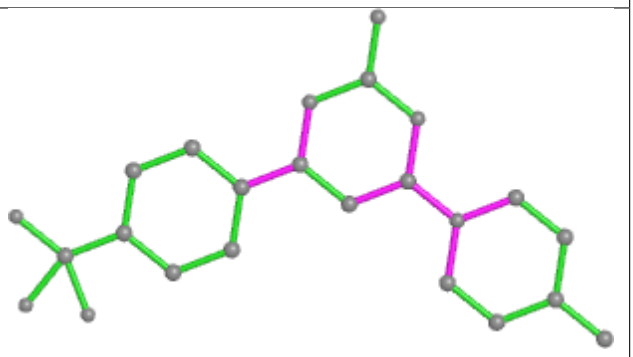


Rings

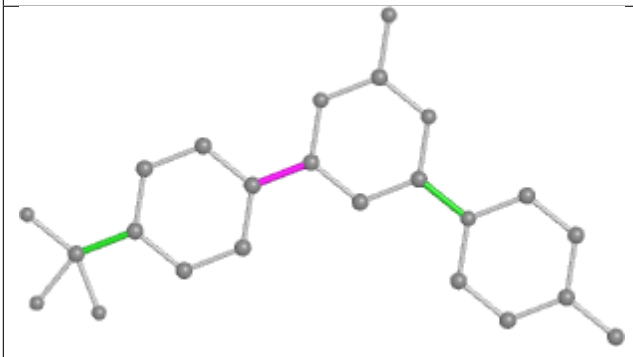
Ligand KK3 D 304



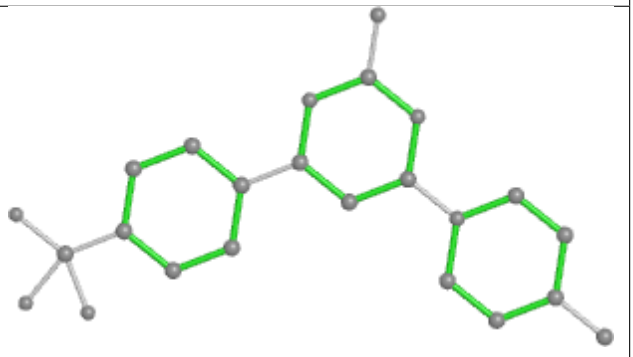
Bond lengths



Bond angles

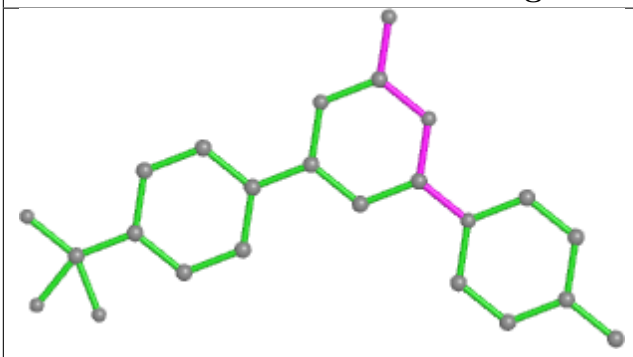


Torsions

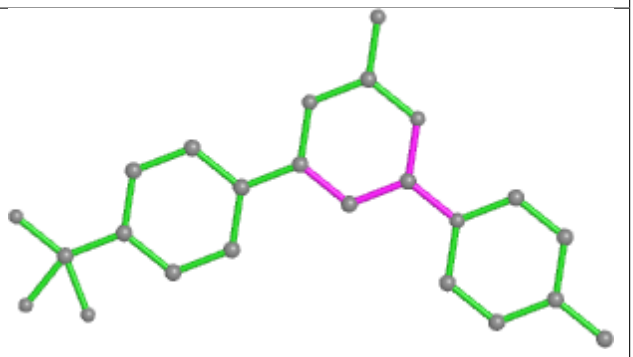


Rings

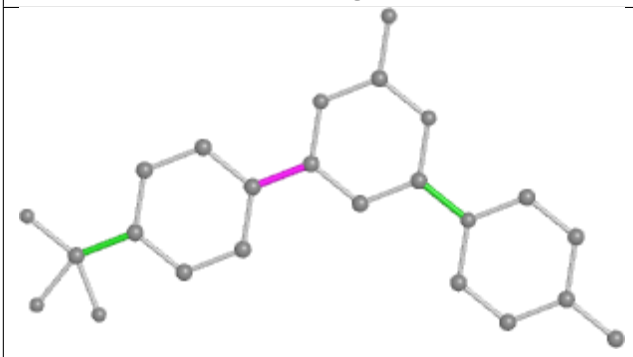
Ligand KK3 B 303



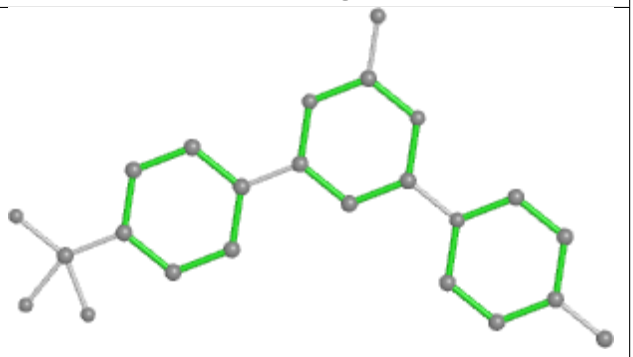
Bond lengths



Bond angles

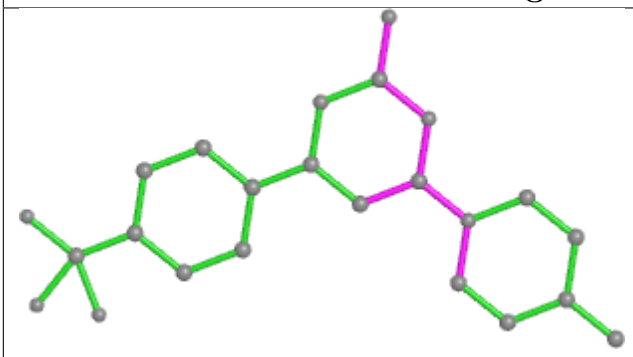


Torsions

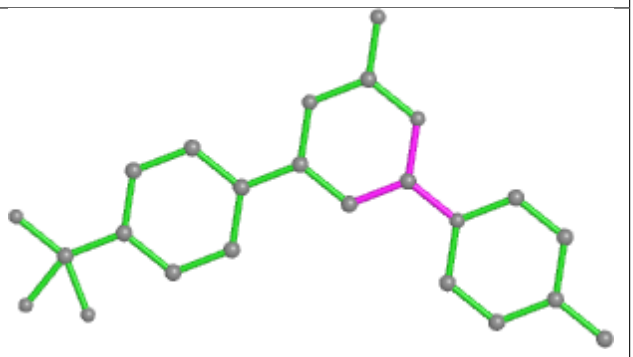


Rings

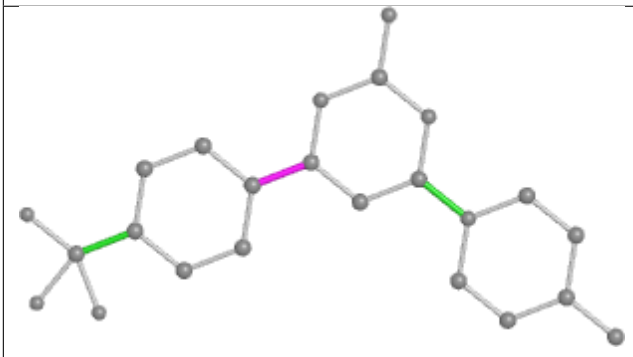
Ligand KK3 F 304



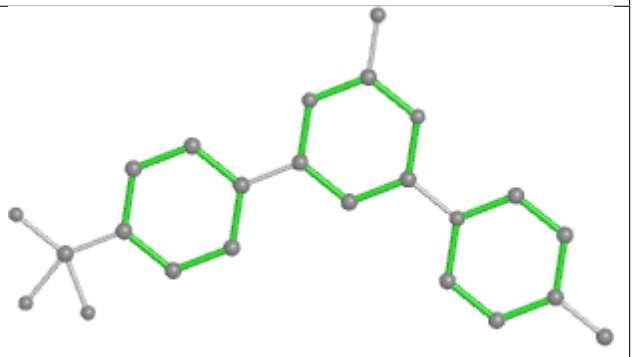
Bond lengths



Bond angles

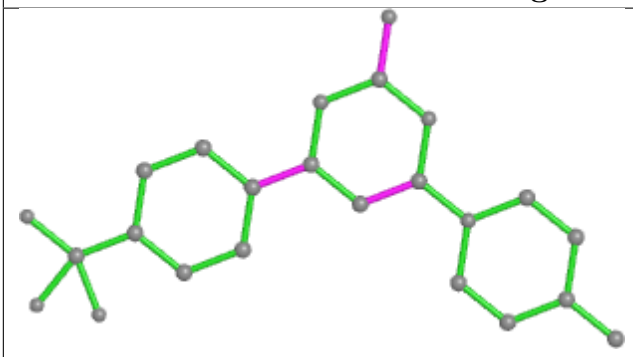


Torsions

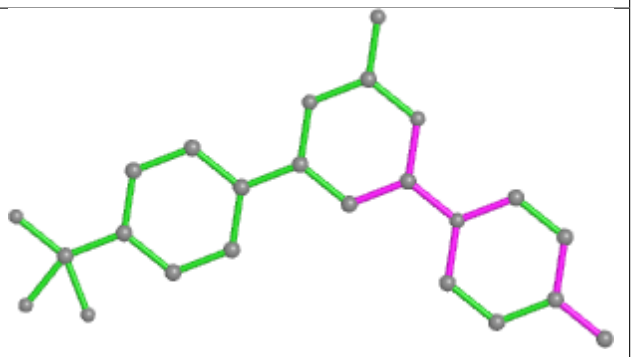


Rings

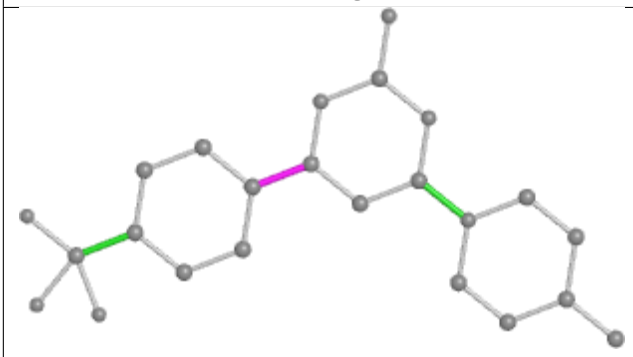
Ligand KK3 I 304



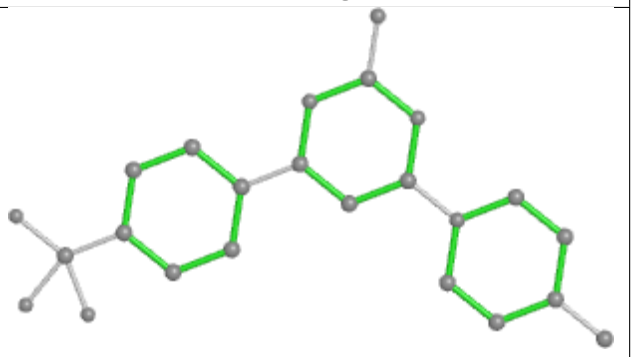
Bond lengths



Bond angles

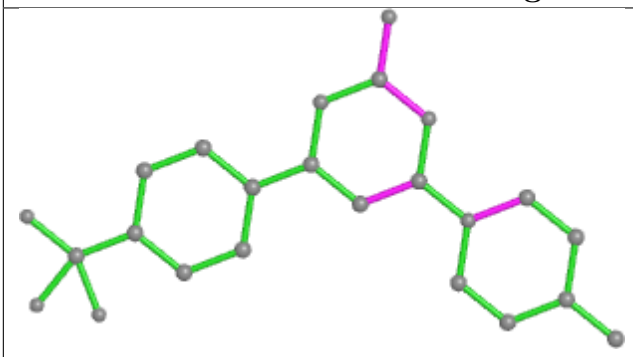


Torsions

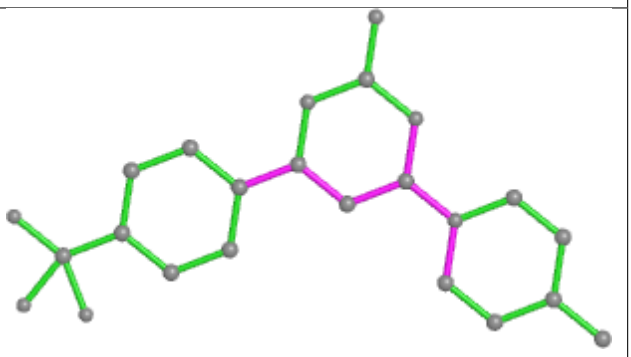


Rings

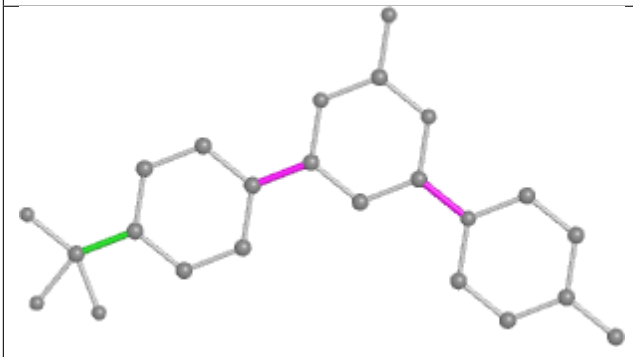
Ligand KK3 A 304



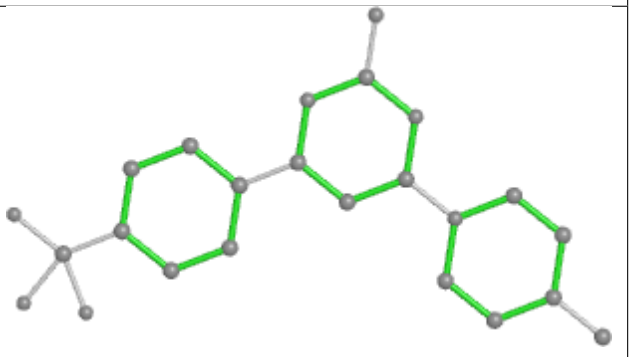
Bond lengths



Bond angles

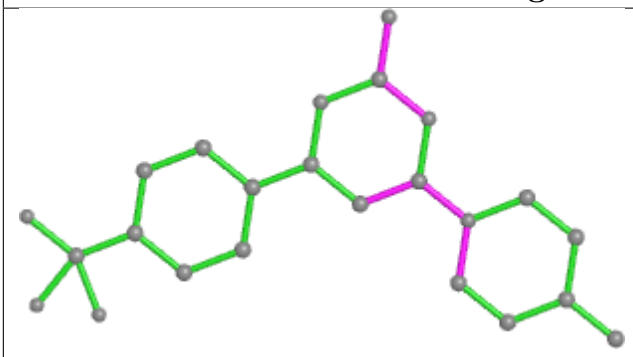


Torsions

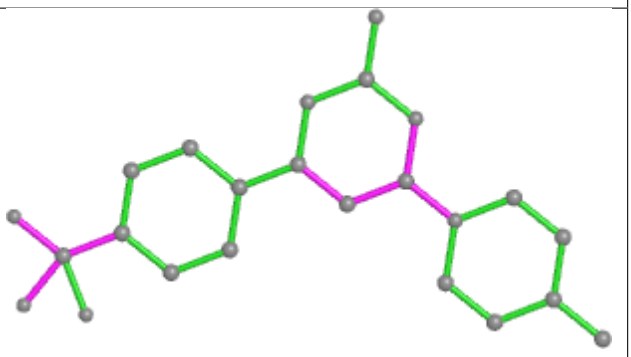


Rings

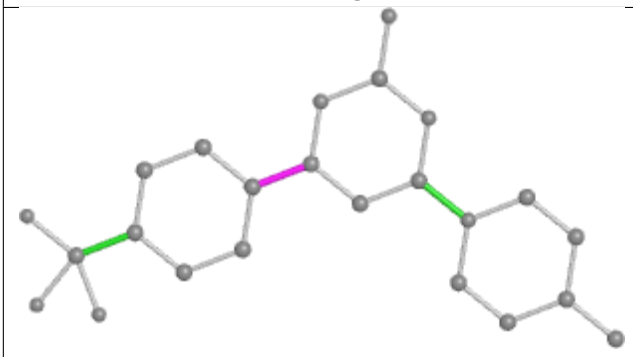
Ligand KK3 J 302



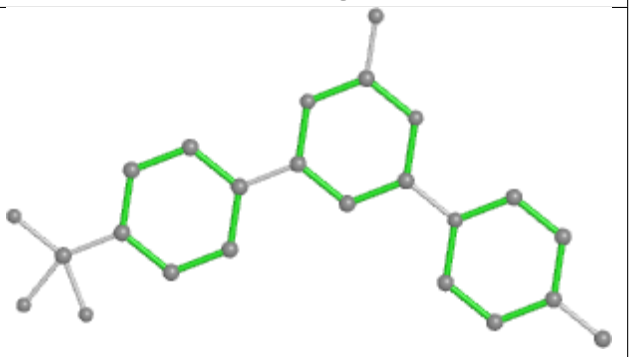
Bond lengths



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

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	209/217 (96%)	-0.04	4 (1%)	66	71	11, 24, 44, 55	0
1	B	205/217 (94%)	0.23	10 (4%)	29	35	13, 26, 46, 58	0
1	C	208/217 (95%)	-0.13	4 (1%)	66	71	11, 20, 37, 57	0
1	D	213/217 (98%)	-0.02	5 (2%)	60	65	10, 21, 41, 57	0
1	E	211/217 (97%)	-0.02	8 (3%)	40	46	11, 21, 41, 55	0
1	F	213/217 (98%)	0.09	10 (4%)	31	37	11, 21, 40, 60	0
1	G	209/217 (96%)	0.03	7 (3%)	46	53	10, 21, 46, 69	0
1	H	210/217 (96%)	-0.12	5 (2%)	59	64	9, 19, 38, 52	0
1	I	208/217 (95%)	-0.16	2 (0%)	82	85	8, 21, 39, 67	0
1	J	205/217 (94%)	0.21	9 (4%)	34	40	13, 24, 44, 64	0
All	All	2091/2170 (96%)	0.01	64 (3%)	49	55	8, 22, 42, 69	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	39	LEU	13.9
1	B	23	ARG	7.6
1	F	-6	TYR	7.2
1	H	186	SER	6.6
1	B	22	GLN	6.3
1	C	-6	TYR	6.1
1	E	199	LEU	5.7
1	G	23	ARG	5.2
1	J	187	CYS	5.2
1	J	23	ARG	5.1
1	F	199	LEU	4.9
1	G	205	GLY	4.7
1	E	-6	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	170	ARG	4.6
1	B	25	ARG	4.5
1	F	71	PRO	4.4
1	J	186	SER	4.3
1	G	162	SER	4.2
1	D	160	ASP	4.1
1	F	23	ARG	4.0
1	D	-6	TYR	3.9
1	D	209	ILE	3.5
1	D	208	GLU	3.5
1	J	189	PRO	3.5
1	J	205	GLY	3.4
1	F	-5	LYS	3.4
1	G	-6	TYR	3.3
1	B	187	CYS	3.3
1	E	205	GLY	3.3
1	G	160	ASP	3.2
1	F	38	ILE	3.2
1	B	156	THR	3.1
1	J	132	SER	3.1
1	F	40	GLU	3.0
1	H	205	GLY	2.9
1	B	154	PRO	2.8
1	H	187	CYS	2.8
1	A	-6	TYR	2.8
1	G	24	ASP	2.7
1	J	-2	ASP	2.7
1	B	174	LEU	2.7
1	A	24	ASP	2.7
1	J	179	LYS	2.7
1	G	112	LEU	2.7
1	E	157	GLU	2.6
1	H	155	THR	2.6
1	A	25	ARG	2.5
1	H	-6	TYR	2.5
1	B	26	PRO	2.4
1	B	205	GLY	2.4
1	A	129	ASP	2.4
1	I	23	ARG	2.3
1	E	158	ASN	2.3
1	C	155	THR	2.3
1	E	131	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	207	SER	2.1
1	F	69	HIS	2.1
1	F	72	ASP	2.1
1	E	200	ASN	2.1
1	E	123	CYS	2.1
1	B	24	ASP	2.1
1	I	187	CYS	2.1
1	C	-7	ASP	2.0
1	C	-5	LYS	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	H	302	14/15	0.52	0.35	39,49,57,60	0
3	NAG	D	303	14/15	0.54	0.28	52,58,63,65	0
3	NAG	F	303	14/15	0.56	0.33	51,61,70,73	0
3	NAG	B	302	14/15	0.64	0.20	57,62,72,72	0
3	NAG	G	301	14/15	0.69	0.40	50,55,60,61	0
3	NAG	E	301	14/15	0.70	0.20	58,66,71,77	0
3	NAG	J	301	14/15	0.71	0.30	43,52,60,61	0
3	NAG	I	303	14/15	0.75	0.20	24,31,38,46	0
3	NAG	A	303	14/15	0.83	0.17	24,28,36,38	0
4	KK3	B	303	24/24	0.92	0.12	15,22,28,34	0
4	KK3	A	304	24/24	0.93	0.12	15,21,27,31	0
4	KK3	G	302	24/24	0.93	0.12	10,16,22,23	0
4	KK3	I	304	24/24	0.93	0.13	14,21,28,31	0
4	KK3	D	304	24/24	0.94	0.12	12,17,26,29	0

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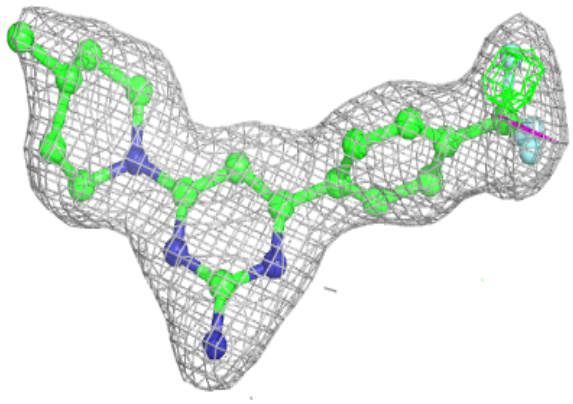
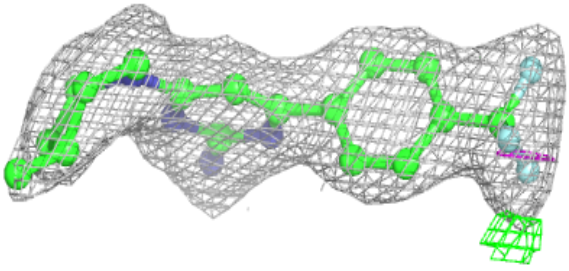
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	KK3	H	303	24/24	0.94	0.12	14,19,24,28	0
4	KK3	E	302	24/24	0.94	0.12	15,21,27,30	0
4	KK3	J	302	24/24	0.94	0.12	15,23,29,30	0
4	KK3	C	301	24/24	0.95	0.10	13,17,22,24	0
4	KK3	F	304	24/24	0.95	0.10	14,20,25,31	0
2	PO4	A	302	5/5	0.98	0.14	20,21,23,23	0
2	PO4	B	301	5/5	0.99	0.11	13,16,17,18	0
2	PO4	D	301	5/5	0.99	0.10	11,12,13,14	0
2	PO4	D	302	5/5	0.99	0.11	11,11,15,17	0
2	PO4	F	301	5/5	0.99	0.09	14,14,17,17	0
2	PO4	F	302	5/5	0.99	0.10	10,13,16,16	0
2	PO4	H	301	5/5	0.99	0.11	10,11,14,15	0
2	PO4	I	301	5/5	0.99	0.10	9,10,12,13	0
2	PO4	I	302	5/5	0.99	0.11	15,18,20,20	0
2	PO4	A	301	5/5	0.99	0.11	12,12,16,16	0

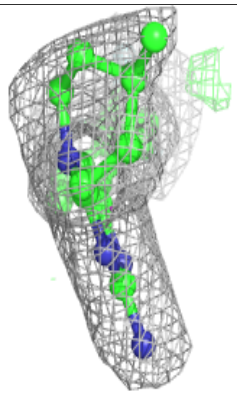
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KK3 B 303:

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

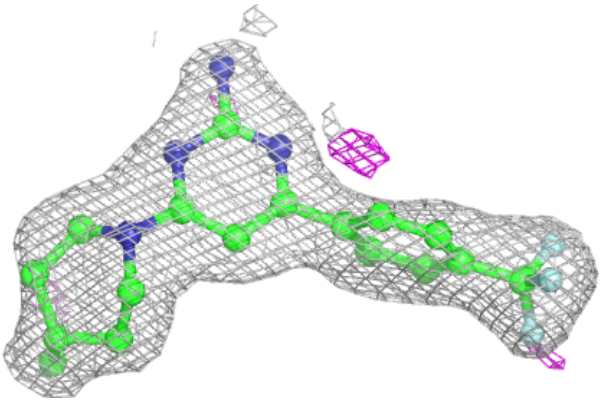


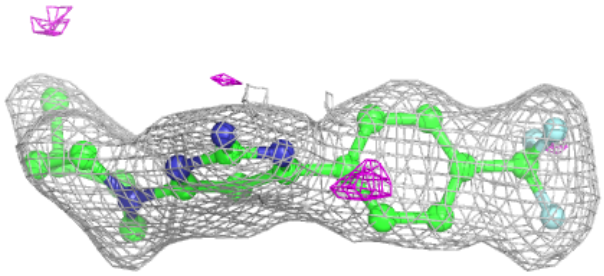


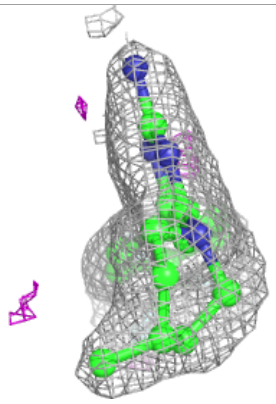


Electron density around KK3 A 304:

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

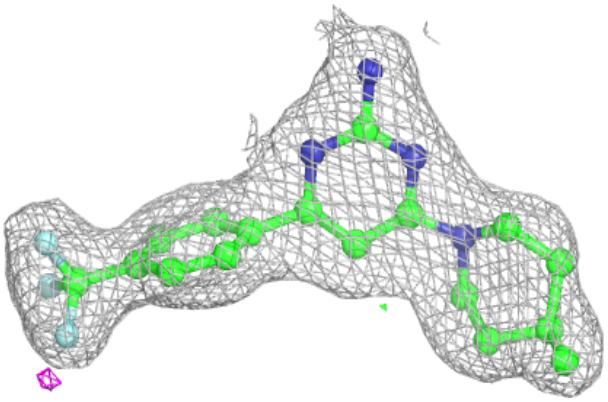


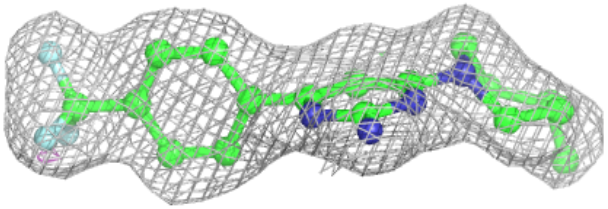


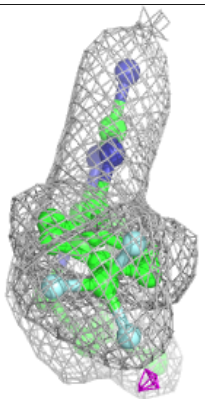


Electron density around KK3 G 302:

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

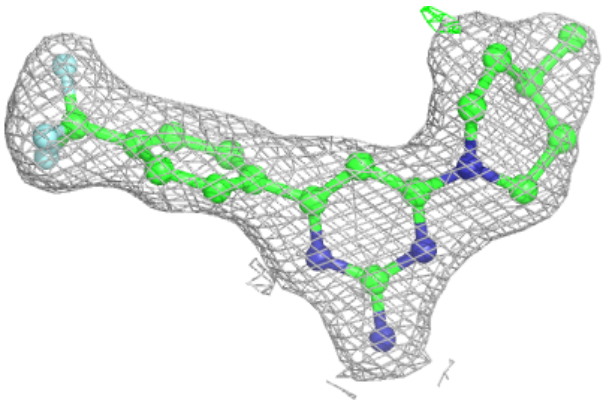


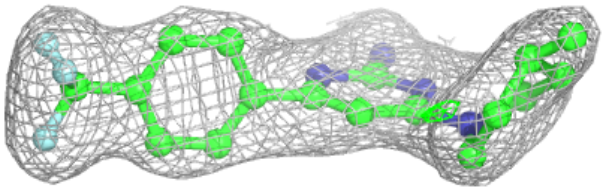


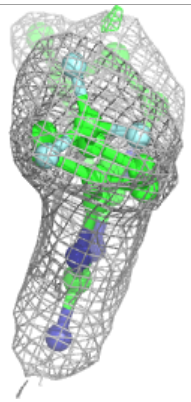


Electron density around KK3 I 304:

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

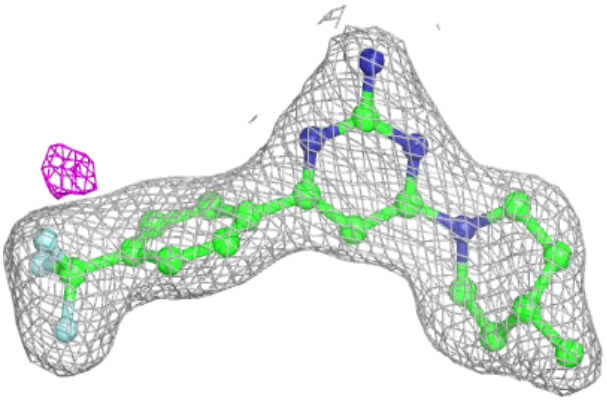


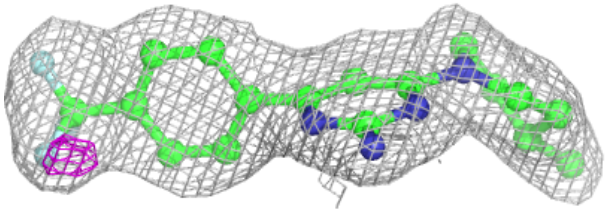


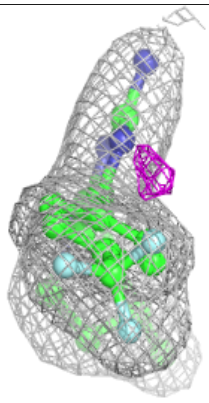


Electron density around KK3 D 304:

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

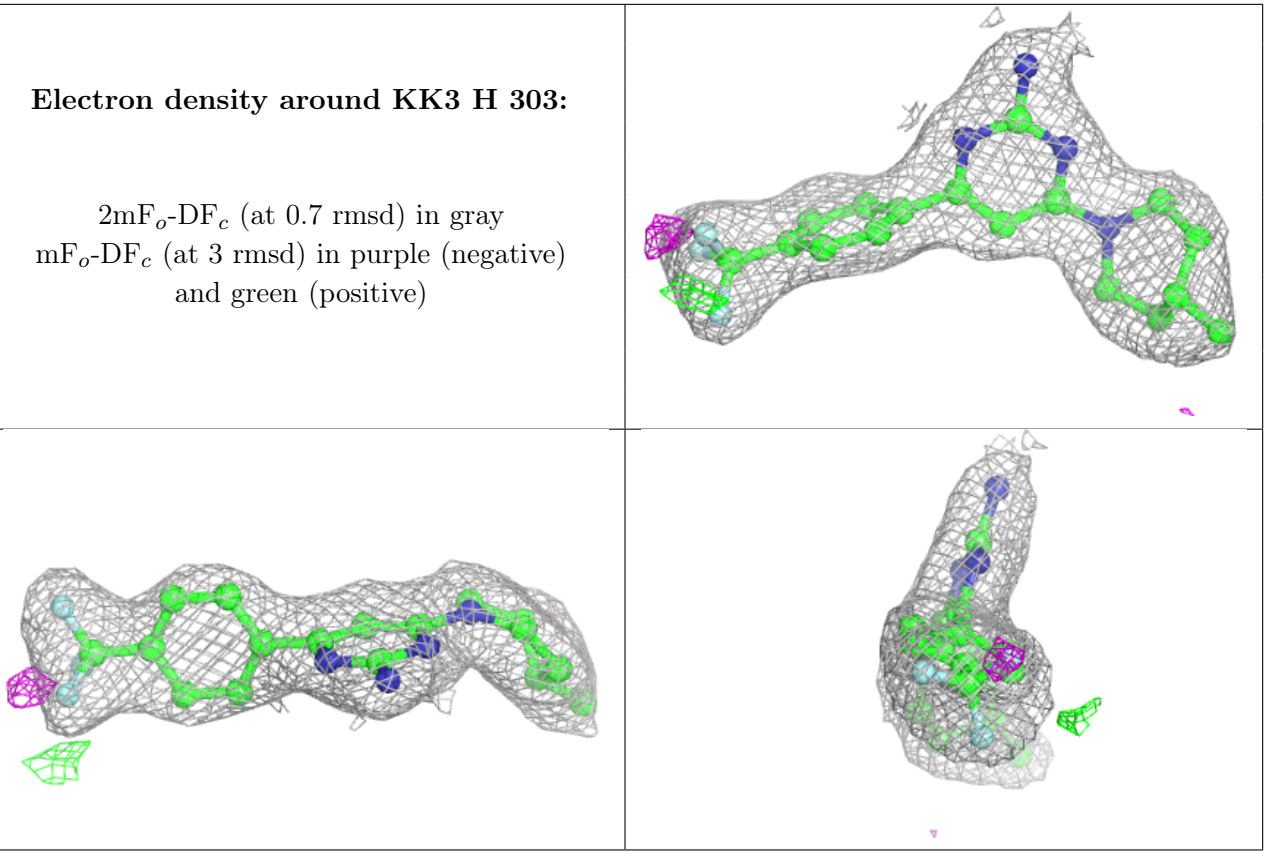






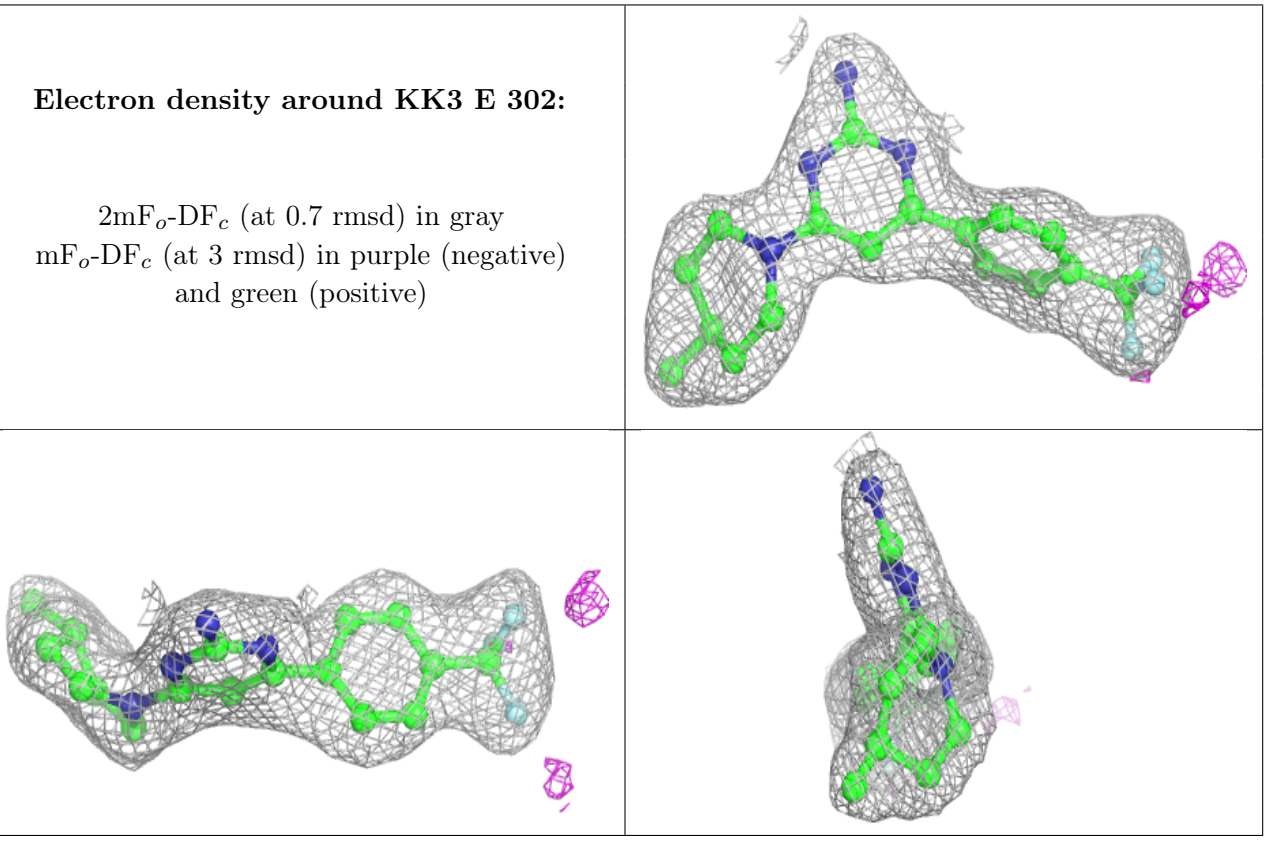
Electron density around KK3 H 303:

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



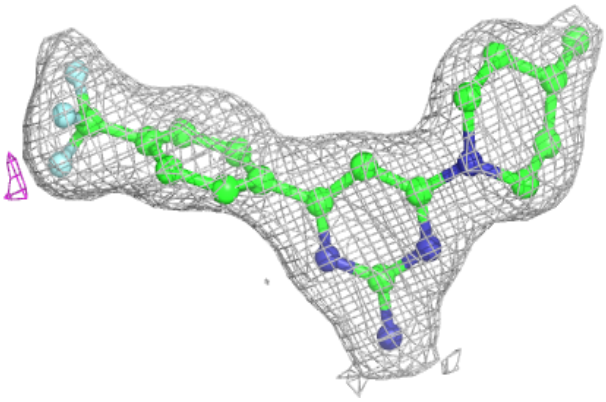
Electron density around KK3 E 302:

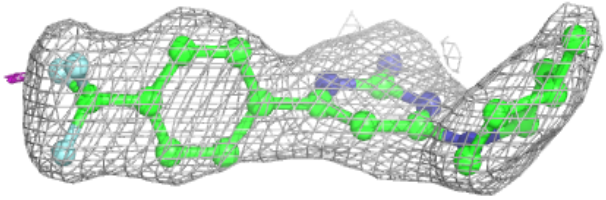
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

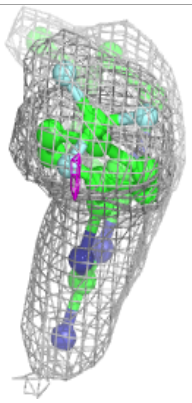


Electron density around KK3 J 302:

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

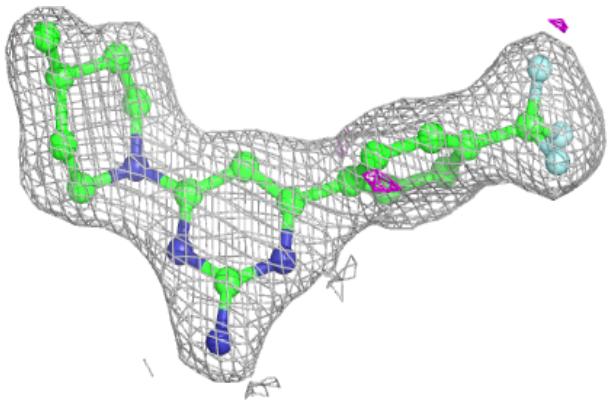


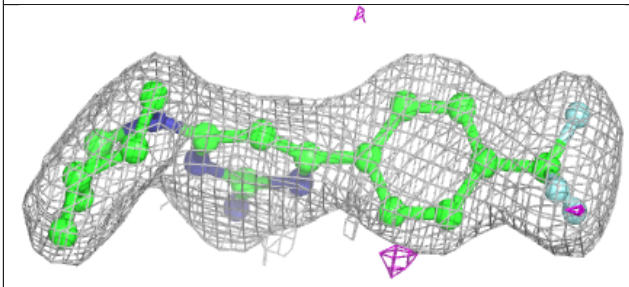


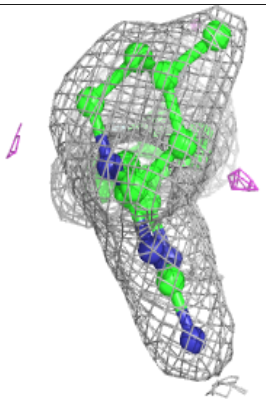


Electron density around KK3 C 301:

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

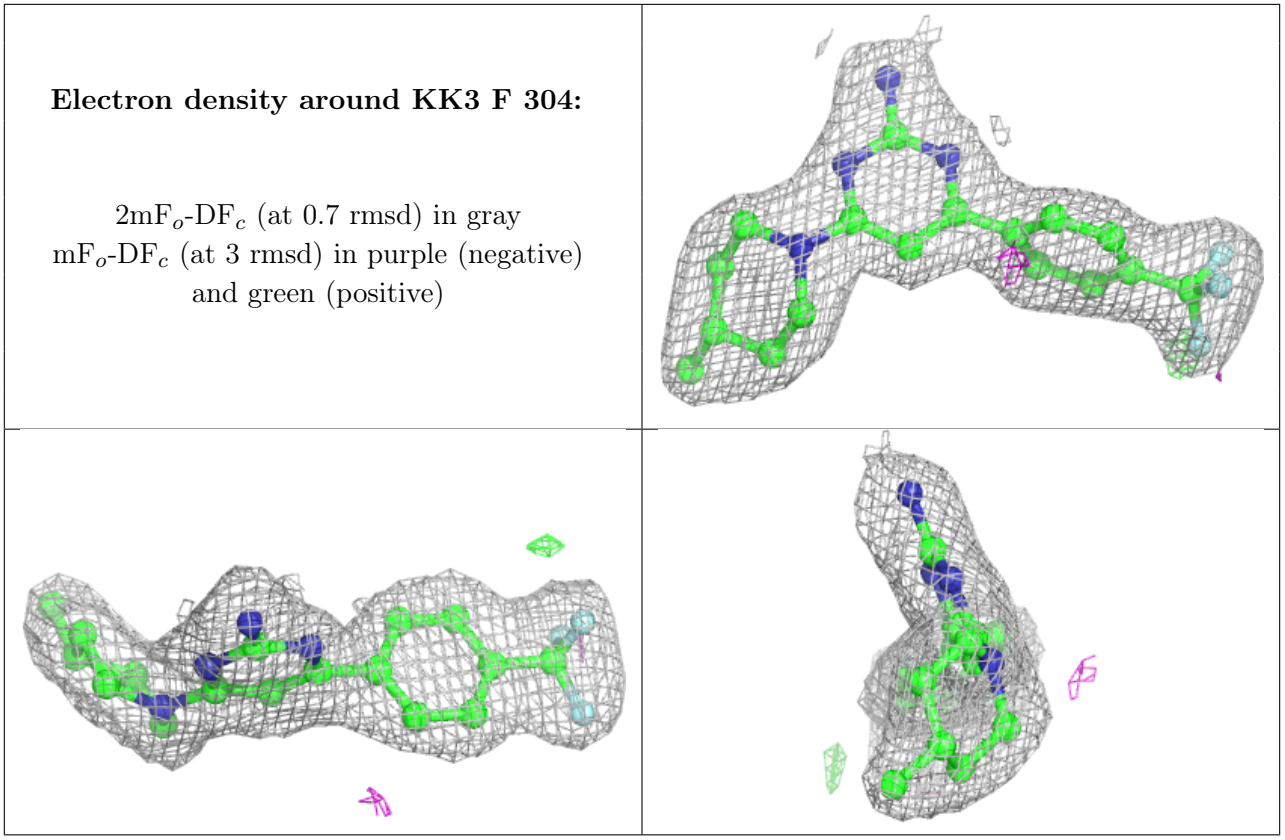






Electron density around KK3 F 304:

$2mF_o$-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.