wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 10:46 am BST

PDB ID	:	5ETY
Title	:	Crystal Structure of human Tankyrase-1 bound to K-756
Authors	:	Takahashi, Y.; Miyagi, H.; Suzuki, M.; Saito, J.
Deposited on	:	2015-11-18
Resolution	:	2.90 Å(reported)

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

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

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

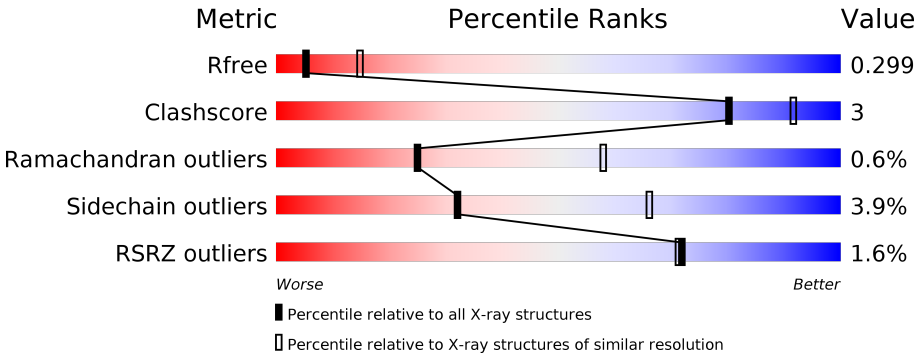
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	257	% 71% 9% • 19%
1	B	257	3% 72% 7% 21%
1	C	257	% 71% 7% • 21%
1	D	257	70% 9% 21%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	1401	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6777 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 Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1662	1048	301	302	11			
1	B	203	Total	C	N	O	S	0	0	0
			1622	1026	293	293	10			
1	C	203	Total	C	N	O	S	0	0	0
			1639	1036	300	293	10			
1	D	204	Total	C	N	O	S	0	0	0
			1648	1041	301	296	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1068	MET	-	initiating methionine	UNP O95271
A	1069	HIS	-	expression tag	UNP O95271
A	1070	HIS	-	expression tag	UNP O95271
A	1071	HIS	-	expression tag	UNP O95271
A	1072	HIS	-	expression tag	UNP O95271
A	1073	HIS	-	expression tag	UNP O95271
A	1074	HIS	-	expression tag	UNP O95271
A	1075	SER	-	expression tag	UNP O95271
A	1076	SER	-	expression tag	UNP O95271
A	1077	GLY	-	expression tag	UNP O95271
A	1078	VAL	-	expression tag	UNP O95271
A	1079	ASP	-	expression tag	UNP O95271
A	1080	LEU	-	expression tag	UNP O95271
A	1081	GLY	-	expression tag	UNP O95271
A	1082	THR	-	expression tag	UNP O95271
A	1083	GLU	-	expression tag	UNP O95271
A	1084	ASN	-	expression tag	UNP O95271
A	1085	LEU	-	expression tag	UNP O95271
A	1086	TYR	-	expression tag	UNP O95271
A	1087	PHE	-	expression tag	UNP O95271
A	1088	GLN	-	expression tag	UNP O95271

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1089	SER	-	expression tag	UNP O95271
A	1090	MET	-	expression tag	UNP O95271
A	1266	ILE	MET	engineered mutation	UNP O95271
B	1068	MET	-	initiating methionine	UNP O95271
B	1069	HIS	-	expression tag	UNP O95271
B	1070	HIS	-	expression tag	UNP O95271
B	1071	HIS	-	expression tag	UNP O95271
B	1072	HIS	-	expression tag	UNP O95271
B	1073	HIS	-	expression tag	UNP O95271
B	1074	HIS	-	expression tag	UNP O95271
B	1075	SER	-	expression tag	UNP O95271
B	1076	SER	-	expression tag	UNP O95271
B	1077	GLY	-	expression tag	UNP O95271
B	1078	VAL	-	expression tag	UNP O95271
B	1079	ASP	-	expression tag	UNP O95271
B	1080	LEU	-	expression tag	UNP O95271
B	1081	GLY	-	expression tag	UNP O95271
B	1082	THR	-	expression tag	UNP O95271
B	1083	GLU	-	expression tag	UNP O95271
B	1084	ASN	-	expression tag	UNP O95271
B	1085	LEU	-	expression tag	UNP O95271
B	1086	TYR	-	expression tag	UNP O95271
B	1087	PHE	-	expression tag	UNP O95271
B	1088	GLN	-	expression tag	UNP O95271
B	1089	SER	-	expression tag	UNP O95271
B	1090	MET	-	expression tag	UNP O95271
B	1266	ILE	MET	engineered mutation	UNP O95271
C	1068	MET	-	initiating methionine	UNP O95271
C	1069	HIS	-	expression tag	UNP O95271
C	1070	HIS	-	expression tag	UNP O95271
C	1071	HIS	-	expression tag	UNP O95271
C	1072	HIS	-	expression tag	UNP O95271
C	1073	HIS	-	expression tag	UNP O95271
C	1074	HIS	-	expression tag	UNP O95271
C	1075	SER	-	expression tag	UNP O95271
C	1076	SER	-	expression tag	UNP O95271
C	1077	GLY	-	expression tag	UNP O95271
C	1078	VAL	-	expression tag	UNP O95271
C	1079	ASP	-	expression tag	UNP O95271
C	1080	LEU	-	expression tag	UNP O95271
C	1081	GLY	-	expression tag	UNP O95271
C	1082	THR	-	expression tag	UNP O95271

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1083	GLU	-	expression tag	UNP O95271
C	1084	ASN	-	expression tag	UNP O95271
C	1085	LEU	-	expression tag	UNP O95271
C	1086	TYR	-	expression tag	UNP O95271
C	1087	PHE	-	expression tag	UNP O95271
C	1088	GLN	-	expression tag	UNP O95271
C	1089	SER	-	expression tag	UNP O95271
C	1090	MET	-	expression tag	UNP O95271
C	1266	ILE	MET	engineered mutation	UNP O95271
D	1068	MET	-	initiating methionine	UNP O95271
D	1069	HIS	-	expression tag	UNP O95271
D	1070	HIS	-	expression tag	UNP O95271
D	1071	HIS	-	expression tag	UNP O95271
D	1072	HIS	-	expression tag	UNP O95271
D	1073	HIS	-	expression tag	UNP O95271
D	1074	HIS	-	expression tag	UNP O95271
D	1075	SER	-	expression tag	UNP O95271
D	1076	SER	-	expression tag	UNP O95271
D	1077	GLY	-	expression tag	UNP O95271
D	1078	VAL	-	expression tag	UNP O95271
D	1079	ASP	-	expression tag	UNP O95271
D	1080	LEU	-	expression tag	UNP O95271
D	1081	GLY	-	expression tag	UNP O95271
D	1082	THR	-	expression tag	UNP O95271
D	1083	GLU	-	expression tag	UNP O95271
D	1084	ASN	-	expression tag	UNP O95271
D	1085	LEU	-	expression tag	UNP O95271
D	1086	TYR	-	expression tag	UNP O95271
D	1087	PHE	-	expression tag	UNP O95271
D	1088	GLN	-	expression tag	UNP O95271
D	1089	SER	-	expression tag	UNP O95271
D	1090	MET	-	expression tag	UNP O95271
D	1266	ILE	MET	engineered mutation	UNP O95271

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

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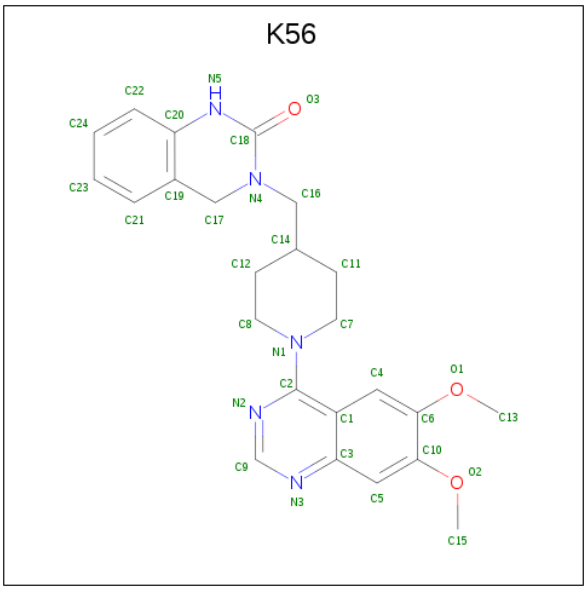
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 3-[[1-(6,7-dimethoxyquinazolin-4-yl)piperidin-4-yl]methyl]-1,4-dihydroquinazolin-2-one (three-letter code: K56) (formula: $C_{24}H_{27}N_5O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 32 24 5 3	0	0
3	B	1	Total C N O 32 24 5 3	0	0
3	C	1	Total C N O 32 24 5 3	0	0
3	D	1	Total C N O 32 24 5 3	0	0

- Molecule 4 is water.

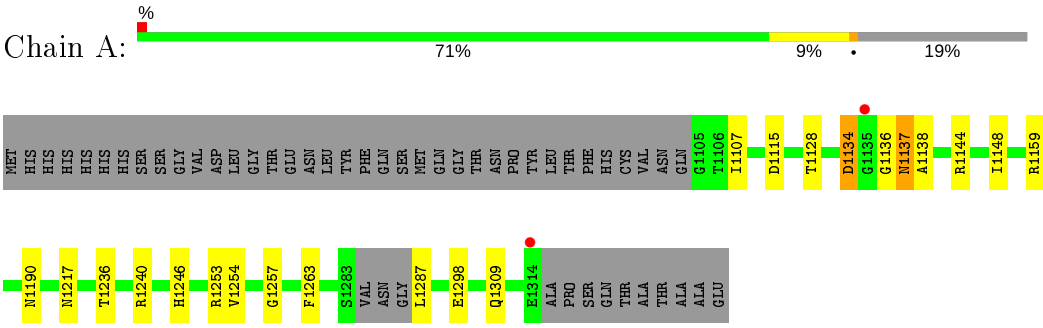
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	20	Total O 20 20	0	0
4	B	20	Total O 20 20	0	0
4	C	15	Total O 15 15	0	0
4	D	19	Total O 19 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

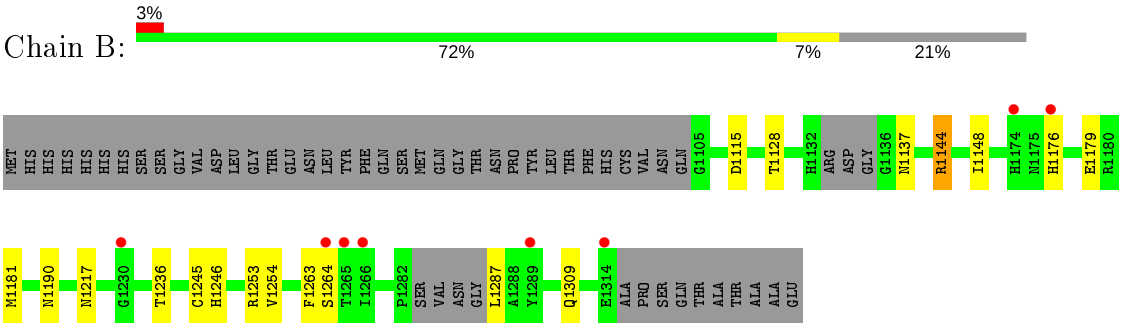
- Molecule 1: Tankyrase-1

Chain A:



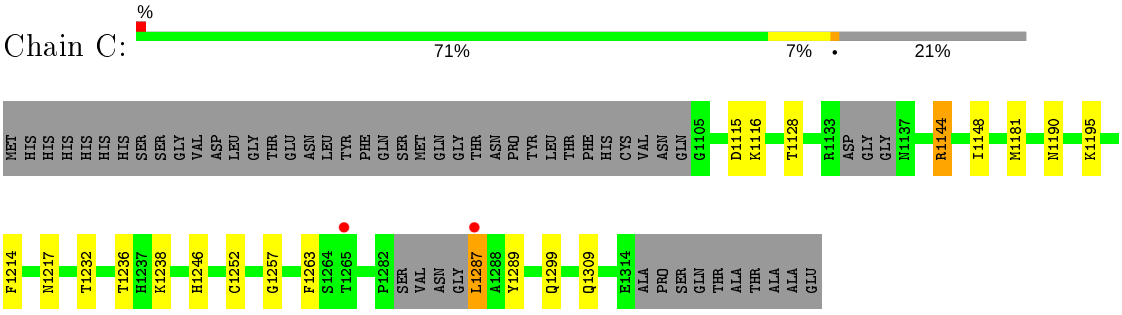
- Molecule 1: Tankyrase-1

Chain B:



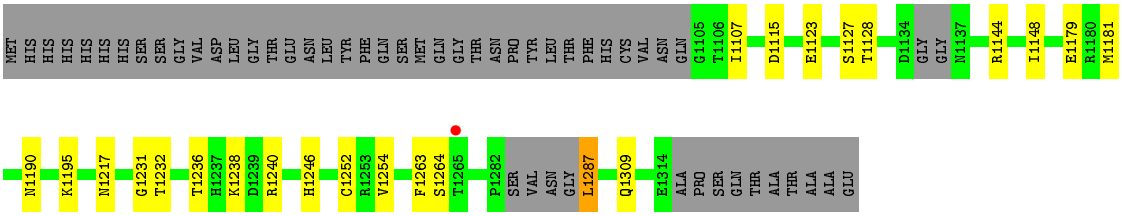
- Molecule 1: Tankyrase-1

Chain C:



- Molecule 1: Tankyrase-1

Chain D:


MET HIS HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET GLN GLY THR ASN PRO TYR LEU THR PHE HIS CYS VAL ASN GLN G1105 T1106 I1107 D1115 E1123 S1127 T1128 D1134 GLY GLY N1137 R1144 I1148 E1179 R1180 M1181
N1190 K1195 N1217 G1231 T1232 T1236 H1237 K1238 D1239 R1240 H1246 C1252 R1253 V1254 F1263 S1264 T1265 P1282 SER VAL ASN GLY L1287 Q1309 E1314 ALA PRO SER GLN THR ALA THR ALA ALA GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	158.85Å 74.68Å 84.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 30.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.8 (50.00-2.90) 92.0 (30.22-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.255 , 0.305 0.257 , 0.299	Depositor DCC
R_{free} test set	1098 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.985	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 29.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6777	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1135e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: K56, ZN

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	0.58	0/1704	0.77	0/2292
1	B	0.58	0/1663	0.73	1/2239 (0.0%)
1	C	0.56	0/1680	0.77	2/2259 (0.1%)
1	D	0.57	0/1689	0.74	0/2271
All	All	0.57	0/6736	0.75	3/9061 (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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1144	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	1144	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	1144	ARG	NE-CZ-NH2	6.38	123.49	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1134	ASP	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	1662	0	1588	8	0
1	B	1622	0	1540	8	0
1	C	1639	0	1571	10	0
1	D	1648	0	1577	11	0
2	A	1	0	0	0	0
2	B	1	0	0	2	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
3	C	32	0	0	0	0
3	D	32	0	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
4	C	15	0	0	1	0
4	D	19	0	0	1	0
All	All	6777	0	6276	35	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 3.

The worst 5 of 35 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:B:1245:CYS:HG	2:B:1401:ZN:ZN	0.87	0.87
1:D:1232:THR:HG22	4:D:1518:HOH:O	1.84	0.77
1:B:1245:CYS:SG	2:B:1401:ZN:ZN	1.77	0.73
1:A:1148:ILE:HD13	1:A:1246:HIS:CE1	2.34	0.63
1:A:1138:ALA:HA	1:A:1240:ARG:HD2	1.81	0.63

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	203/257 (79%)	197 (97%)	3 (2%)	3 (2%)	10	34
1	B	197/257 (77%)	193 (98%)	3 (2%)	1 (0%)	29	61
1	C	197/257 (77%)	189 (96%)	7 (4%)	1 (0%)	29	61
1	D	198/257 (77%)	192 (97%)	6 (3%)	0	100	100
All	All	795/1028 (77%)	771 (97%)	19 (2%)	5 (1%)	25	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1137	ASN
1	B	1137	ASN
1	A	1136	GLY
1	A	1257	GLY
1	C	1257	GLY

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	174/218 (80%)	167 (96%)	7 (4%)	31	65
1	B	168/218 (77%)	162 (96%)	6 (4%)	35	69
1	C	171/218 (78%)	164 (96%)	7 (4%)	30	64
1	D	172/218 (79%)	165 (96%)	7 (4%)	30	64
All	All	685/872 (79%)	658 (96%)	27 (4%)	32	66

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1309	GLN
1	C	1144	ARG
1	D	1264	SER
1	C	1115	ASP
1	A	1236	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1217	ASN
1	C	1132	HIS
1	C	1246	HIS
1	B	1143	ASN
1	C	1217	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	K56	D	1402	-	35,36,36	1.16	5 (14%)	49,51,51	1.63	11 (22%)
3	K56	B	1402	-	35,36,36	1.00	3 (8%)	49,51,51	1.63	10 (20%)
3	K56	C	1402	-	35,36,36	1.17	3 (8%)	49,51,51	1.67	11 (22%)
3	K56	A	1402	-	35,36,36	1.04	3 (8%)	49,51,51	1.76	7 (14%)

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	K56	D	1402	-	-	2/12/34/34	0/5/5/5
3	K56	B	1402	-	-	3/12/34/34	0/5/5/5
3	K56	C	1402	-	-	6/12/34/34	0/5/5/5
3	K56	A	1402	-	-	6/12/34/34	0/5/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1402	K56	C18-N5	-3.33	1.32	1.36
3	A	1402	K56	C5-C10	3.08	1.42	1.36
3	D	1402	K56	C18-N5	-3.06	1.32	1.36
3	D	1402	K56	C4-C6	3.05	1.42	1.36
3	A	1402	K56	C4-C6	2.47	1.41	1.36

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1402	K56	C14-C16-N4	-5.28	105.43	113.80
3	C	1402	K56	C14-C16-N4	-5.00	105.87	113.80
3	A	1402	K56	C15-O2-C10	4.80	124.77	117.53
3	D	1402	K56	C14-C16-N4	-4.68	106.37	113.80
3	B	1402	K56	C14-C16-N4	-4.40	106.82	113.80

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1402	K56	N2-C2-N1-C7
3	C	1402	K56	C1-C2-N1-C7

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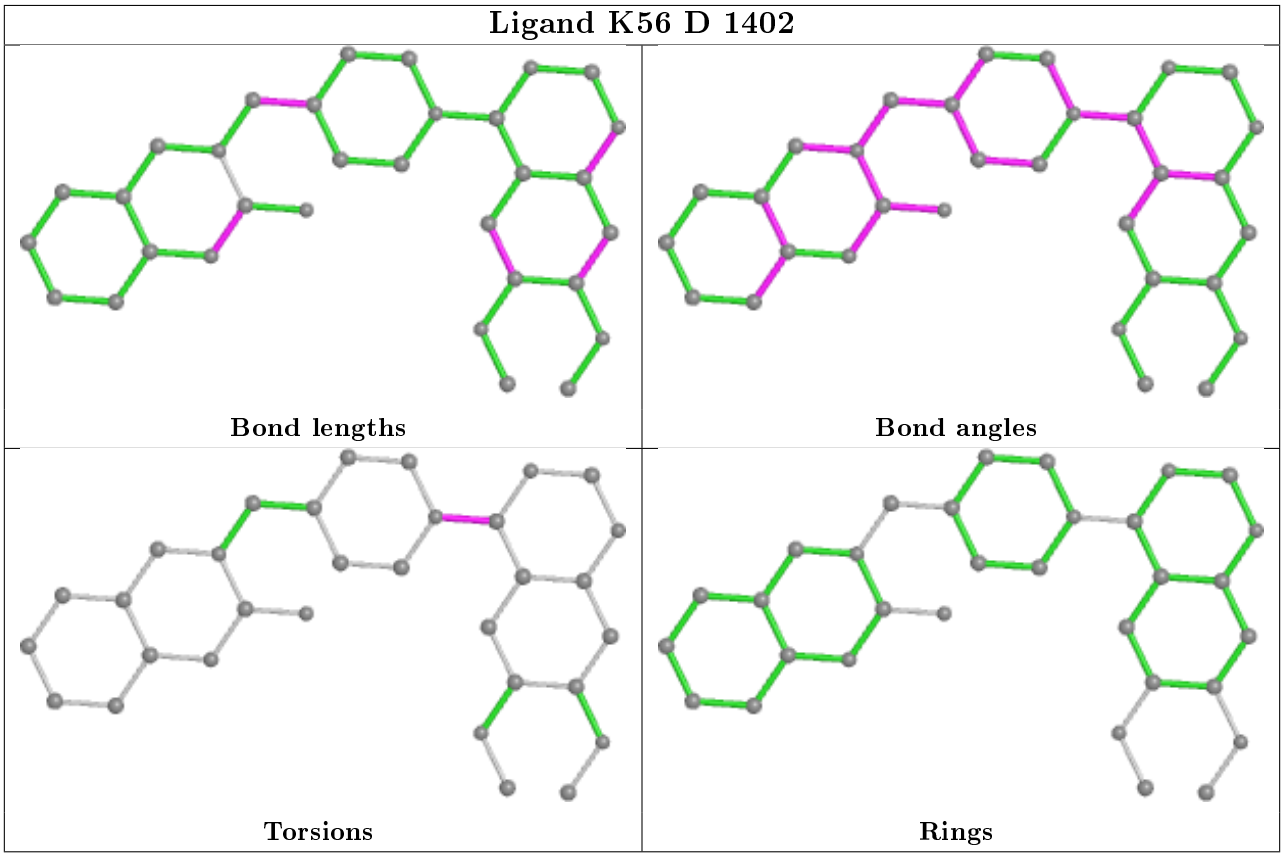
Mol	Chain	Res	Type	Atoms
3	D	1402	K56	N2-C2-N1-C7
3	D	1402	K56	C1-C2-N1-C7
3	B	1402	K56	N2-C2-N1-C7

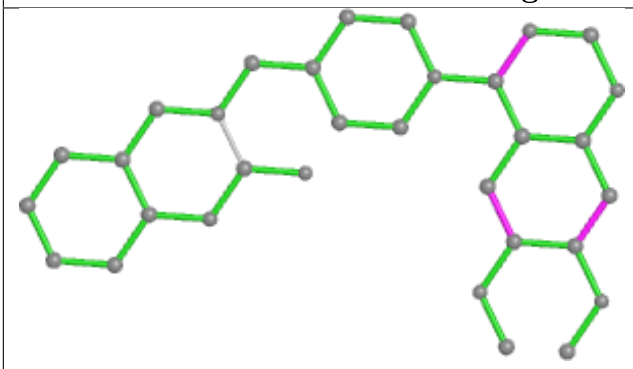
There are no ring outliers.

No monomer is involved in short contacts.

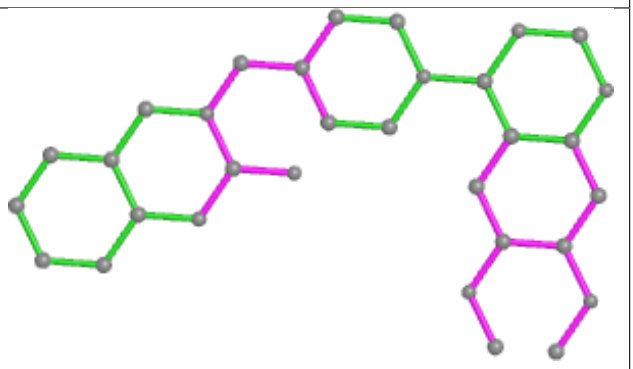
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



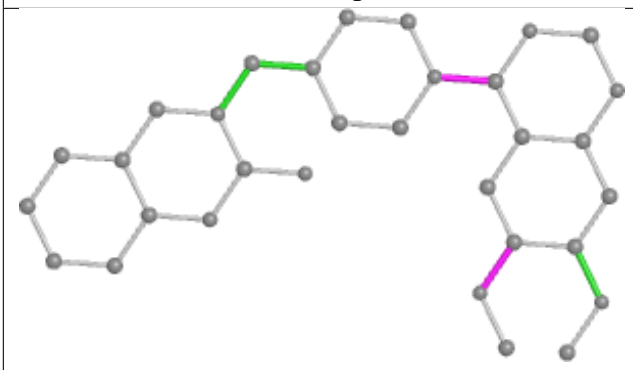
Ligand K56 B 1402



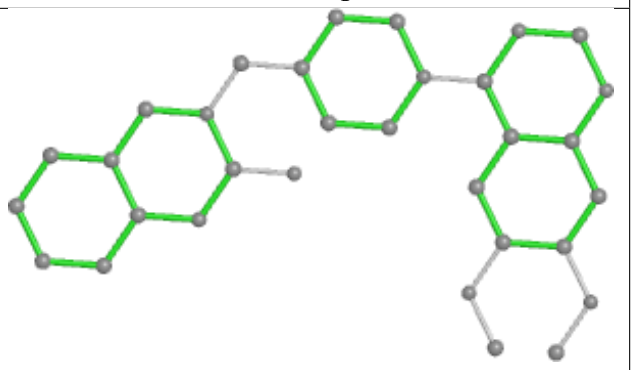
Bond lengths



Bond angles

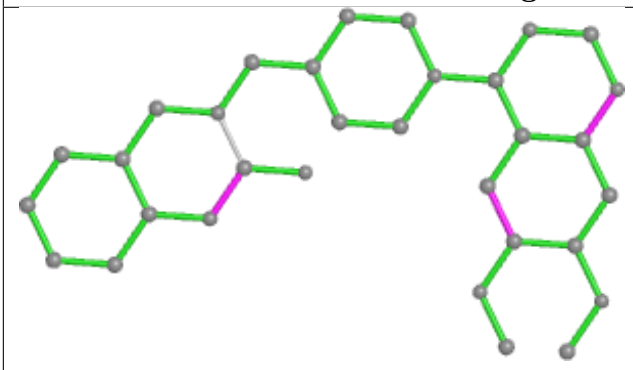


Torsions

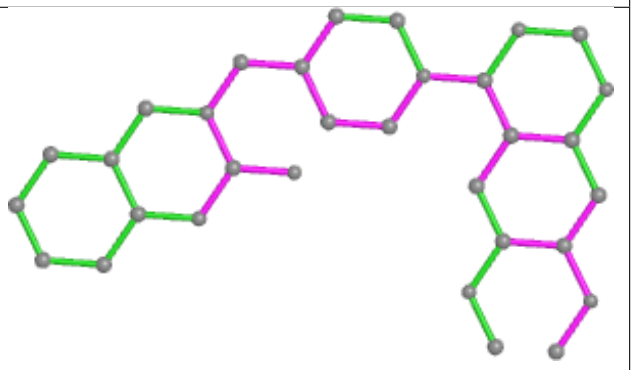


Rings

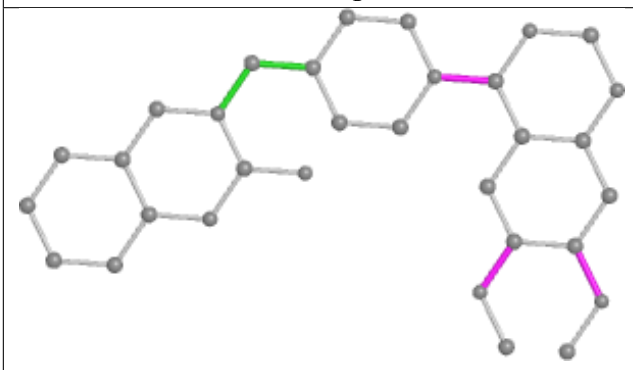
Ligand K56 C 1402



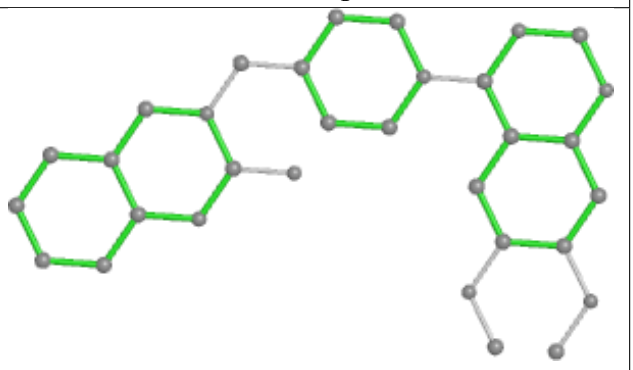
Bond lengths



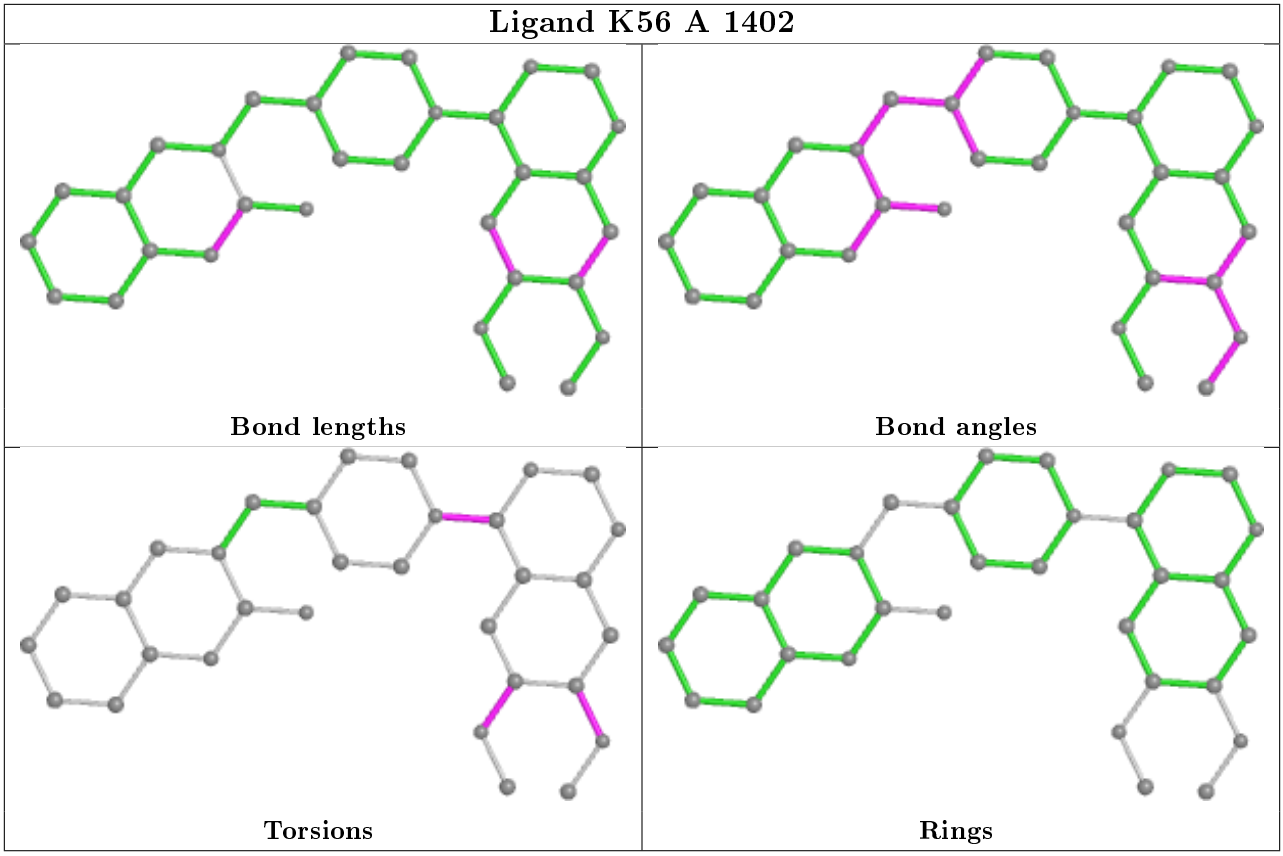
Bond angles



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	207/257 (80%)	-0.10	2 (0%)	82	82	38, 54, 82, 101	0
1	B	203/257 (78%)	-0.03	8 (3%)	39	35	33, 52, 90, 102	0
1	C	203/257 (78%)	-0.20	2 (0%)	82	82	40, 53, 79, 99	0
1	D	204/257 (79%)	-0.19	1 (0%)	91	91	36, 51, 79, 90	0
All	All	817/1028 (79%)	-0.13	13 (1%)	72	71	33, 53, 83, 102	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1266	ILE	3.1
1	A	1314	GLU	3.0
1	C	1265	THR	2.9
1	B	1230	GLY	2.7
1	B	1289	TYR	2.5

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

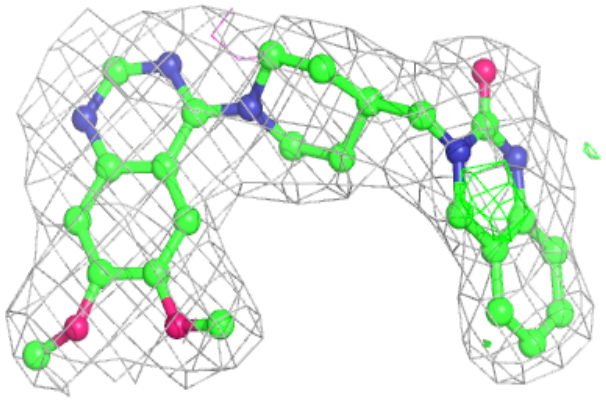
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

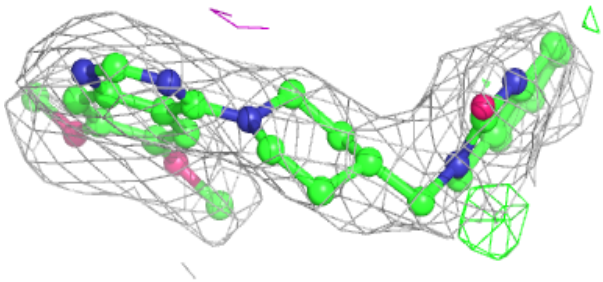
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K56	A	1402	32/32	0.94	0.14	35,40,45,46	0
3	K56	B	1402	32/32	0.95	0.14	31,35,46,47	0
3	K56	D	1402	32/32	0.95	0.16	41,43,47,48	0
3	K56	C	1402	32/32	0.96	0.15	39,43,45,47	0
2	ZN	D	1401	1/1	0.99	0.03	48,48,48,48	0
2	ZN	B	1401	1/1	0.99	0.04	70,70,70,70	0
2	ZN	C	1401	1/1	0.99	0.03	50,50,50,50	0
2	ZN	A	1401	1/1	0.99	0.03	65,65,65,65	0

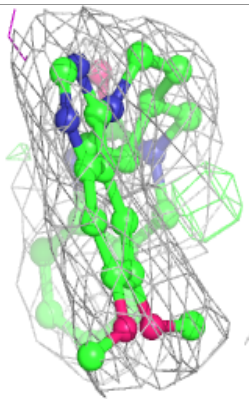
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K56 A 1402:

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

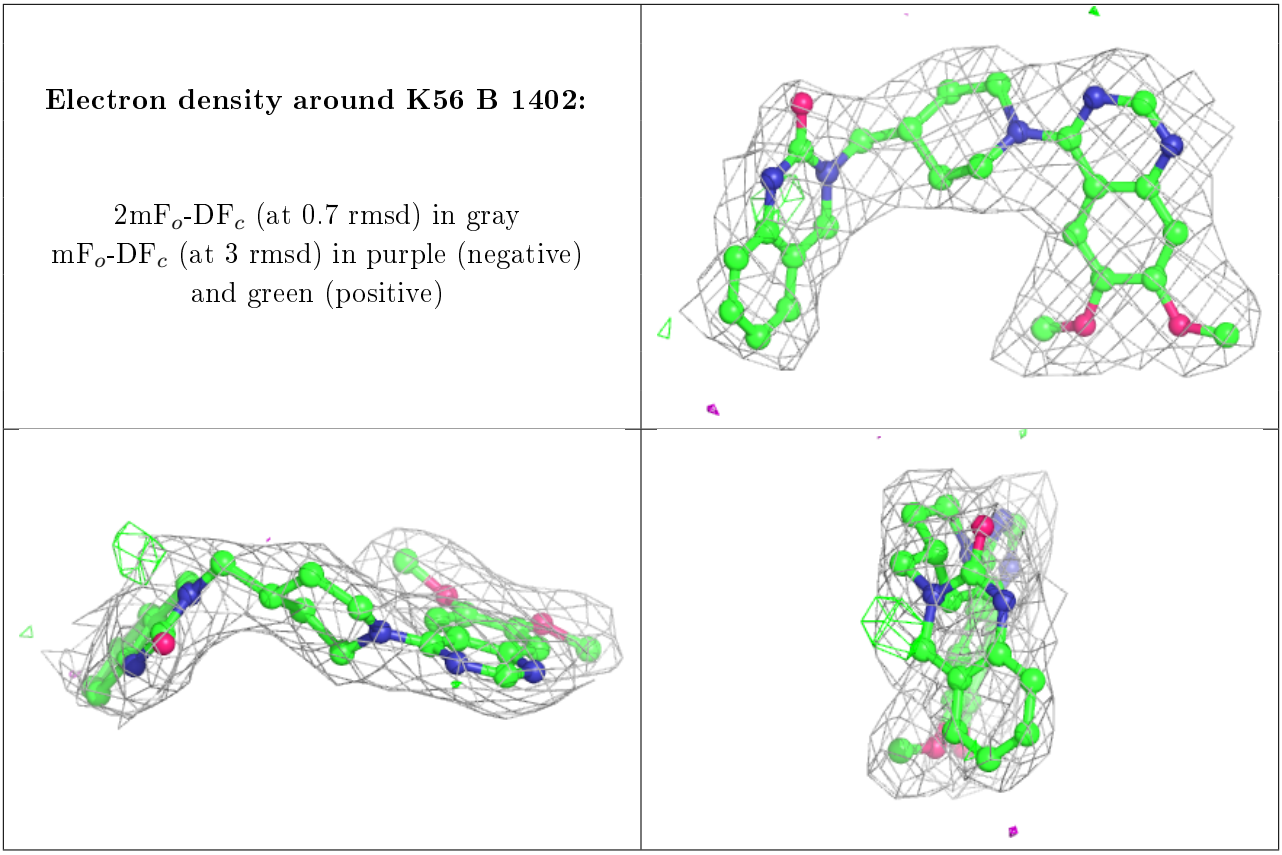






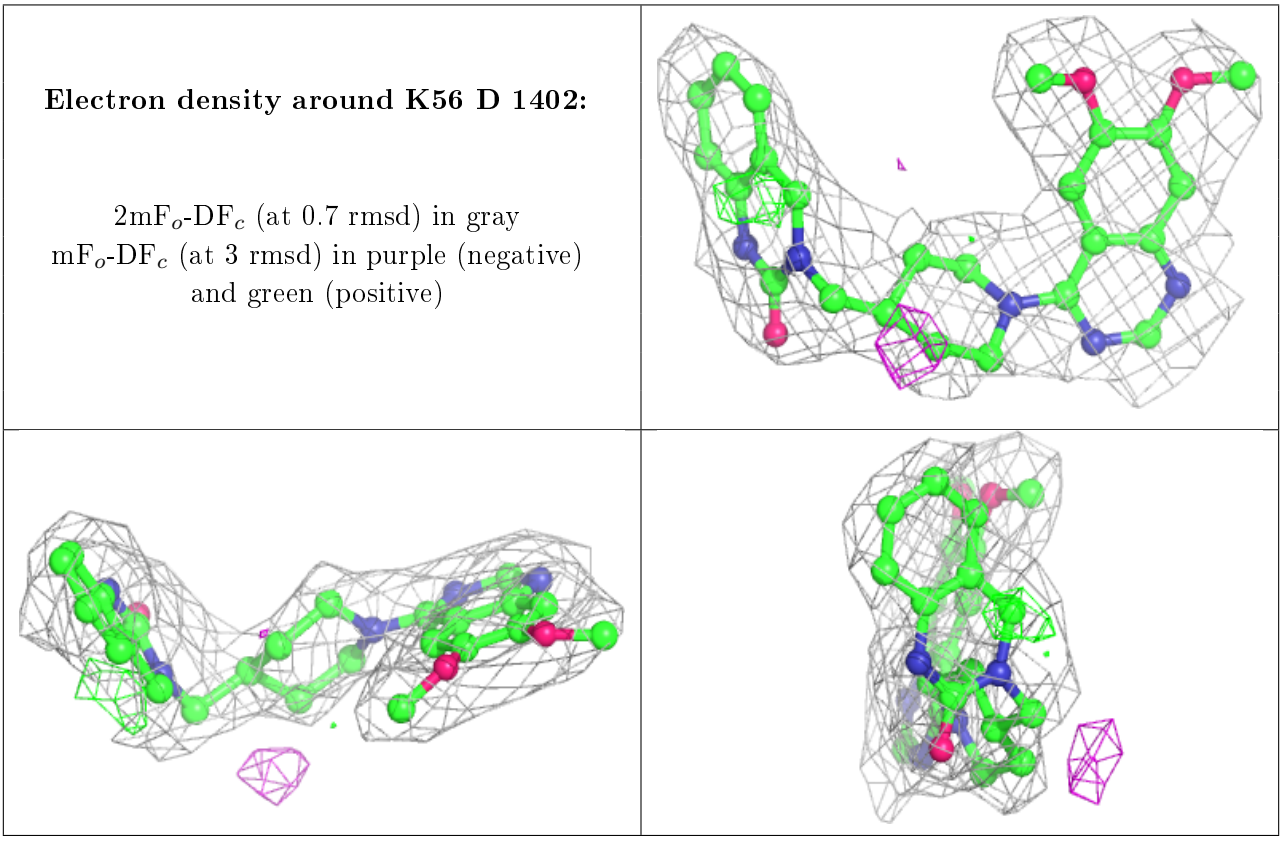
Electron density around K56 B 1402:

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



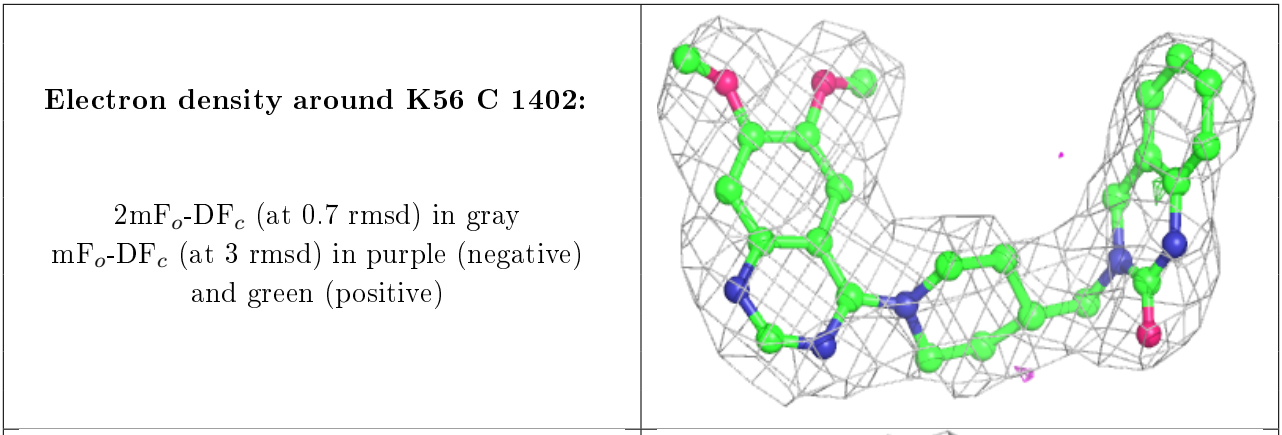
Electron density around K56 D 1402:

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



Electron density around K56 C 1402:

$2mF_o$-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.