wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 10:18 PM EDT

PDB ID	:	2FUM
Title	:	Catalytic domain of protein kinase PknB from Mycobacterium tuberculosis in complex with mitoxantrone
Authors	:	Wehenkel, A.; Alzari, P.M.
Deposited on	:	2006-01-27
Resolution	:	2.89 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

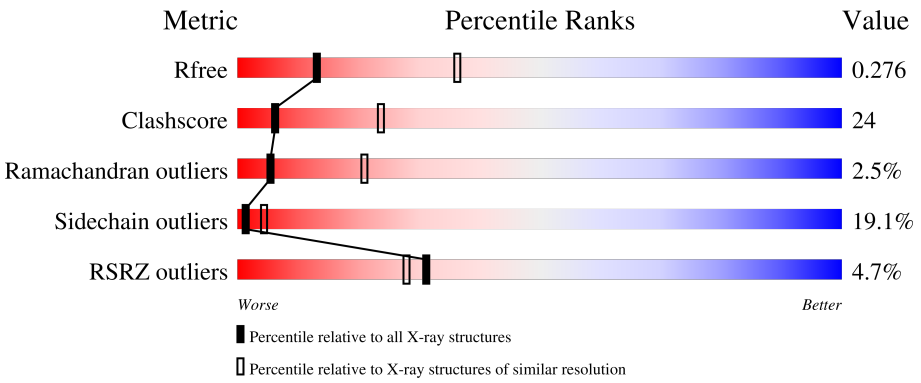
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.89 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 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	299	.% 47% 32% 8% • 12%
1	B	299	4% 44% 33% 9% • 12%
1	C	299	2% 44% 33% 7% • 15%
1	D	299	10% 45% 33% 7% 14%

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
2	MIX	D	3539	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7998 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 Probable serine/threonine-protein kinase pknB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	1994	1249	354	383	8	0	0	0
1	B	262	1991	1247	357	379	8	0	0	0
1	C	254	1931	1211	340	372	8	0	0	0
1	D	258	1954	1225	347	374	8	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	cloning artifact	UNP P0A5S4
A	-18	GLY	-	cloning artifact	UNP P0A5S4
A	-17	SER	-	cloning artifact	UNP P0A5S4
A	-16	SER	-	cloning artifact	UNP P0A5S4
A	-15	HIS	-	cloning artifact	UNP P0A5S4
A	-14	HIS	-	cloning artifact	UNP P0A5S4
A	-13	HIS	-	cloning artifact	UNP P0A5S4
A	-12	HIS	-	cloning artifact	UNP P0A5S4
A	-11	HIS	-	cloning artifact	UNP P0A5S4
A	-10	HIS	-	cloning artifact	UNP P0A5S4
A	-9	SER	-	cloning artifact	UNP P0A5S4
A	-8	SER	-	cloning artifact	UNP P0A5S4
A	-7	GLY	-	cloning artifact	UNP P0A5S4
A	-6	LEU	-	cloning artifact	UNP P0A5S4
A	-5	VAL	-	cloning artifact	UNP P0A5S4
A	-4	PRO	-	cloning artifact	UNP P0A5S4
A	-3	ARG	-	cloning artifact	UNP P0A5S4
A	-2	GLY	-	cloning artifact	UNP P0A5S4
A	-1	SER	-	cloning artifact	UNP P0A5S4
A	0	HIS	-	cloning artifact	UNP P0A5S4
B	-19	MET	-	cloning artifact	UNP P0A5S4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	cloning artifact	UNP P0A5S4
B	-17	SER	-	cloning artifact	UNP P0A5S4
B	-16	SER	-	cloning artifact	UNP P0A5S4
B	-15	HIS	-	cloning artifact	UNP P0A5S4
B	-14	HIS	-	cloning artifact	UNP P0A5S4
B	-13	HIS	-	cloning artifact	UNP P0A5S4
B	-12	HIS	-	cloning artifact	UNP P0A5S4
B	-11	HIS	-	cloning artifact	UNP P0A5S4
B	-10	HIS	-	cloning artifact	UNP P0A5S4
B	-9	SER	-	cloning artifact	UNP P0A5S4
B	-8	SER	-	cloning artifact	UNP P0A5S4
B	-7	GLY	-	cloning artifact	UNP P0A5S4
B	-6	LEU	-	cloning artifact	UNP P0A5S4
B	-5	VAL	-	cloning artifact	UNP P0A5S4
B	-4	PRO	-	cloning artifact	UNP P0A5S4
B	-3	ARG	-	cloning artifact	UNP P0A5S4
B	-2	GLY	-	cloning artifact	UNP P0A5S4
B	-1	SER	-	cloning artifact	UNP P0A5S4
B	0	HIS	-	cloning artifact	UNP P0A5S4
C	-19	MET	-	cloning artifact	UNP P0A5S4
C	-18	GLY	-	cloning artifact	UNP P0A5S4
C	-17	SER	-	cloning artifact	UNP P0A5S4
C	-16	SER	-	cloning artifact	UNP P0A5S4
C	-15	HIS	-	cloning artifact	UNP P0A5S4
C	-14	HIS	-	cloning artifact	UNP P0A5S4
C	-13	HIS	-	cloning artifact	UNP P0A5S4
C	-12	HIS	-	cloning artifact	UNP P0A5S4
C	-11	HIS	-	cloning artifact	UNP P0A5S4
C	-10	HIS	-	cloning artifact	UNP P0A5S4
C	-9	SER	-	cloning artifact	UNP P0A5S4
C	-8	SER	-	cloning artifact	UNP P0A5S4
C	-7	GLY	-	cloning artifact	UNP P0A5S4
C	-6	LEU	-	cloning artifact	UNP P0A5S4
C	-5	VAL	-	cloning artifact	UNP P0A5S4
C	-4	PRO	-	cloning artifact	UNP P0A5S4
C	-3	ARG	-	cloning artifact	UNP P0A5S4
C	-2	GLY	-	cloning artifact	UNP P0A5S4
C	-1	SER	-	cloning artifact	UNP P0A5S4
C	0	HIS	-	cloning artifact	UNP P0A5S4
D	-19	MET	-	cloning artifact	UNP P0A5S4
D	-18	GLY	-	cloning artifact	UNP P0A5S4
D	-17	SER	-	cloning artifact	UNP P0A5S4

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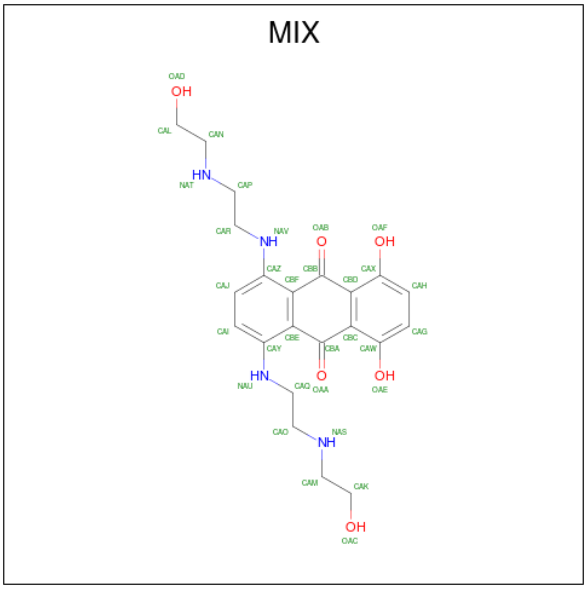
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	cloning artifact	UNP P0A5S4
D	-15	HIS	-	cloning artifact	UNP P0A5S4
D	-14	HIS	-	cloning artifact	UNP P0A5S4
D	-13	HIS	-	cloning artifact	UNP P0A5S4
D	-12	HIS	-	cloning artifact	UNP P0A5S4
D	-11	HIS	-	cloning artifact	UNP P0A5S4
D	-10	HIS	-	cloning artifact	UNP P0A5S4
D	-9	SER	-	cloning artifact	UNP P0A5S4
D	-8	SER	-	cloning artifact	UNP P0A5S4
D	-7	GLY	-	cloning artifact	UNP P0A5S4
D	-6	LEU	-	cloning artifact	UNP P0A5S4
D	-5	VAL	-	cloning artifact	UNP P0A5S4
D	-4	PRO	-	cloning artifact	UNP P0A5S4
D	-3	ARG	-	cloning artifact	UNP P0A5S4
D	-2	GLY	-	cloning artifact	UNP P0A5S4
D	-1	SER	-	cloning artifact	UNP P0A5S4
D	0	HIS	-	cloning artifact	UNP P0A5S4

- Molecule 2 is 1,4-DIHYDROXY-5,8-BIS({2-[(2-HYDROXYETHYL)AMINO]ETHYL}AMINO)-9,10-ANTHRACENEDIONE (three-letter code: MIX) (formula: $C_{22}H_{28}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	22	4	6	0	0
			Total	C	N	O		
2	B	1	32	22	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	32	22	4	6	0	0
			Total	C	N	O		
2	D	1	32	22	4	6	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: Probable serine/threonine-protein kinase pknB

Chain A: %
47% 32% 8% • 12%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR T3 H6 L7 S8 D9 R10 Y11 E12 E15 I16 L17 G18 F19 G20 G21 M22 S23 E24 V25 D30 L31 R32 L33 H34 K40 R43 A44 D45 L46 D49 P50

L54 R57 A60 N67 H68 P69 V72 A73 V74 Y75 D76 P83 P86 Y89 I90 E93 T99 L100 R101 D102 I103 V104 H105 T106 E107 G108 P109 M110 T111 R114 A115 I116 E117 V118 I119 A120 L126 M127 F128 Q131 I134 I135 H136 R137 D138 V139 K140

P141 A142 N143 S147 V154 M155 D156 F157 G158 I159 A160 R161 A162 I163 A164 D165 SER GLY ASN SER VAL THR GLN THR ALA ALA VAL ILE G178 T179 A180 Q181 Y182 L183 S184 P185 E186 Q187 A188 R189 G190 D191 S192 V193 R196 V199 Y200 S201 L202 G203 C204 V205 L206 Y207 E208 V209

E213 P214 P215 F216 T217 P221 V222 Q227 R230 E231 H240 E241 D246 L247 V250 A256 K257 N258 P259 E260 N261 R262 Y263 Q264 A271 D272 L273 V274 R275 V276 H277 ASN GLY

• Molecule 1: Probable serine/threonine-protein kinase pknB

Chain B: 4%
44% 33% 9% • 12%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR T3 P4 S8 D9 R10 L13 G18 F19 G20 G21 M22 S23 R29 R32 L33 H34 K40 V41 L42 R43 A44 D45 L46 A47 R48 D49 P50 S51 F52 Y53 L54 R55

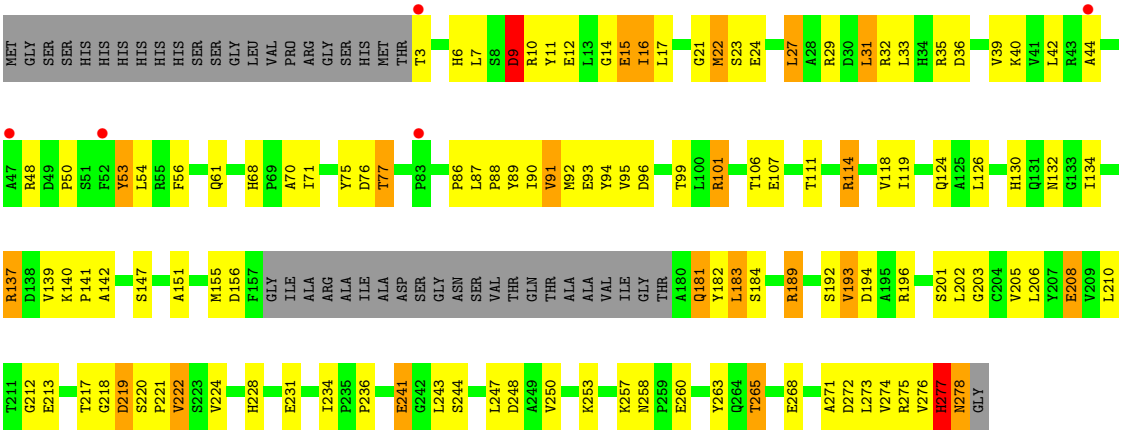
E59 N67 H68 P69 A73 V74 Y75 D76 E81 T82 P83 A84 L87 P88 Y89 M92 E93 V98 T99 L100 R101 D102 I103 T106 E107 M110 T111 P112 K113 R114 A115 I116 E117 V118 I119 N127 F128 Q131 I135 H136 R137 D138 V139 K140 P141 A142 N143 I144

M145 I146 S147 A148 T149 N150 A151 M155 D156 F157 G158 I159 A160 R161 A162 I163 ALA ASP SER GLY ASN SER VAL THR GLN THR ALA ALA VAL ILE G178 T179 A180 Q181 Y182 L183 S184 P185 E186 Q187 A188 R189 G190 D191 S192 V193 D194 A195 R196 V199 Y200 S201 L202 L206 Y207 E208 V209

E213 P214 P221 V224 A225 V229 R230 E231 I234 R239 H240 D246 V251 L252 K253 A254 L255 A256 K257 N258 P259 E260 N261 R262 T265 E268 M269 R270 A271 D272 L273 V274 R275 V276 H277 N278 GLY

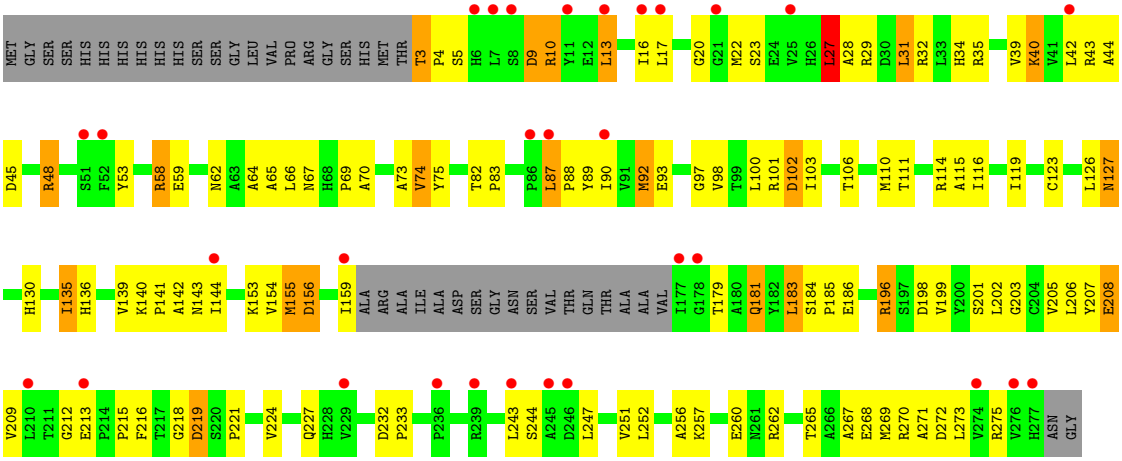
• Molecule 1: Probable serine/threonine-protein kinase pknB

Chain C: 2%
44% 33% 7% • 15%



- Molecule 1: Probable serine/threonine-protein kinase pknB

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.86Å 116.86Å 260.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.84 – 2.89 58.43 – 2.89	Depositor EDS
% Data completeness (in resolution range)	68.1 (69.84-2.89) 68.1 (58.43-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.218 , 0.278 0.214 , 0.276	Depositor DCC
R_{free} test set	1426 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	97.6	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 114.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7998	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MIX

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	0.74	0/2035	0.89	1/2775 (0.0%)
1	B	0.78	0/2032	0.93	7/2770 (0.3%)
1	C	0.69	0/1972	0.85	0/2691
1	D	0.63	0/1994	0.76	1/2719 (0.0%)
All	All	0.71	0/8033	0.86	9/10955 (0.1%)

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	2

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	180	ALA	N-CA-C	7.83	132.14	111.00
1	A	179	THR	N-CA-C	7.64	131.64	111.00
1	B	179	THR	N-CA-C	6.64	128.94	111.00
1	B	183	LEU	CB-CG-CD1	-6.29	100.30	111.00
1	B	22	MET	N-CA-C	5.67	126.31	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	180	ALA	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	1994	0	1940	101	0
1	B	1991	0	1944	100	0
1	C	1931	0	1868	86	0
1	D	1954	0	1908	99	0
2	A	32	0	26	2	0
2	B	32	0	27	4	0
2	C	32	0	27	1	0
2	D	32	0	28	6	0
All	All	7998	0	7768	384	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 24.

The worst 5 of 384 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ILE:CD1	1:D:116:ILE:CG1	1.76	1.63
1:B:99:THR:HG21	1:B:142:ALA:HA	1.16	1.16
1:C:189:ARG:HB2	1:C:189:ARG:NH1	1.64	1.12
1:B:180:ALA:HB2	1:B:221:PRO:HA	1.39	1.04
1:C:181:GLN:HG3	1:C:224:VAL:HG11	1.39	1.02

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	259/299 (87%)	222 (86%)	32 (12%)	5 (2%)	8	28
1	B	258/299 (86%)	223 (86%)	29 (11%)	6 (2%)	6	23
1	C	250/299 (84%)	216 (86%)	26 (10%)	8 (3%)	4	16
1	D	254/299 (85%)	217 (85%)	30 (12%)	7 (3%)	5	19
All	All	1021/1196 (85%)	878 (86%)	117 (12%)	26 (2%)	5	21

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	44	ALA
1	A	180	ALA
1	B	22	MET
1	B	44	ALA

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	208/242 (86%)	165 (79%)	43 (21%)	1	3
1	B	208/242 (86%)	170 (82%)	38 (18%)	1	5
1	C	203/242 (84%)	161 (79%)	42 (21%)	1	3
1	D	205/242 (85%)	171 (83%)	34 (17%)	2	7
All	All	824/968 (85%)	667 (81%)	157 (19%)	1	4

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	241	GLU
1	D	127	ASN

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Mol	Chain	Res	Type
1	C	265	THR
1	D	31	LEU
1	D	196	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	277	HIS
1	C	124	GLN
1	D	143	ASN
1	C	68	HIS
1	C	132	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	MIX	C	2539	-	34,34,34	1.06	4 (11%)	44,46,46	1.06	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MIX	A	539	-	34,34,34	1.46	4 (11%)	44,46,46	1.03	4 (9%)
2	MIX	D	3539	-	34,34,34	1.08	4 (11%)	44,46,46	0.81	1 (2%)
2	MIX	B	1539	-	34,34,34	1.25	4 (11%)	44,46,46	1.48	6 (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
2	MIX	C	2539	-	-	6/14/30/30	0/3/3/3
2	MIX	A	539	-	-	7/14/30/30	0/3/3/3
2	MIX	D	3539	-	-	9/14/30/30	0/3/3/3
2	MIX	B	1539	-	-	11/14/30/30	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1539	MIX	CBC-CBA	-3.90	1.38	1.47
2	A	539	MIX	CBD-CBB	-3.79	1.38	1.47
2	A	539	MIX	CBE-CBA	-3.62	1.39	1.47
2	A	539	MIX	CBC-CBA	-3.56	1.39	1.47
2	A	539	MIX	CBF-CBB	-3.13	1.40	1.47

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1539	MIX	CAJ-CAZ-NAV	-4.61	113.94	121.80
2	B	1539	MIX	CBF-CAZ-NAV	4.39	126.53	121.32
2	B	1539	MIX	OAA-CBA-CBC	-2.90	116.74	121.43
2	A	539	MIX	CAJ-CAZ-NAV	-2.63	117.31	121.80
2	A	539	MIX	CAP-CAR-NAV	-2.60	106.04	111.46

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1539	MIX	OAD-CAL-CAN-NAT
2	C	2539	MIX	OAC-CAK-CAM-NAS
2	C	2539	MIX	CAK-CAM-NAS-CAO

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Mol	Chain	Res	Type	Atoms
2	B	1539	MIX	CAJ-CAZ-NAV-CAR
2	D	3539	MIX	CAI-CAY-NAU-CAQ

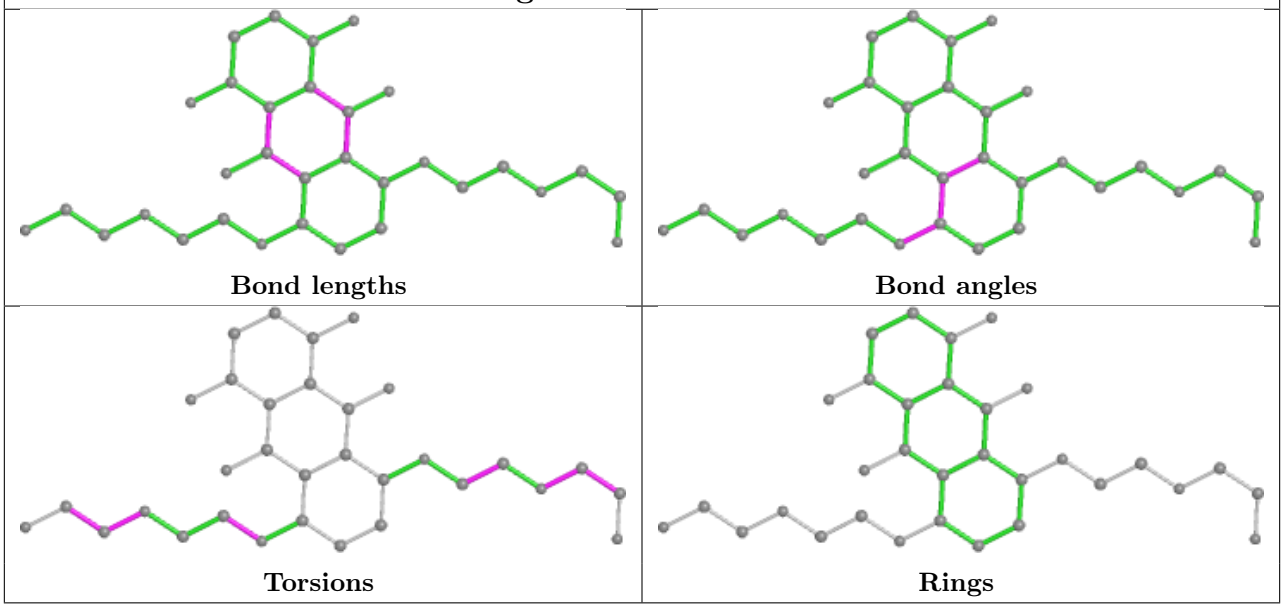
There are no ring outliers.

4 monomers are involved in 13 short contacts:

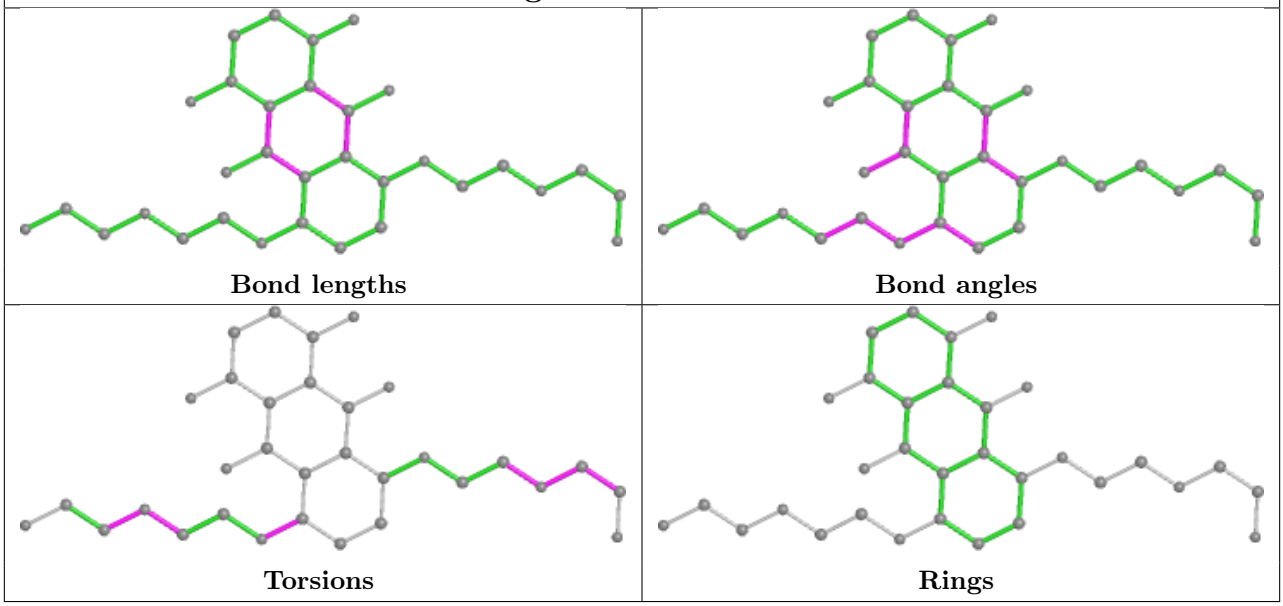
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2539	MIX	1	0
2	A	539	MIX	2	0
2	D	3539	MIX	6	0
2	B	1539	MIX	4	0

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.

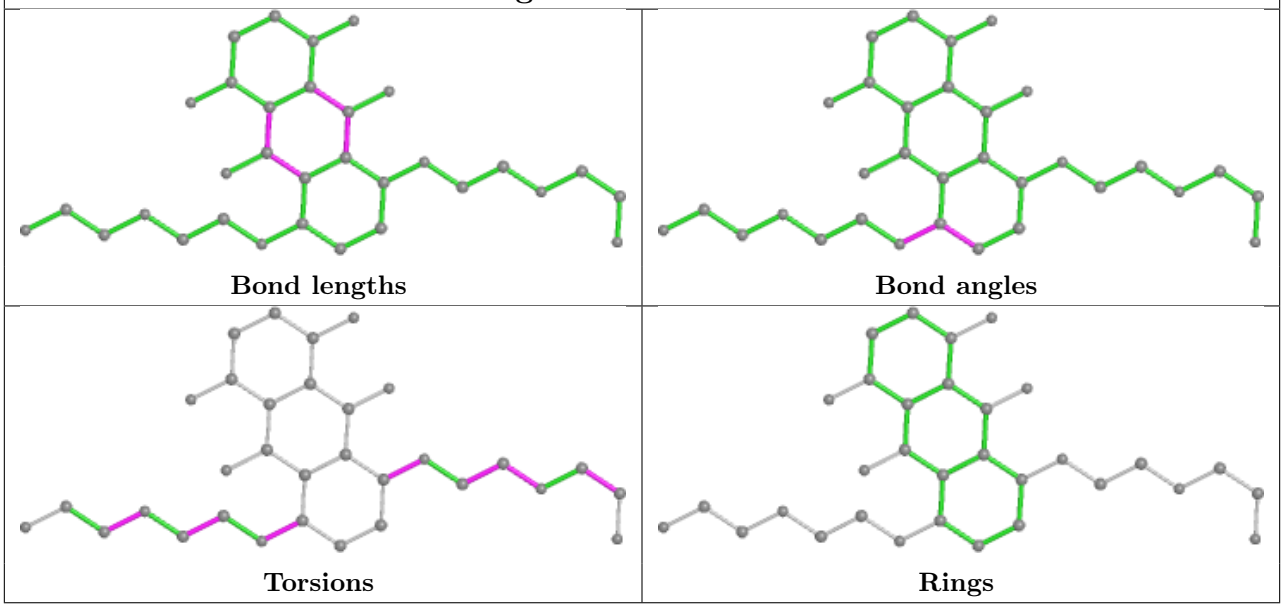
Ligand MIX C 2539

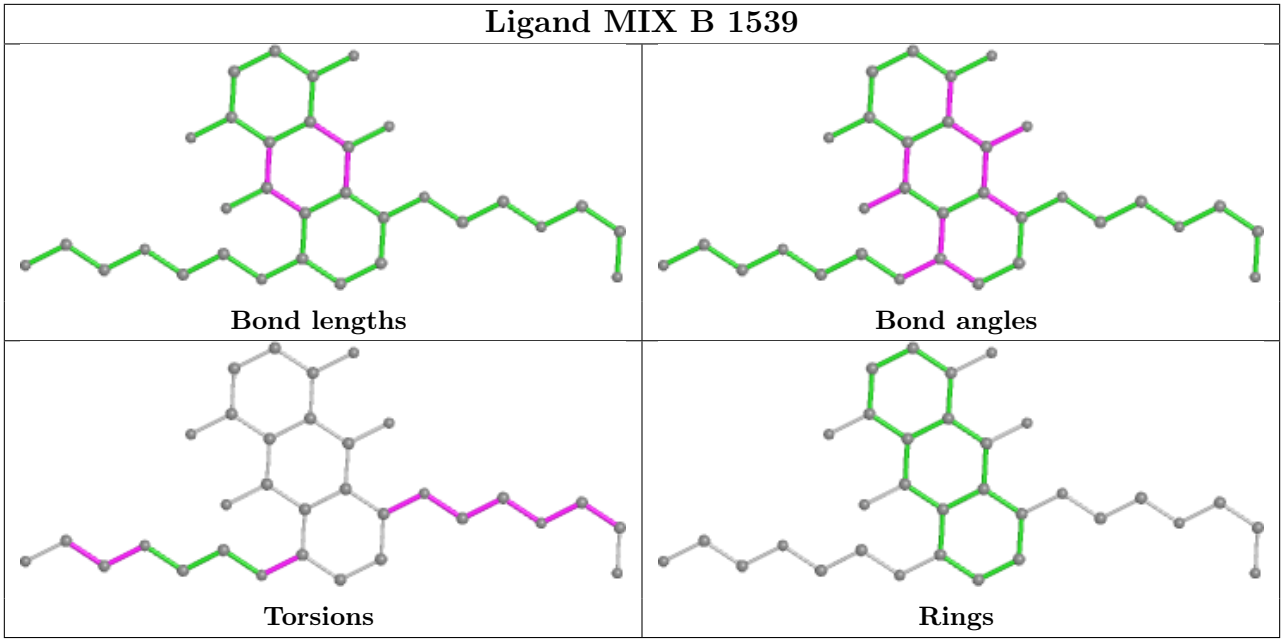


Ligand MIX A 539



Ligand MIX D 3539





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	263/299 (87%)	0.31	3 (1%)	80	80	76, 79, 83, 89	0
1	B	262/299 (87%)	0.42	11 (4%)	36	32	75, 79, 83, 89	0
1	C	254/299 (84%)	0.27	5 (1%)	65	63	77, 79, 81, 86	0
1	D	258/299 (86%)	0.66	30 (11%)	4	3	76, 79, 82, 86	0
All	All	1037/1196 (86%)	0.42	49 (4%)	31	28	75, 79, 83, 89	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	ILE	7.0
1	D	7	LEU	6.3
1	B	84	ALA	4.9
1	D	210	LEU	4.9
1	D	276	VAL	4.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

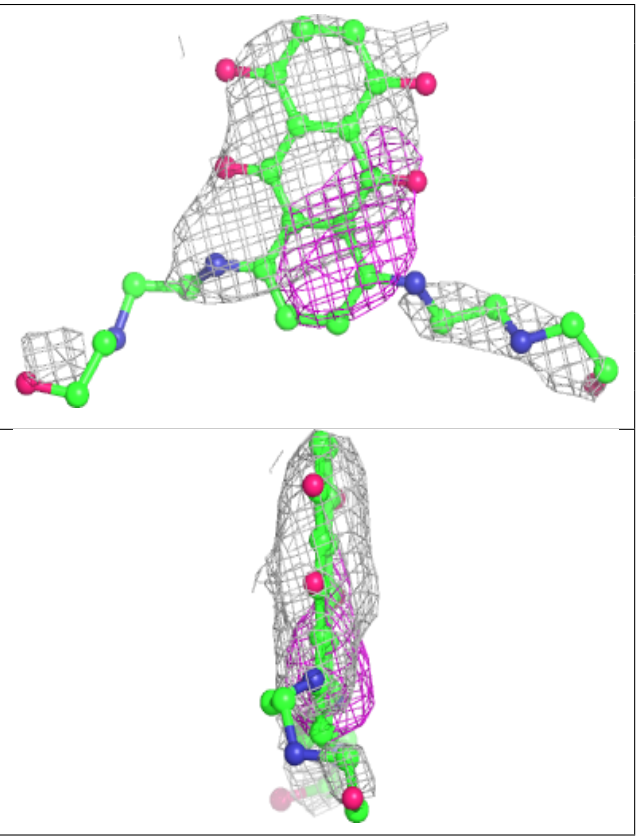
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MIX	D	3539	32/32	0.77	0.54	158,163,164,164	0
2	MIX	C	2539	32/32	0.89	0.19	122,127,130,132	0
2	MIX	A	539	32/32	0.95	0.23	91,91,103,105	0
2	MIX	B	1539	32/32	0.97	0.16	80,81,87,87	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.

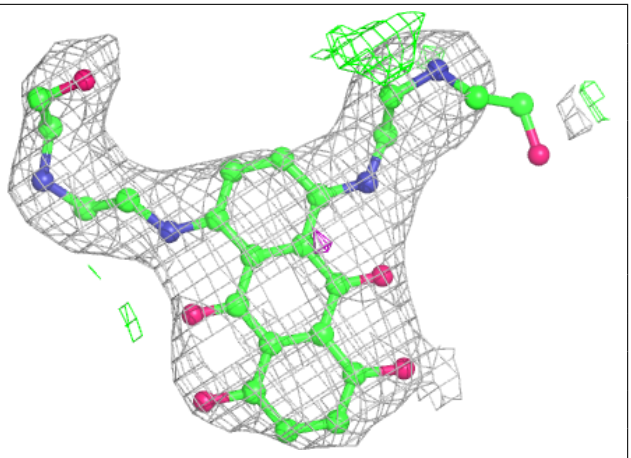
Electron density around MIX D 3539:

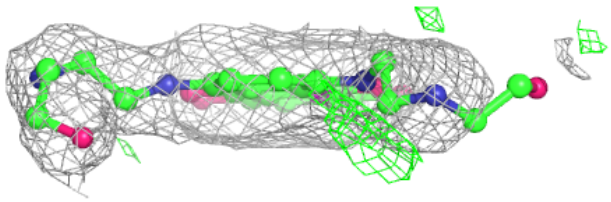
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

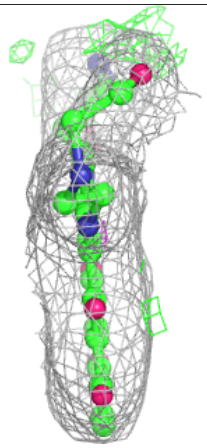


Electron density around MIX C 2539:

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

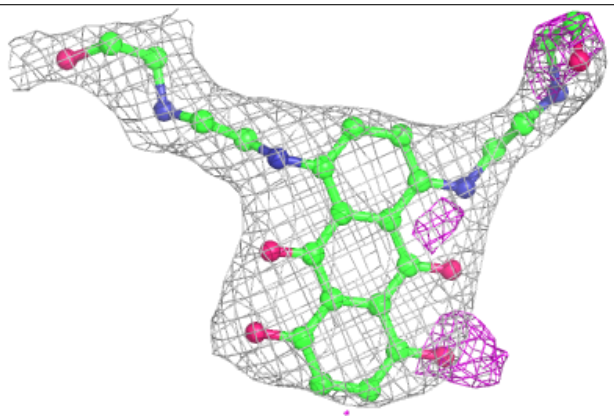


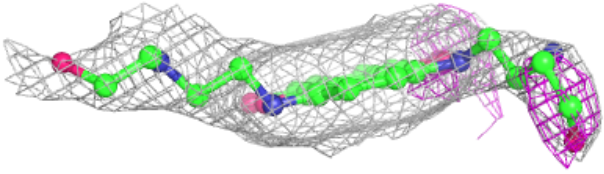


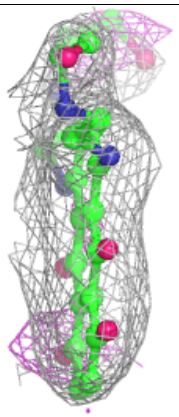


Electron density around MIX A 539:

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

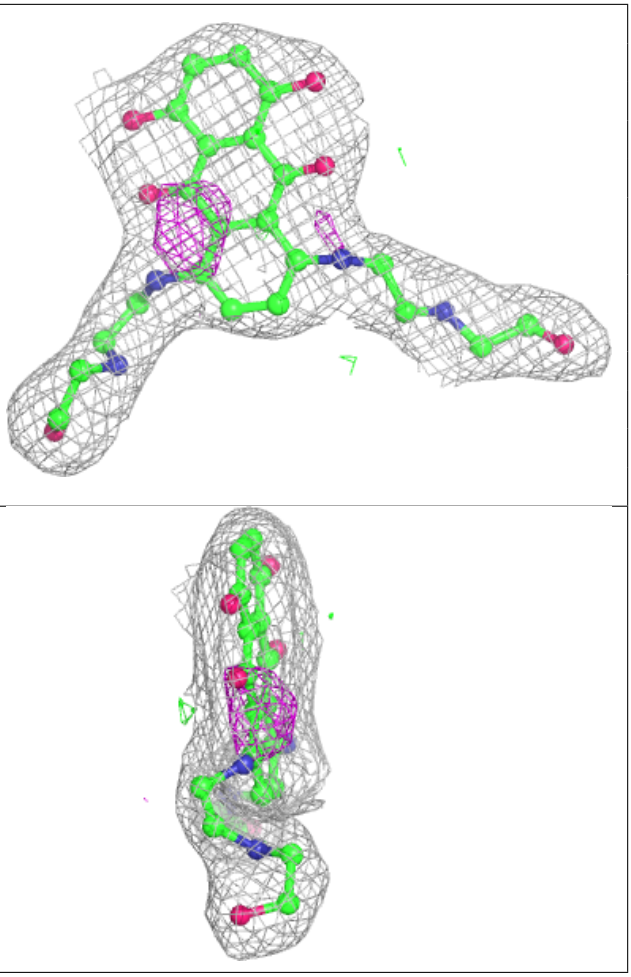






Electron density around MIX B 1539:

$2mF_o$-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.