wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2023 – 03:06 AM EDT

PDB ID	:	3F5P
Title	:	Complex Structure of Insulin-like Growth Factor Receptor and 3-Cyanoquinoline Inhibitor
Authors	:	Xu, W.; Miller, L.M.; Mayer, S.C.; Berger, D.M.; Boschelli, D.H.; Boschelli, F.
Deposited on	:	2008-11-04
Resolution	:	2.90 Å(reported)

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

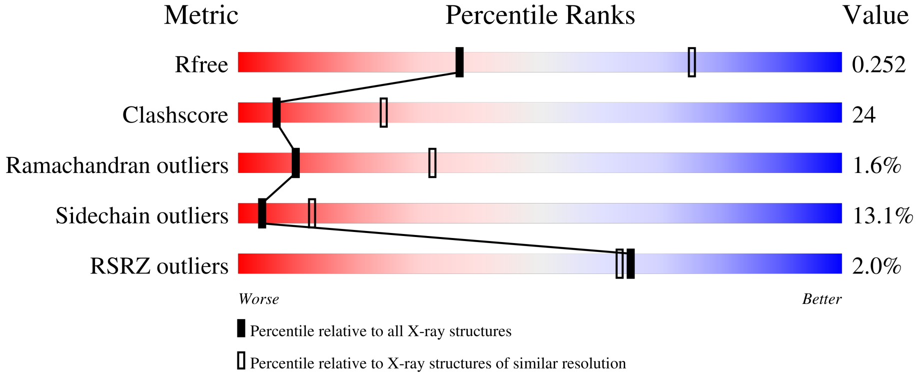
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

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

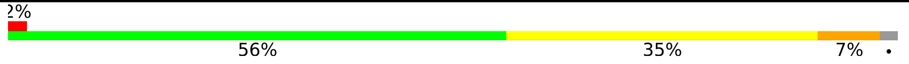
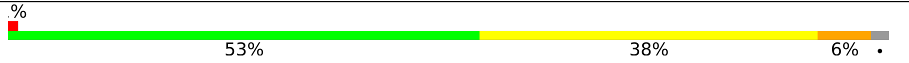
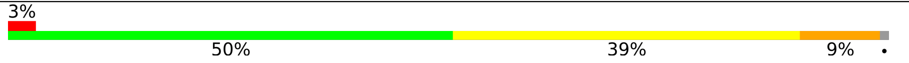
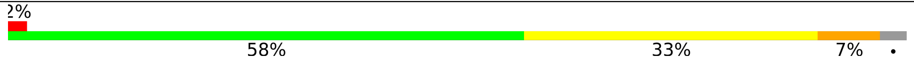
The reported resolution of this entry is 2.90 Å.

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 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	308	
1	B	308	
1	C	308	
1	D	308	

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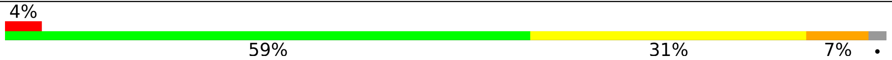
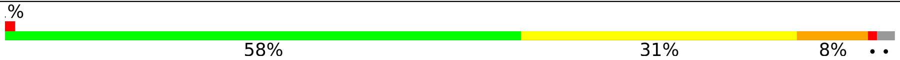
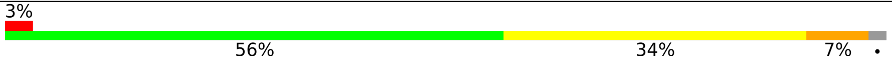
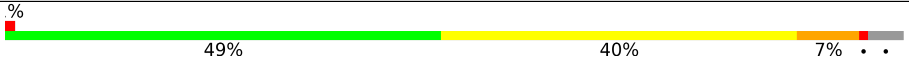
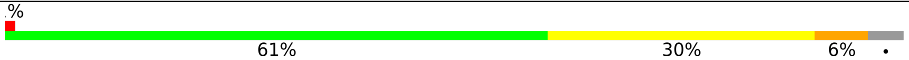
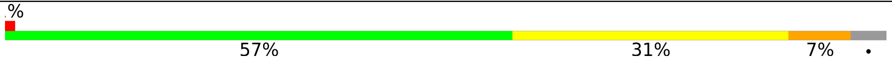
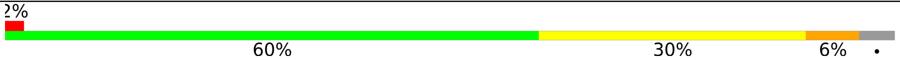
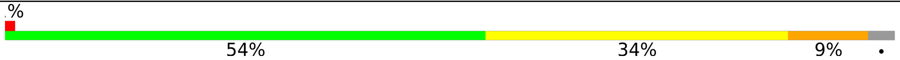
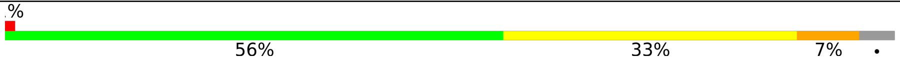
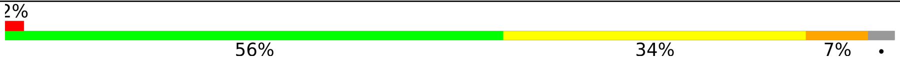
Mol	Chain	Length	Quality of chain
1	E	308	
1	F	308	
1	G	308	
1	H	308	
1	I	308	
1	J	308	
1	K	308	
1	L	308	
1	M	308	
1	R	308	
1	S	308	
1	T	308	

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
1	PTR	M	1166	-	-	X	-
1	PTR	S	1161	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39086 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.

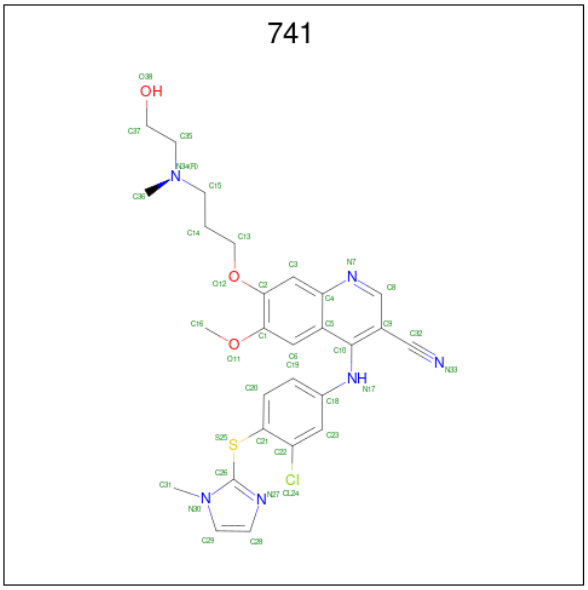
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	302	2420	1530	400	464	3	23	0	0	0
1	B	301	2408	1525	399	460	2	22	0	0	0
1	C	304	2420	1531	402	463	2	22	0	0	0
1	D	300	2399	1520	398	457	2	22	0	0	0
1	E	302	2405	1522	399	460	2	22	0	0	0
1	F	302	2412	1529	399	460	2	22	0	0	0
1	G	302	2416	1532	400	460	2	22	0	0	0
1	H	302	2416	1530	400	461	2	23	0	0	0
1	I	297	2380	1508	395	453	2	22	0	0	0
1	J	296	2369	1500	393	452	2	22	0	0	0
1	K	296	2369	1500	393	452	2	22	0	0	0
1	M	298	2381	1508	395	454	2	22	0	0	0
1	L	296	2369	1500	393	452	2	22	0	0	0
1	R	297	2376	1505	394	453	2	22	0	0	0
1	S	298	2386	1511	396	455	2	22	0	0	0
1	T	298	2386	1511	396	455	2	22	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	-	expression tag	UNP P08069
A	980	SER	-	expression tag	UNP P08069
B	979	GLY	-	expression tag	UNP P08069
B	980	SER	-	expression tag	UNP P08069
C	979	GLY	-	expression tag	UNP P08069
C	980	SER	-	expression tag	UNP P08069
D	979	GLY	-	expression tag	UNP P08069
D	980	SER	-	expression tag	UNP P08069
E	979	GLY	-	expression tag	UNP P08069
E	980	SER	-	expression tag	UNP P08069
F	979	GLY	-	expression tag	UNP P08069
F	980	SER	-	expression tag	UNP P08069
G	979	GLY	-	expression tag	UNP P08069
G	980	SER	-	expression tag	UNP P08069
H	979	GLY	-	expression tag	UNP P08069
H	980	SER	-	expression tag	UNP P08069
I	979	GLY	-	expression tag	UNP P08069
I	980	SER	-	expression tag	UNP P08069
J	979	GLY	-	expression tag	UNP P08069
J	980	SER	-	expression tag	UNP P08069
K	979	GLY	-	expression tag	UNP P08069
K	980	SER	-	expression tag	UNP P08069
M	979	GLY	-	expression tag	UNP P08069
M	980	SER	-	expression tag	UNP P08069
L	979	GLY	-	expression tag	UNP P08069
L	980	SER	-	expression tag	UNP P08069
R	979	GLY	-	expression tag	UNP P08069
R	980	SER	-	expression tag	UNP P08069
S	979	GLY	-	expression tag	UNP P08069
S	980	SER	-	expression tag	UNP P08069
T	979	GLY	-	expression tag	UNP P08069
T	980	SER	-	expression tag	UNP P08069

- Molecule 2 is 4-[[3-chloro-4-(1-methylimidazol-2-yl)sulfanyl-phenyl]amino]-7-[3-(2-hydroxy ethyl-methyl-amino)propoxy]-6-methoxy-quinoline-3-carbonitrile (three-letter code: 741) (formula: $C_{27}H_{29}ClN_6O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	B	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	C	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	D	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	E	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	F	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	G	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	H	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	I	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	J	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	K	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	M	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	L	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0
2	R	1	Total 38	C 27	Cl 1	N 6	O 3	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	S	1	Total C Cl N O S 38 27 1 6 3 1	0	0
2	T	1	Total C Cl N O S 38 27 1 6 3 1	0	0

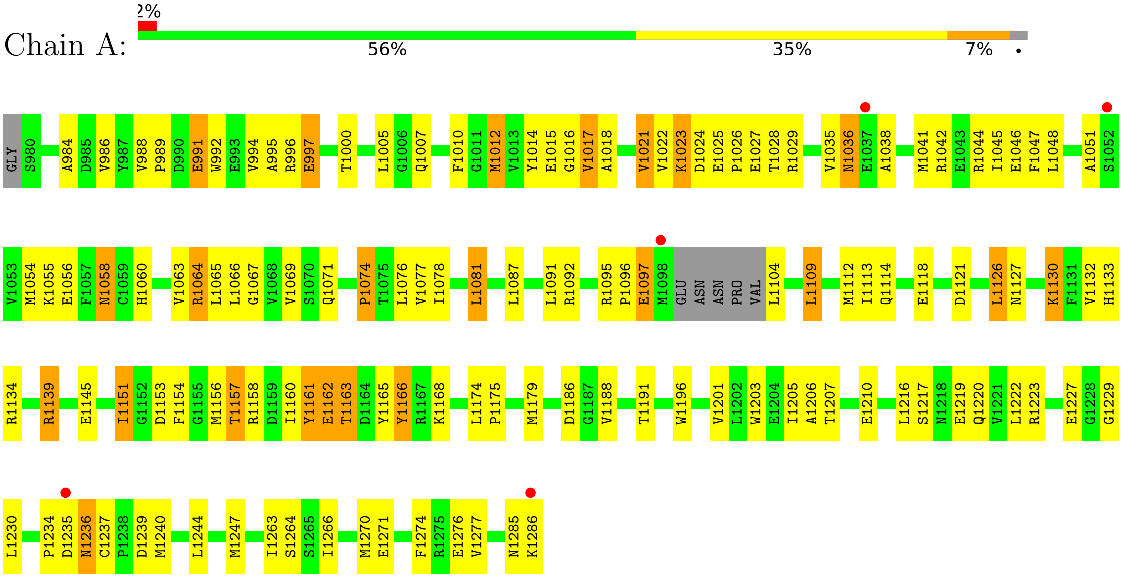
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	19	Total O 19 19	0	0
3	C	18	Total O 18 18	0	0
3	D	7	Total O 7 7	0	0
3	E	1	Total O 1 1	0	0
3	F	4	Total O 4 4	0	0
3	G	14	Total O 14 14	0	0
3	H	19	Total O 19 19	0	0
3	I	19	Total O 19 19	0	0
3	J	29	Total O 29 29	0	0
3	K	1	Total O 1 1	0	0
3	M	1	Total O 1 1	0	0
3	L	6	Total O 6 6	0	0
3	R	16	Total O 16 16	0	0
3	S	6	Total O 6 6	0	0
3	T	1	Total O 1 1	0	0

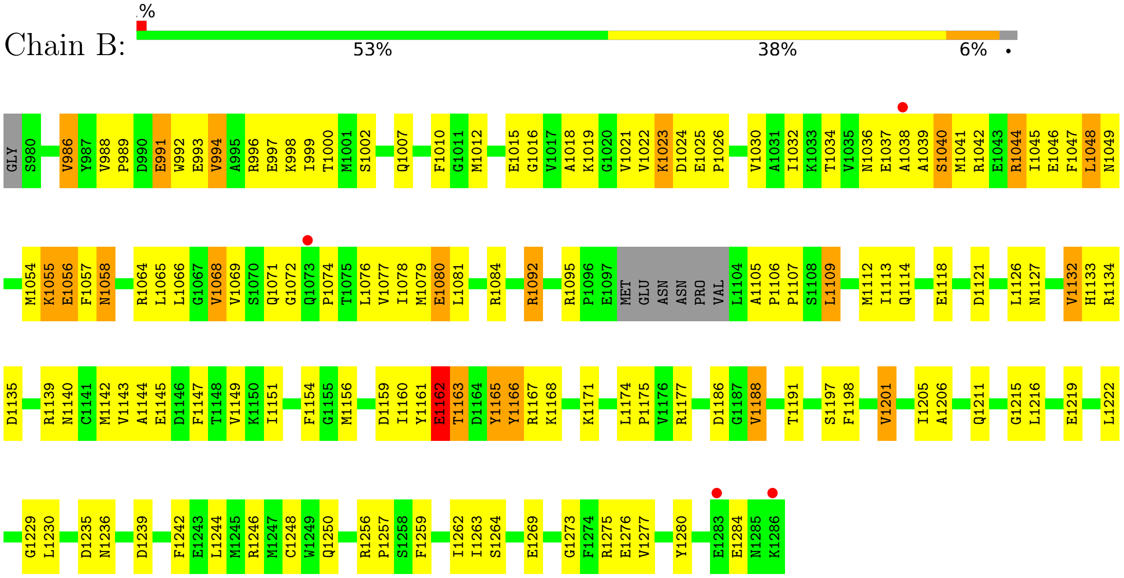
3 Residue-property plots ⓘ

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: Insulin-like growth factor 1 receptor

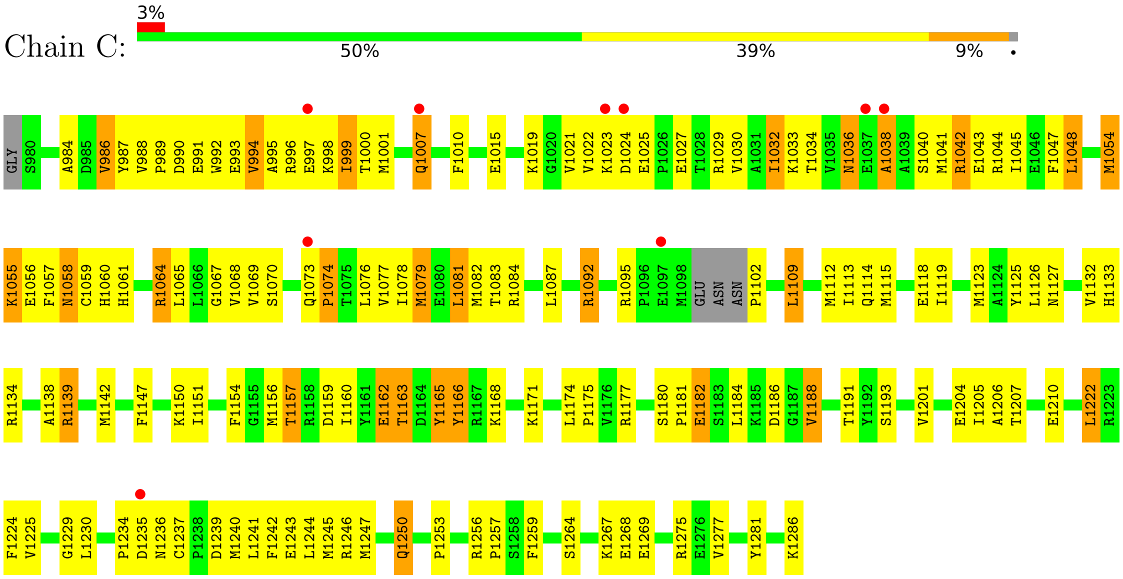


- Molecule 1: Insulin-like growth factor 1 receptor



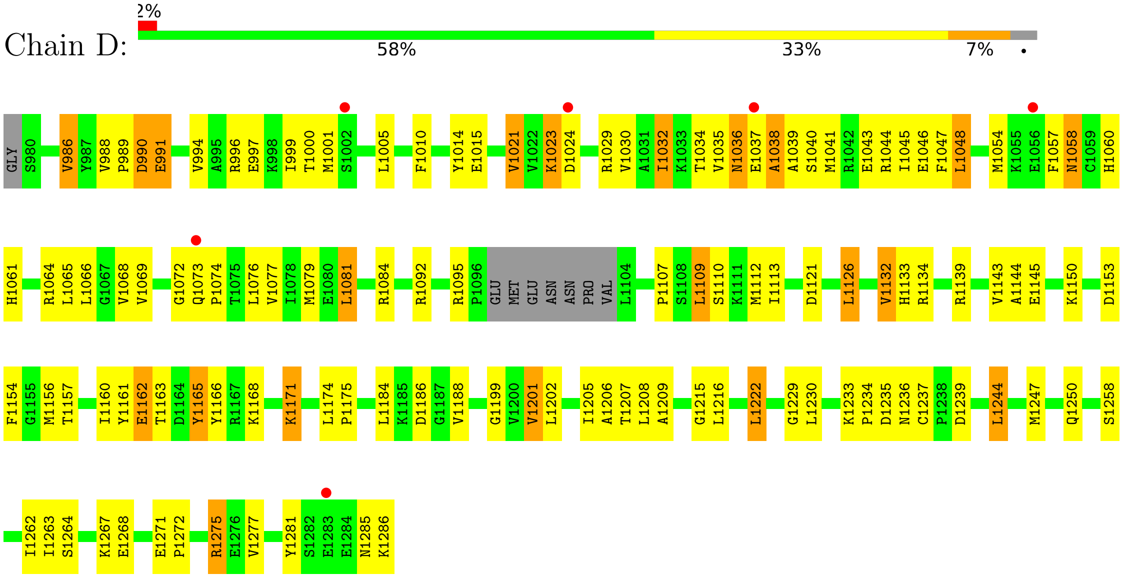
- Molecule 1: Insulin-like growth factor 1 receptor

Chain C:



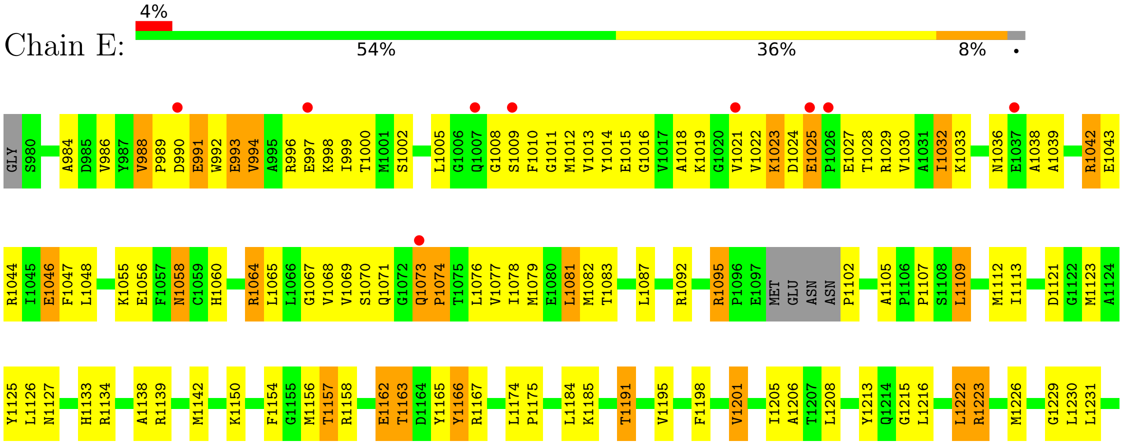
- Molecule 1: Insulin-like growth factor 1 receptor

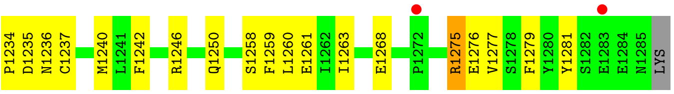
Chain D:



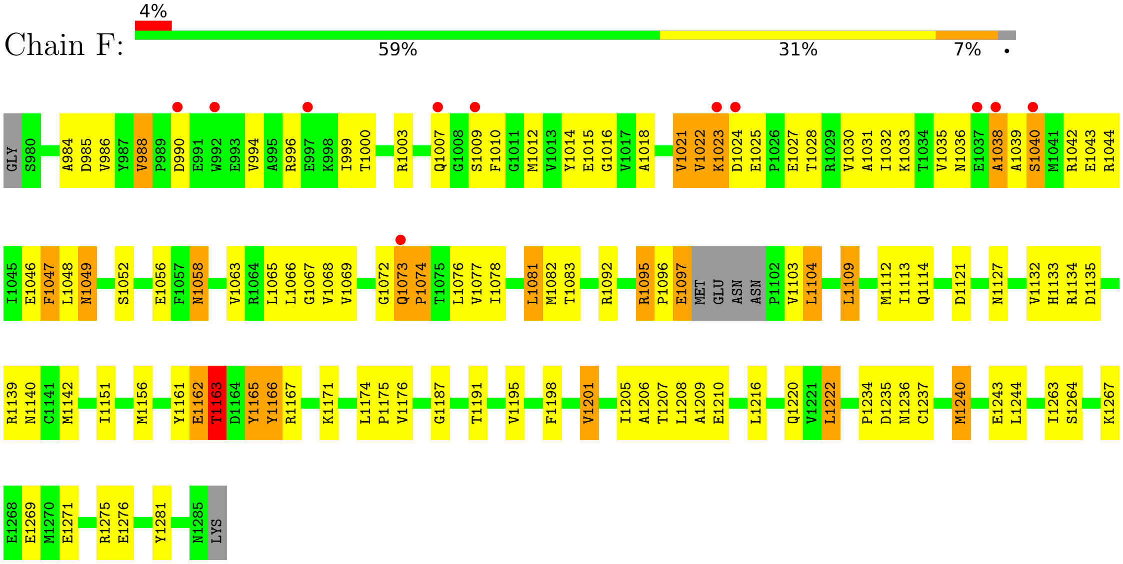
- Molecule 1: Insulin-like growth factor 1 receptor

Chain E:

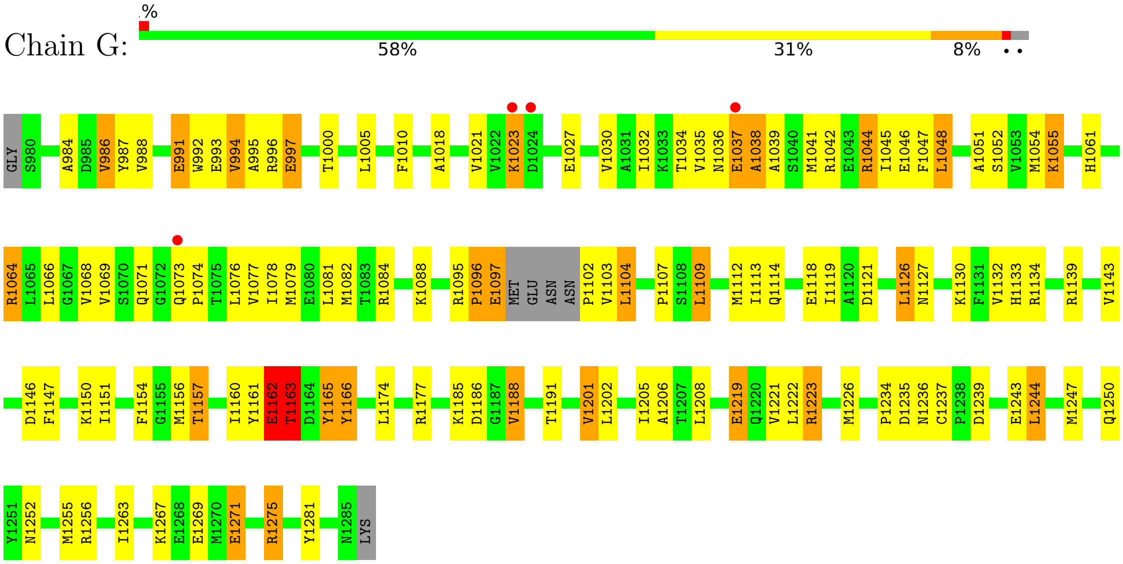




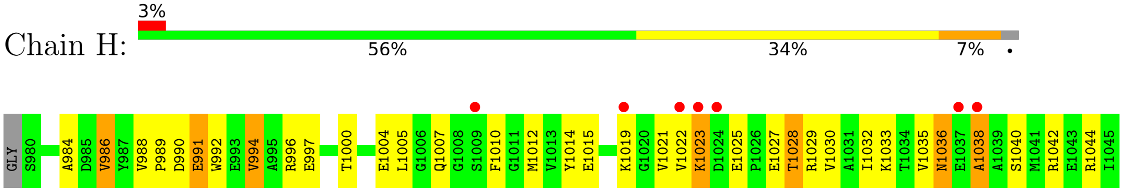
- Molecule 1: Insulin-like growth factor 1 receptor

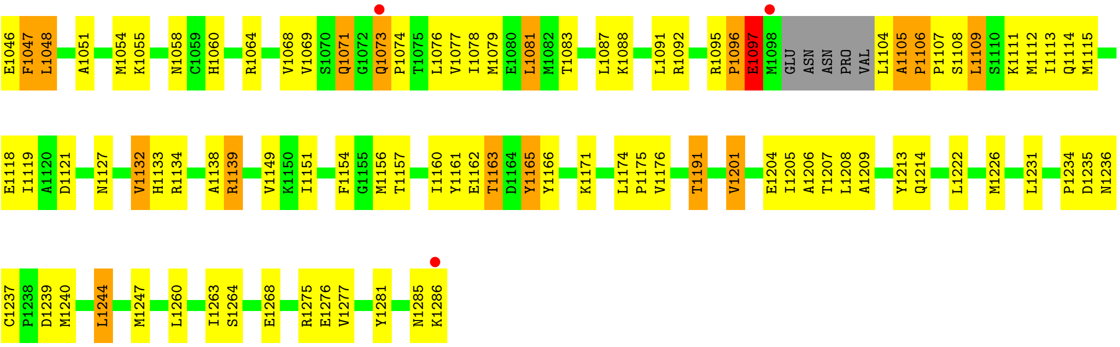


- Molecule 1: Insulin-like growth factor 1 receptor



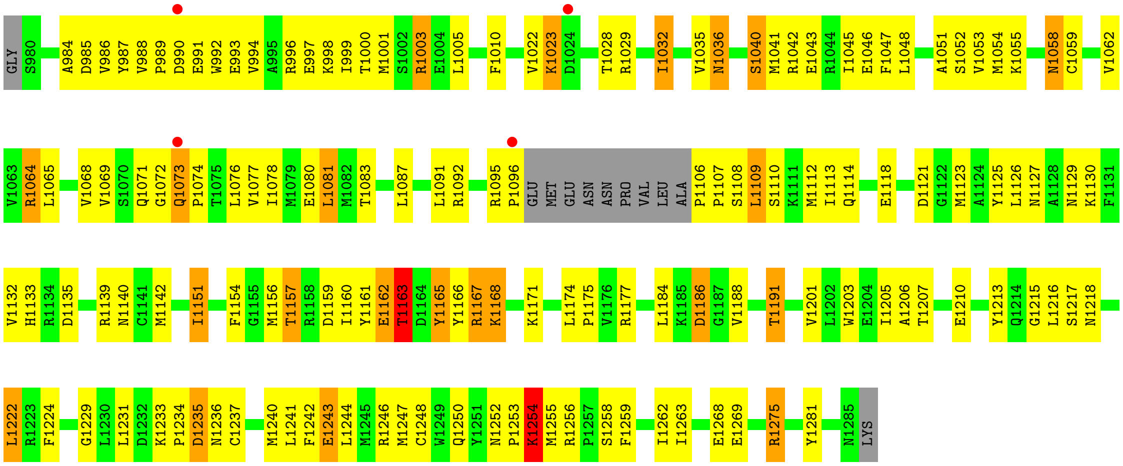
- Molecule 1: Insulin-like growth factor 1 receptor





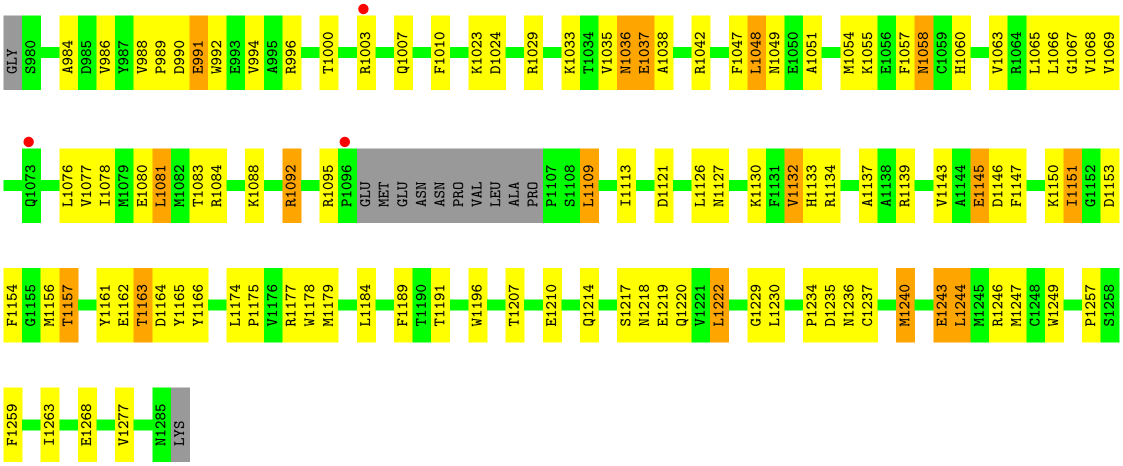
- Molecule 1: Insulin-like growth factor 1 receptor

Chain I:



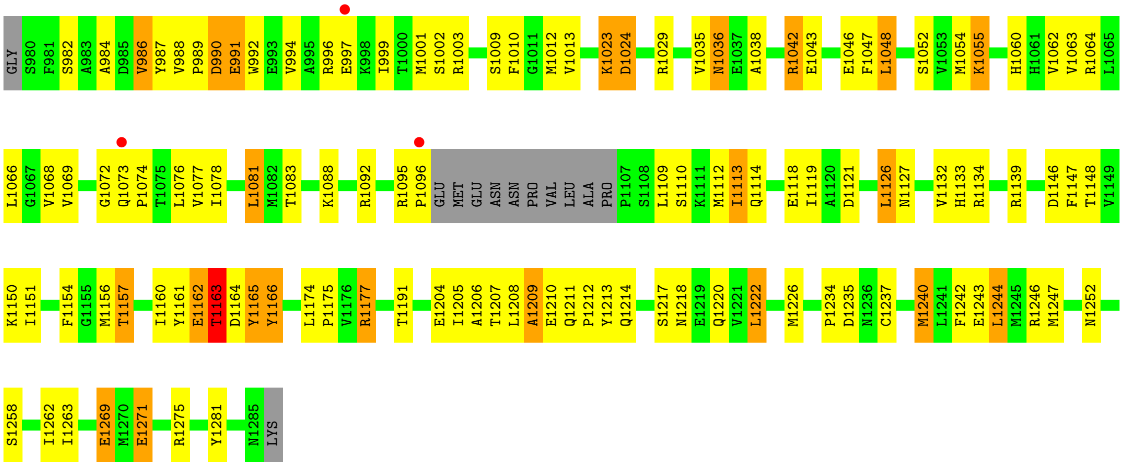
- Molecule 1: Insulin-like growth factor 1 receptor

Chain J:



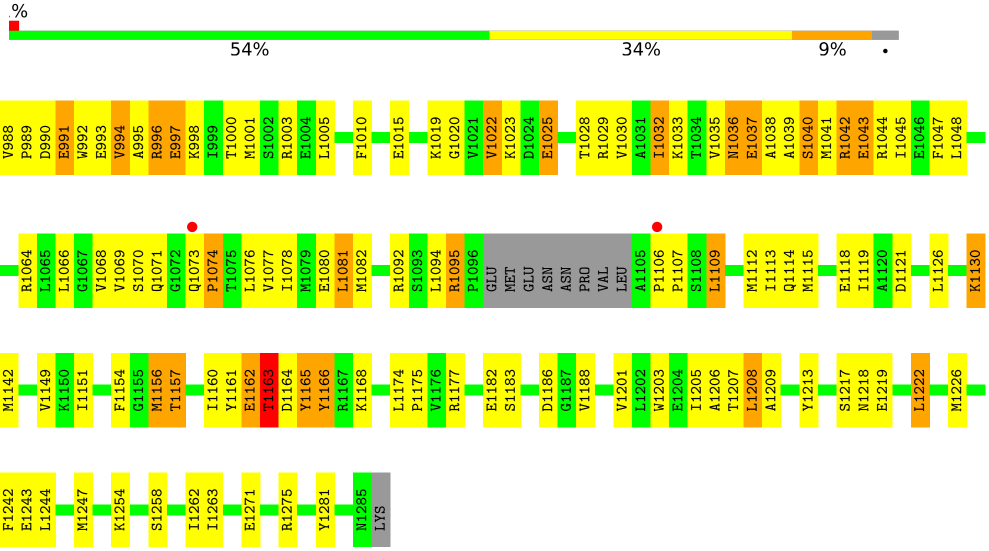
- Molecule 1: Insulin-like growth factor 1 receptor

Chain K:



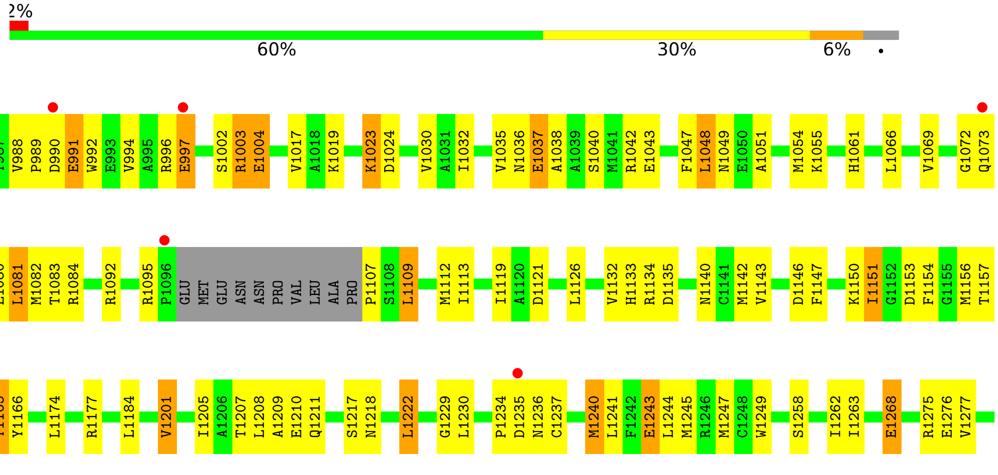
- Molecule 1: Insulin-like growth factor 1 receptor

Chain M:



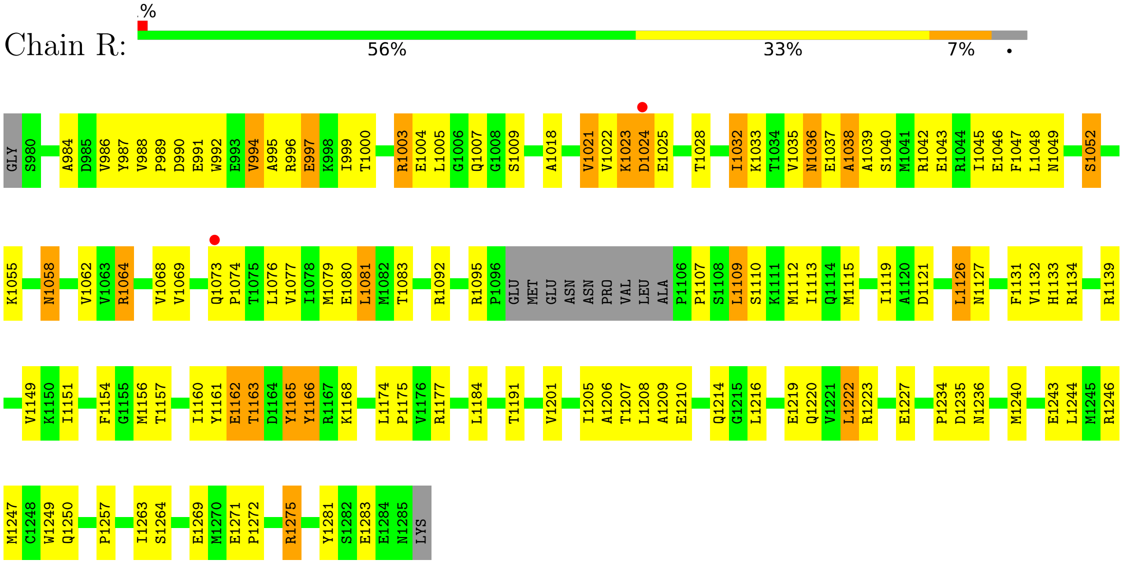
- Molecule 1: Insulin-like growth factor 1 receptor

Chain L:



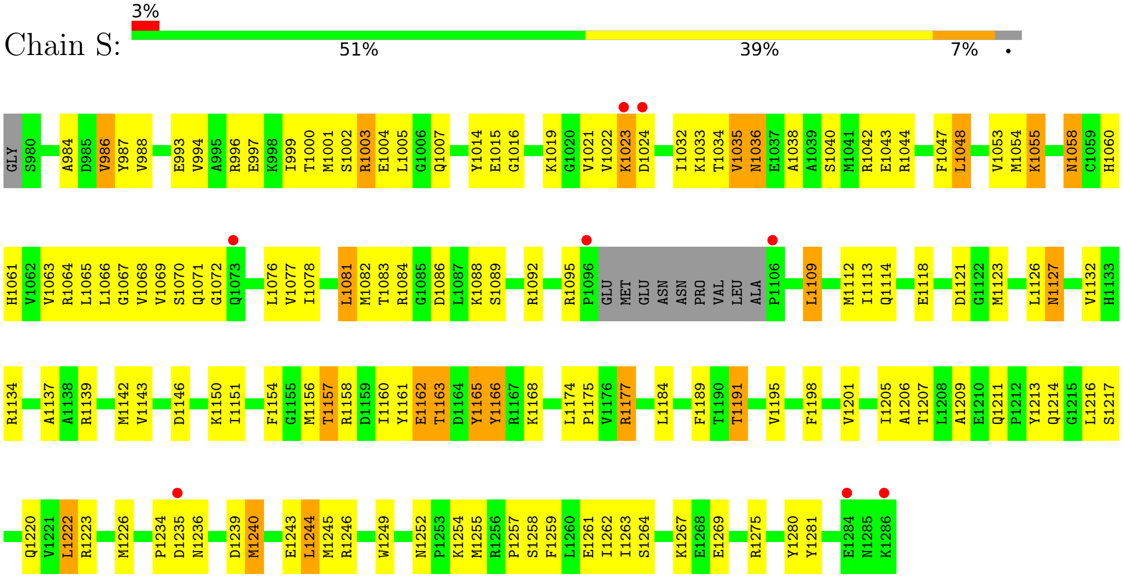
- Molecule 1: Insulin-like growth factor 1 receptor

Chain R:



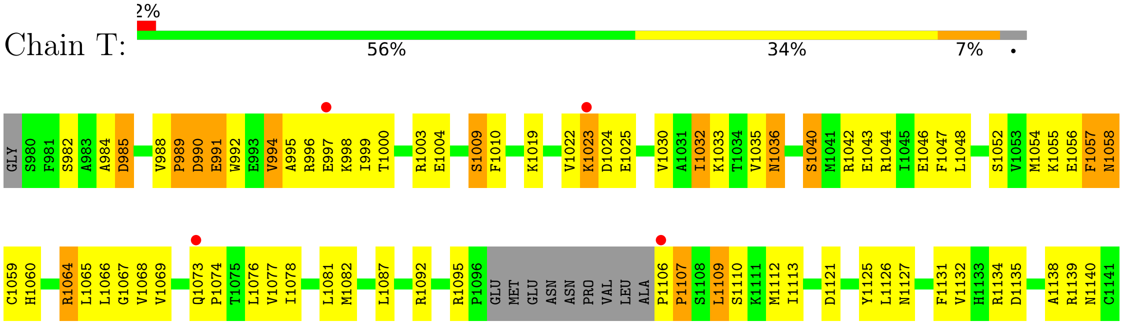
- Molecule 1: Insulin-like growth factor 1 receptor

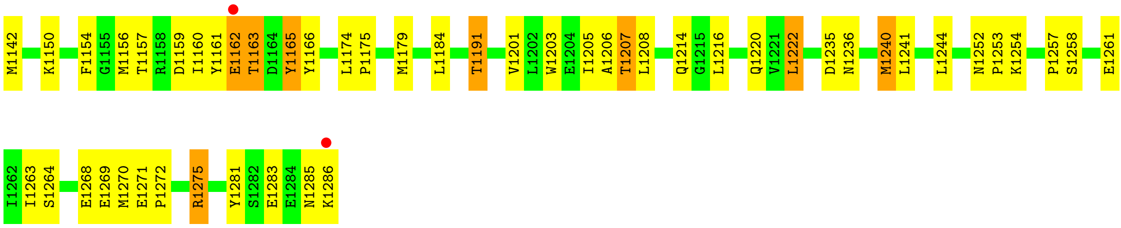
Chain S:



- Molecule 1: Insulin-like growth factor 1 receptor

Chain T:




M1142
K1150
F1154
G1155
M1156
T1157
R1158
D1159
I1160
Y1161
E1162
T1163
D1164
Y1165
Y1166
L1174
P1175
M1179
L1184
T1191
V1201
L1202
W1203
E1204
I1205
A1206
T1207
L1208
Q1214
G1215
L1216
Q1220
V1221
L1222
D1235
N1236
M1240
L1241
L1244
N1252
P1253
K1254
P1257
S1258
E1261
I1262
I1263
S1264
E1268
E1269
M1270
E1271
P1272
R1275
Y1281
S1282
E1283
E1284
N1285
K1286

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	137.34Å 137.02Å 178.99Å 90.00° 110.36° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-2.90) 97.1 (19.99-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.88Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.258 0.206 , 0.252	Depositor DCC
R_{free} test set	6715 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.8	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.47, $< L^2 >$ = 0.30	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	39086	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 42.03 % 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 2.1640e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: PTR, 741

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	0.40	0/2418	0.57	0/3255
1	B	0.39	0/2410	0.55	0/3245
1	C	0.39	0/2422	0.56	1/3262 (0.0%)
1	D	0.39	0/2401	0.55	1/3233 (0.0%)
1	E	0.39	0/2407	0.58	1/3244 (0.0%)
1	F	0.39	0/2415	0.57	0/3255
1	G	0.37	0/2419	0.53	0/3259
1	H	0.37	0/2418	0.55	0/3255
1	I	0.46	1/2382 (0.0%)	0.59	0/3207
1	J	0.39	0/2370	0.55	0/3191
1	K	0.41	0/2370	0.56	0/3191
1	L	0.38	0/2370	0.54	0/3191
1	M	0.40	0/2383	0.56	0/3211
1	R	0.39	0/2378	0.55	0/3203
1	S	0.39	0/2388	0.56	0/3214
1	T	0.42	0/2388	0.58	0/3214
All	All	0.40	1/38339 (0.0%)	0.56	3/51630 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1254	LYS	CE-NZ	-5.91	1.34	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1102	PRO	N-CA-CB	6.57	111.19	103.30
1	C	1102	PRO	N-CA-CB	6.10	110.62	103.30
1	D	1048	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2420	0	2358	111	0
1	B	2408	0	2349	110	0
1	C	2420	0	2346	145	0
1	D	2399	0	2343	112	0
1	E	2405	0	2331	125	0
1	F	2412	0	2353	112	0
1	G	2416	0	2364	118	0
1	H	2416	0	2358	112	0
1	I	2380	0	2326	139	0
1	J	2369	0	2308	104	0
1	K	2369	0	2308	102	0
1	L	2369	0	2308	87	0
1	M	2381	0	2319	126	0
1	R	2376	0	2315	114	0
1	S	2386	0	2328	118	0
1	T	2386	0	2328	114	0
2	A	38	0	29	5	0
2	B	38	0	29	3	0
2	C	38	0	29	2	0
2	D	38	0	29	1	0
2	E	38	0	29	5	0
2	F	38	0	29	5	0
2	G	38	0	29	2	0
2	H	38	0	29	4	0
2	I	38	0	29	9	0
2	J	38	0	29	2	0
2	K	38	0	29	2	0
2	L	38	0	29	3	0
2	M	38	0	29	1	0
2	R	38	0	29	6	0
2	S	38	0	29	4	0
2	T	38	0	29	3	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	0	1	0
3	C	18	0	0	2	0
3	D	7	0	0	3	0
3	E	1	0	0	1	0
3	F	4	0	0	1	0
3	G	14	0	0	0	0
3	H	19	0	0	1	0
3	I	19	0	0	0	0
3	J	29	0	0	7	0
3	K	1	0	0	0	0
3	L	6	0	0	0	0
3	M	1	0	0	0	0
3	R	16	0	0	3	0
3	S	6	0	0	0	0
3	T	1	0	0	0	0
All	All	39086	0	37806	1849	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 1849 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1254:LYS:N	1:I:1254:LYS:HE3	1.61	1.13
1:C:1092:ARG:HH11	1:C:1092:ARG:HG3	0.99	1.13
1:K:989:PRO:HG2	1:K:992:TRP:HD1	1.09	1.11
1:H:1023:LYS:H	1:H:1023:LYS:HD2	1.17	1.09
1:M:996:ARG:HH12	1:M:1074:PRO:HD2	0.93	1.09

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	295/308 (96%)	267 (90%)	22 (8%)	6 (2%)	7	27
1	B	294/308 (96%)	273 (93%)	17 (6%)	4 (1%)	11	36
1	C	297/308 (96%)	271 (91%)	20 (7%)	6 (2%)	7	27
1	D	293/308 (95%)	271 (92%)	18 (6%)	4 (1%)	11	36
1	E	295/308 (96%)	271 (92%)	20 (7%)	4 (1%)	11	36
1	F	295/308 (96%)	268 (91%)	21 (7%)	6 (2%)	7	27
1	G	295/308 (96%)	275 (93%)	16 (5%)	4 (1%)	11	36
1	H	295/308 (96%)	265 (90%)	22 (8%)	8 (3%)	5	19
1	I	290/308 (94%)	272 (94%)	15 (5%)	3 (1%)	15	45
1	J	289/308 (94%)	266 (92%)	20 (7%)	3 (1%)	15	45
1	K	289/308 (94%)	266 (92%)	17 (6%)	6 (2%)	7	26
1	L	289/308 (94%)	270 (93%)	16 (6%)	3 (1%)	15	45
1	M	291/308 (94%)	268 (92%)	14 (5%)	9 (3%)	4	16
1	R	290/308 (94%)	268 (92%)	19 (7%)	3 (1%)	15	45
1	S	291/308 (94%)	264 (91%)	24 (8%)	3 (1%)	15	45
1	T	291/308 (94%)	265 (91%)	21 (7%)	5 (2%)	9	31
All	All	4679/4928 (95%)	4300 (92%)	302 (6%)	77 (2%)	9	32

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1097	GLU
1	C	1055	LYS
1	C	1163	THR
1	D	1038	ALA
1	D	1163	THR

5.3.2 Protein sidechains ⓘ

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	259/265 (98%)	228 (88%)	31 (12%)	5	15
1	B	258/265 (97%)	217 (84%)	41 (16%)	2	7
1	C	257/265 (97%)	222 (86%)	35 (14%)	3	11
1	D	257/265 (97%)	231 (90%)	26 (10%)	7	23
1	E	256/265 (97%)	219 (86%)	37 (14%)	3	9
1	F	259/265 (98%)	223 (86%)	36 (14%)	3	10
1	G	260/265 (98%)	223 (86%)	37 (14%)	3	10
1	H	259/265 (98%)	226 (87%)	33 (13%)	4	13
1	I	256/265 (97%)	212 (83%)	44 (17%)	2	6
1	J	254/265 (96%)	230 (91%)	24 (9%)	8	26
1	K	254/265 (96%)	224 (88%)	30 (12%)	5	16
1	L	254/265 (96%)	226 (89%)	28 (11%)	6	19
1	M	255/265 (96%)	220 (86%)	35 (14%)	3	11
1	R	255/265 (96%)	223 (88%)	32 (12%)	4	14
1	S	256/265 (97%)	223 (87%)	33 (13%)	4	13
1	T	256/265 (97%)	220 (86%)	36 (14%)	3	10
All	All	4105/4240 (97%)	3567 (87%)	538 (13%)	4	12

5 of 538 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	1222	LEU
1	S	1035	VAL
1	R	1219	GLU
1	T	1058	ASN
1	F	1132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	1214	GLN
1	S	1236	ASN
1	L	1058	ASN
1	R	1236	ASN
1	T	1073	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PTR	E	1161	1	11,12,17	0.72	0	12,15,24	0.52	0
1	PTR	A	1166	1	15,16,17	2.01	2 (13%)	19,22,24	0.78	1 (5%)
1	PTR	R	1165	1	15,16,17	1.97	2 (13%)	19,22,24	0.63	0
1	PTR	G	1161	1	11,12,17	0.57	0	12,15,24	0.29	0
1	PTR	H	1166	1	15,16,17	1.92	2 (13%)	19,22,24	0.70	0
1	PTR	C	1166	1	15,16,17	2.07	1 (6%)	19,22,24	0.69	1 (5%)
1	PTR	R	1166	1	15,16,17	1.90	2 (13%)	19,22,24	0.66	0
1	PTR	K	1161	1	11,12,17	0.66	0	12,15,24	0.27	0
1	PTR	D	1166	1	15,16,17	2.00	2 (13%)	19,22,24	0.80	1 (5%)
1	PTR	T	1161	1	11,12,17	0.61	0	12,15,24	0.51	0
1	PTR	L	1161	1	11,12,17	0.75	0	12,15,24	0.34	0
1	PTR	B	1161	1	11,12,17	0.70	0	12,15,24	0.22	0
1	PTR	J	1161	1	11,12,17	0.70	0	12,15,24	0.19	0
1	PTR	R	1161	1	11,12,17	0.63	0	12,15,24	0.29	0
1	PTR	T	1165	1	15,16,17	1.99	1 (6%)	19,22,24	0.65	0
1	PTR	G	1165	1	15,16,17	1.95	2 (13%)	19,22,24	0.81	1 (5%)
1	PTR	I	1161	1	11,12,17	0.61	0	12,15,24	0.29	0
1	PTR	C	1165	1	15,16,17	2.01	2 (13%)	19,22,24	0.60	0
1	PTR	J	1166	1	15,16,17	1.95	2 (13%)	19,22,24	0.97	1 (5%)
1	PTR	D	1165	1	15,16,17	1.96	1 (6%)	19,22,24	0.65	1 (5%)
1	PTR	B	1166	1	15,16,17	2.16	2 (13%)	19,22,24	1.11	2 (10%)
1	PTR	A	1165	1	15,16,17	1.93	1 (6%)	19,22,24	0.52	0
1	PTR	F	1165	1	15,16,17	1.93	1 (6%)	19,22,24	0.81	1 (5%)
1	PTR	I	1166	1	15,16,17	1.99	2 (13%)	19,22,24	1.01	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PTR	G	1166	1	15,16,17	2.03	2 (13%)	19,22,24	0.71	1 (5%)
1	PTR	F	1161	1	11,12,17	0.77	0	12,15,24	0.29	0
1	PTR	K	1166	1	15,16,17	1.91	2 (13%)	19,22,24	0.88	0
1	PTR	S	1165	1	15,16,17	1.94	1 (6%)	19,22,24	0.73	1 (5%)
1	PTR	S	1161	1	11,12,17	0.55	0	12,15,24	0.24	0
1	PTR	C	1161	1	11,12,17	0.76	0	12,15,24	0.30	0
1	PTR	M	1161	1	11,12,17	0.77	0	12,15,24	0.31	0
1	PTR	L	1166	1	15,16,17	2.01	2 (13%)	19,22,24	0.94	2 (10%)
1	PTR	E	1165	1	15,16,17	2.03	1 (6%)	19,22,24	0.91	2 (10%)
1	PTR	A	1161	1	15,16,17	1.98	2 (13%)	19,22,24	0.86	1 (5%)
1	PTR	F	1166	1	15,16,17	1.97	2 (13%)	19,22,24	0.86	1 (5%)
1	PTR	I	1165	1	15,16,17	2.02	1 (6%)	19,22,24	0.54	0
1	PTR	D	1161	1	11,12,17	0.68	0	12,15,24	0.46	0
1	PTR	S	1166	1	15,16,17	1.96	2 (13%)	19,22,24	0.76	1 (5%)
1	PTR	K	1165	1	15,16,17	1.97	1 (6%)	19,22,24	0.48	0
1	PTR	H	1165	1	15,16,17	1.93	2 (13%)	19,22,24	0.69	0
1	PTR	E	1166	1	15,16,17	1.97	2 (13%)	19,22,24	0.60	0
1	PTR	J	1165	1	15,16,17	2.00	2 (13%)	19,22,24	0.75	1 (5%)
1	PTR	B	1165	1	15,16,17	1.98	1 (6%)	19,22,24	0.65	1 (5%)
1	PTR	M	1166	1	15,16,17	2.13	3 (20%)	19,22,24	1.72	6 (31%)
1	PTR	M	1165	1	15,16,17	1.95	1 (6%)	19,22,24	0.64	1 (5%)
1	PTR	L	1165	1	15,16,17	1.96	1 (6%)	19,22,24	0.49	0
1	PTR	T	1166	1	15,16,17	1.91	2 (13%)	19,22,24	0.81	1 (5%)
1	PTR	H	1161	1	11,12,17	0.68	0	12,15,24	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	E	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	A	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	R	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	G	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	H	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	C	1166	1	-	2/10/11/13	0/1/1/1
1	PTR	R	1166	1	-	2/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	K	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	D	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	T	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	L	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	B	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	J	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	R	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	T	1165	1	-	2/10/11/13	0/1/1/1
1	PTR	G	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	I	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	C	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	J	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	D	1165	1	-	1/10/11/13	0/1/1/1
1	PTR	B	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	F	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	I	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	G	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	F	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	K	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	S	1165	1	-	1/10/11/13	0/1/1/1
1	PTR	S	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	C	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	M	1161	1	-	2/5/6/13	0/1/1/1
1	PTR	L	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	E	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1161	1	-	0/10/11/13	0/1/1/1
1	PTR	F	1166	1	-	1/10/11/13	0/1/1/1
1	PTR	I	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	D	1161	1	-	0/5/6/13	0/1/1/1
1	PTR	S	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	K	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	H	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	E	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	J	1165	1	-	1/10/11/13	0/1/1/1
1	PTR	B	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	M	1166	1	-	2/10/11/13	0/1/1/1
1	PTR	M	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	L	1165	1	-	0/10/11/13	0/1/1/1
1	PTR	T	1166	1	-	0/10/11/13	0/1/1/1
1	PTR	H	1161	1	-	1/5/6/13	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1166	PTR	OH-CZ	-7.68	1.23	1.40
1	E	1165	PTR	OH-CZ	-7.59	1.23	1.40
1	G	1166	PTR	OH-CZ	-7.47	1.23	1.40
1	I	1165	PTR	OH-CZ	-7.46	1.23	1.40
1	T	1165	PTR	OH-CZ	-7.36	1.23	1.40

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	1166	PTR	OH-CZ-CE1	3.60	129.95	119.23
1	I	1166	PTR	O3P-P-OH	3.26	115.43	105.24
1	M	1166	PTR	O3P-P-OH	2.97	114.52	105.24
1	J	1166	PTR	O2P-P-OH	2.82	114.06	105.24
1	A	1161	PTR	CB-CA-C	-2.65	106.50	111.47

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1166	PTR	CZ-OH-P-O1P
1	F	1166	PTR	CZ-OH-P-O1P
1	D	1165	PTR	N-CA-CB-CG
1	S	1165	PTR	N-CA-CB-CG
1	M	1161	PTR	CA-CB-CG-CD1

There are no ring outliers.

37 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1166	PTR	2	0
1	R	1165	PTR	2	0
1	G	1161	PTR	3	0
1	C	1166	PTR	2	0
1	R	1166	PTR	1	0
1	K	1161	PTR	1	0
1	T	1161	PTR	5	0
1	L	1161	PTR	4	0
1	B	1161	PTR	1	0
1	J	1161	PTR	1	0
1	R	1161	PTR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	T	1165	PTR	2	0
1	G	1165	PTR	4	0
1	I	1161	PTR	4	0
1	C	1165	PTR	3	0
1	D	1165	PTR	1	0
1	B	1166	PTR	2	0
1	F	1165	PTR	2	0
1	G	1166	PTR	1	0
1	F	1161	PTR	1	0
1	K	1166	PTR	1	0
1	S	1165	PTR	1	0
1	S	1161	PTR	8	0
1	M	1161	PTR	5	0
1	A	1161	PTR	1	0
1	F	1166	PTR	1	0
1	I	1165	PTR	3	0
1	D	1161	PTR	1	0
1	S	1166	PTR	1	0
1	K	1165	PTR	2	0
1	H	1165	PTR	1	0
1	E	1166	PTR	4	0
1	B	1165	PTR	4	0
1	M	1166	PTR	6	0
1	M	1165	PTR	2	0
1	L	1165	PTR	4	0
1	H	1161	PTR	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	741	K	11	-	39,41,41	0.99	1 (2%)	47,56,56	2.40	14 (29%)
2	741	F	6	-	39,41,41	1.05	3 (7%)	47,56,56	2.29	16 (34%)
2	741	H	8	-	39,41,41	0.97	2 (5%)	47,56,56	2.24	14 (29%)
2	741	A	1	-	39,41,41	1.05	3 (7%)	47,56,56	2.25	14 (29%)
2	741	S	15	-	39,41,41	0.98	2 (5%)	47,56,56	2.43	18 (38%)
2	741	E	5	-	39,41,41	1.10	2 (5%)	47,56,56	2.33	13 (27%)
2	741	T	16	-	39,41,41	1.01	2 (5%)	47,56,56	2.57	14 (29%)
2	741	G	7	-	39,41,41	0.97	2 (5%)	47,56,56	2.33	15 (31%)
2	741	B	2	-	39,41,41	1.01	2 (5%)	47,56,56	2.49	14 (29%)
2	741	R	14	-	39,41,41	1.16	4 (10%)	47,56,56	2.21	13 (27%)
2	741	C	3	-	39,41,41	1.04	2 (5%)	47,56,56	2.18	13 (27%)
2	741	I	9	-	39,41,41	0.95	2 (5%)	47,56,56	2.37	13 (27%)
2	741	M	12	-	39,41,41	1.01	2 (5%)	47,56,56	2.14	11 (23%)
2	741	D	4	-	39,41,41	1.14	2 (5%)	47,56,56	2.15	15 (31%)
2	741	J	10	-	39,41,41	1.13	3 (7%)	47,56,56	2.23	15 (31%)
2	741	L	13	-	39,41,41	1.12	4 (10%)	47,56,56	2.48	15 (31%)

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	741	K	11	-	-	6/20/22/22	0/4/4/4
2	741	F	6	-	-	7/20/22/22	0/4/4/4
2	741	H	8	-	-	8/20/22/22	0/4/4/4
2	741	A	1	-	-	11/20/22/22	0/4/4/4
2	741	S	15	-	-	11/20/22/22	0/4/4/4
2	741	E	5	-	-	6/20/22/22	0/4/4/4
2	741	T	16	-	-	8/20/22/22	0/4/4/4
2	741	G	7	-	-	12/20/22/22	0/4/4/4
2	741	B	2	-	-	8/20/22/22	0/4/4/4
2	741	R	14	-	-	7/20/22/22	0/4/4/4
2	741	C	3	-	-	9/20/22/22	0/4/4/4
2	741	I	9	-	-	5/20/22/22	0/4/4/4
2	741	M	12	-	-	5/20/22/22	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	741	D	4	-	-	7/20/22/22	0/4/4/4
2	741	J	10	-	-	7/20/22/22	0/4/4/4
2	741	L	13	-	-	10/20/22/22	0/4/4/4

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	13	741	C3-C2	2.88	1.41	1.36
2	C	3	741	C3-C2	2.87	1.41	1.36
2	D	4	741	C3-C2	2.80	1.41	1.36
2	R	14	741	C3-C2	2.79	1.41	1.36
2	L	13	741	C6-C1	2.72	1.41	1.36

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	16	741	O11-C1-C6	-8.35	114.45	125.24
2	J	10	741	O11-C1-C6	-6.97	116.22	125.24
2	L	13	741	O11-C1-C6	-6.90	116.31	125.24
2	B	2	741	O11-C1-C6	-6.90	116.32	125.24
2	E	5	741	C29-N30-C26	-6.87	102.03	108.56

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	741	C14-C15-N34-C35
2	B	2	741	N34-C35-C37-O38
2	C	3	741	N33-C32-C9-C8
2	C	3	741	N33-C32-C9-C10
2	C	3	741	C13-C14-C15-N34

There are no ring outliers.

16 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	11	741	2	0
2	F	6	741	5	0
2	H	8	741	4	0
2	A	1	741	5	0

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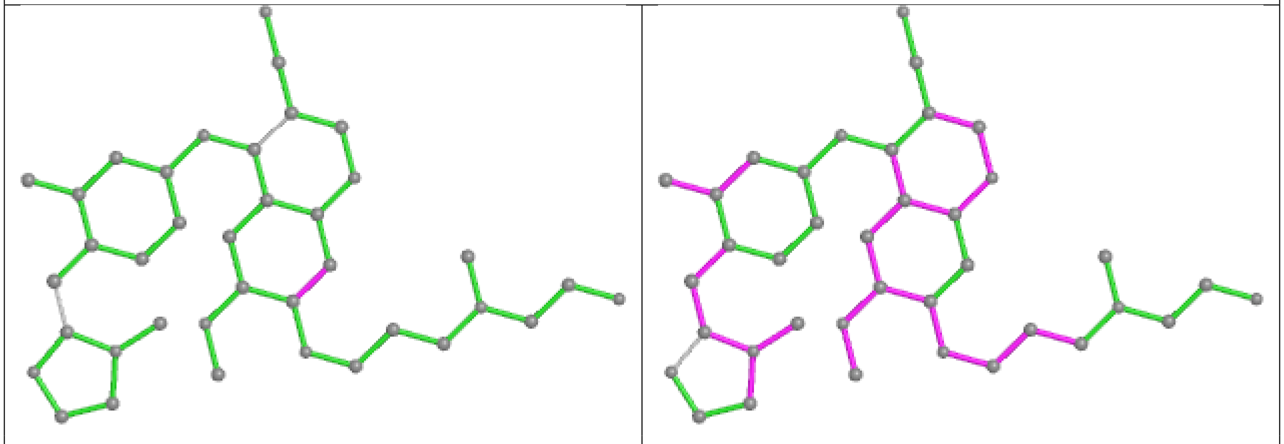
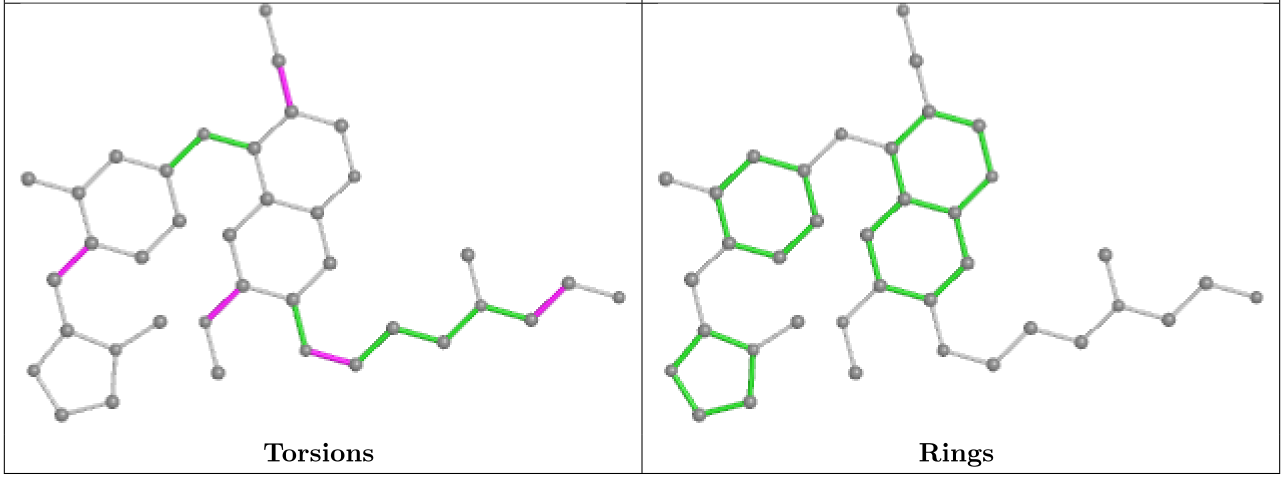
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	15	741	4	0
2	E	5	741	5	0
2	T	16	741	3	0
2	G	7	741	2	0
2	B	2	741	3	0
2	R	14	741	6	0
2	C	3	741	2	0
2	I	9	741	9	0
2	M	12	741	1	0
2	D	4	741	1	0
2	J	10	741	2	0
2	L	13	741	3	0

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

Ligand 741 K 11

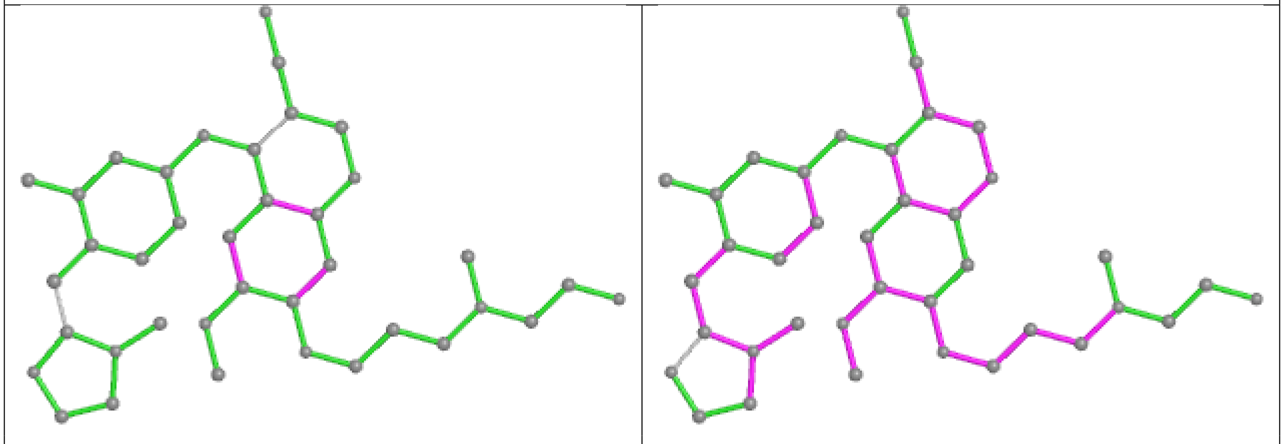


Bond lengths **Bond angles**



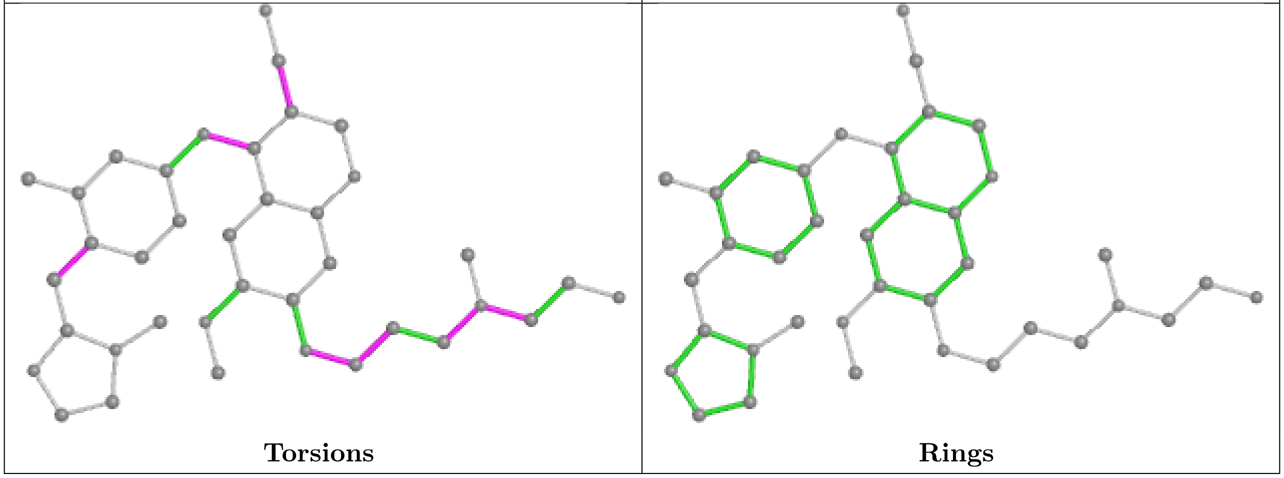
Torsions **Rings**

Ligand 741 F 6



Bond lengths

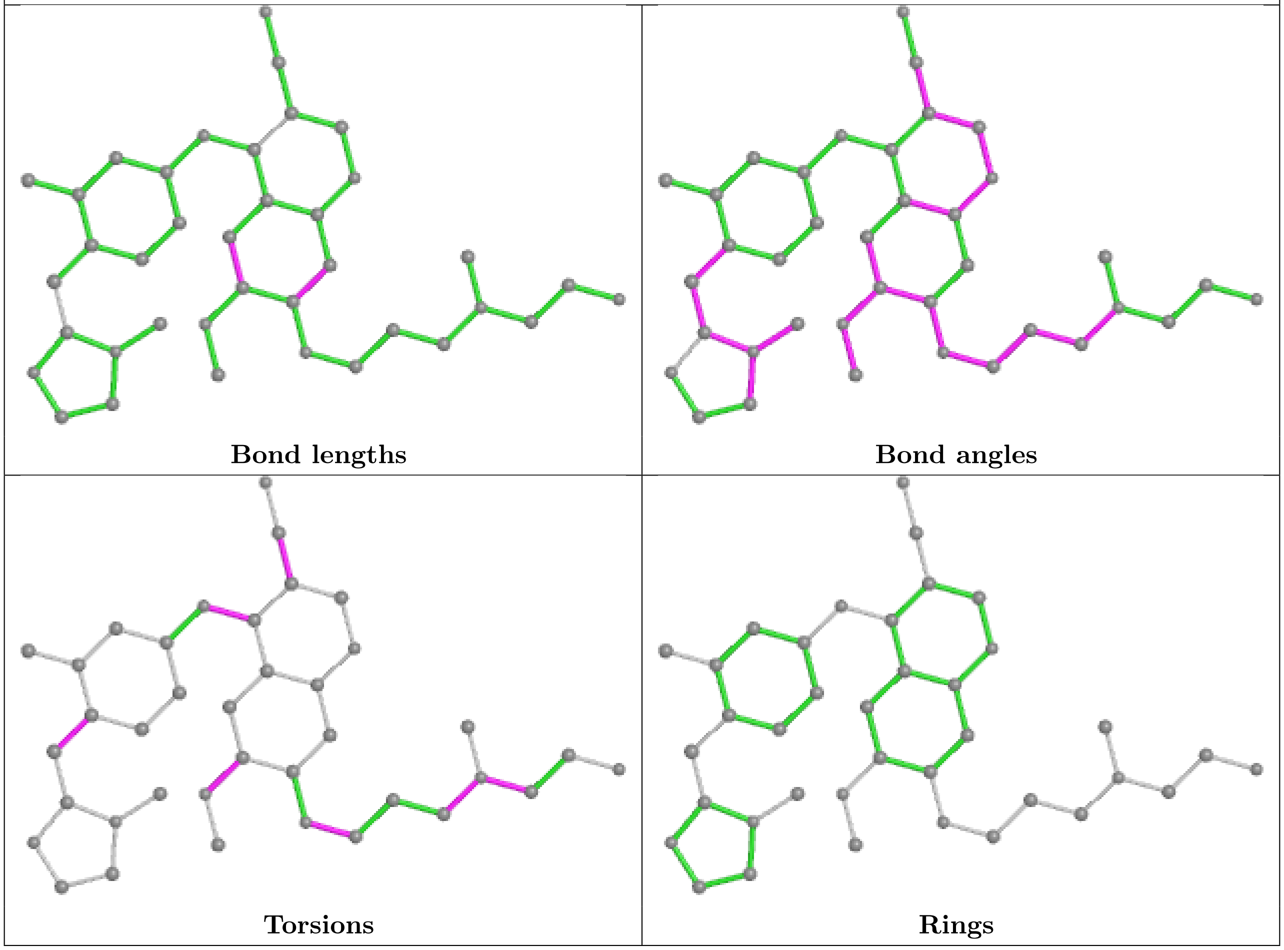
Bond angles



Torsions

Rings

Ligand 741 H 8



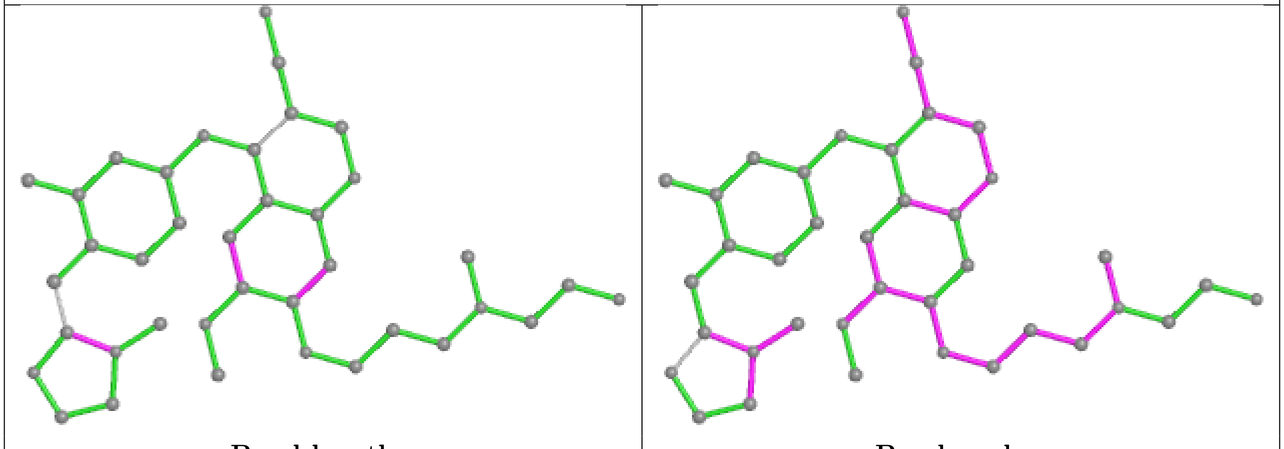
Bond lengths

Bond angles

Torsions

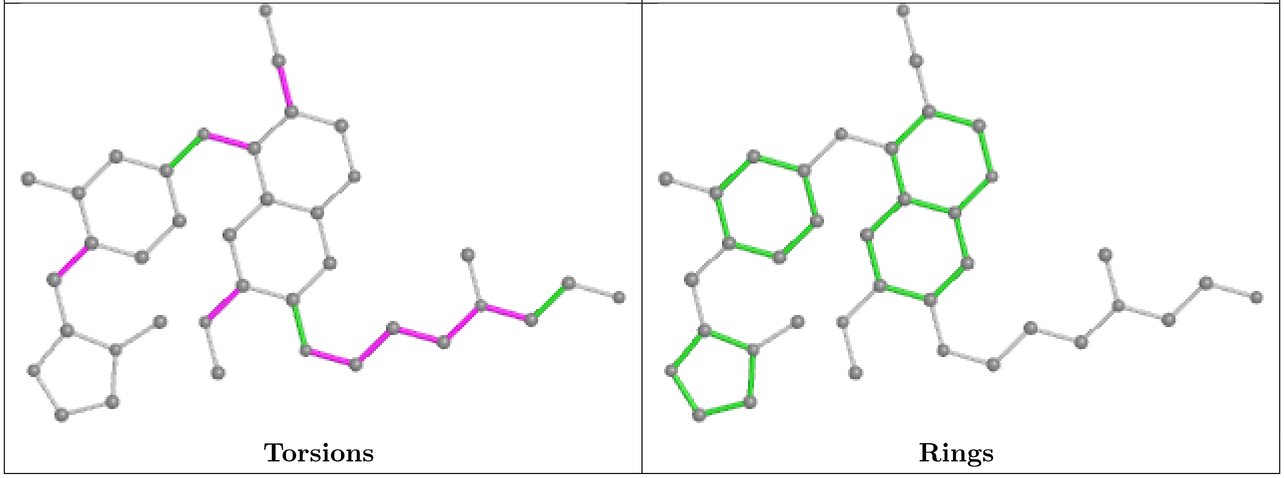
Rings

Ligand 741 A 1



Bond lengths

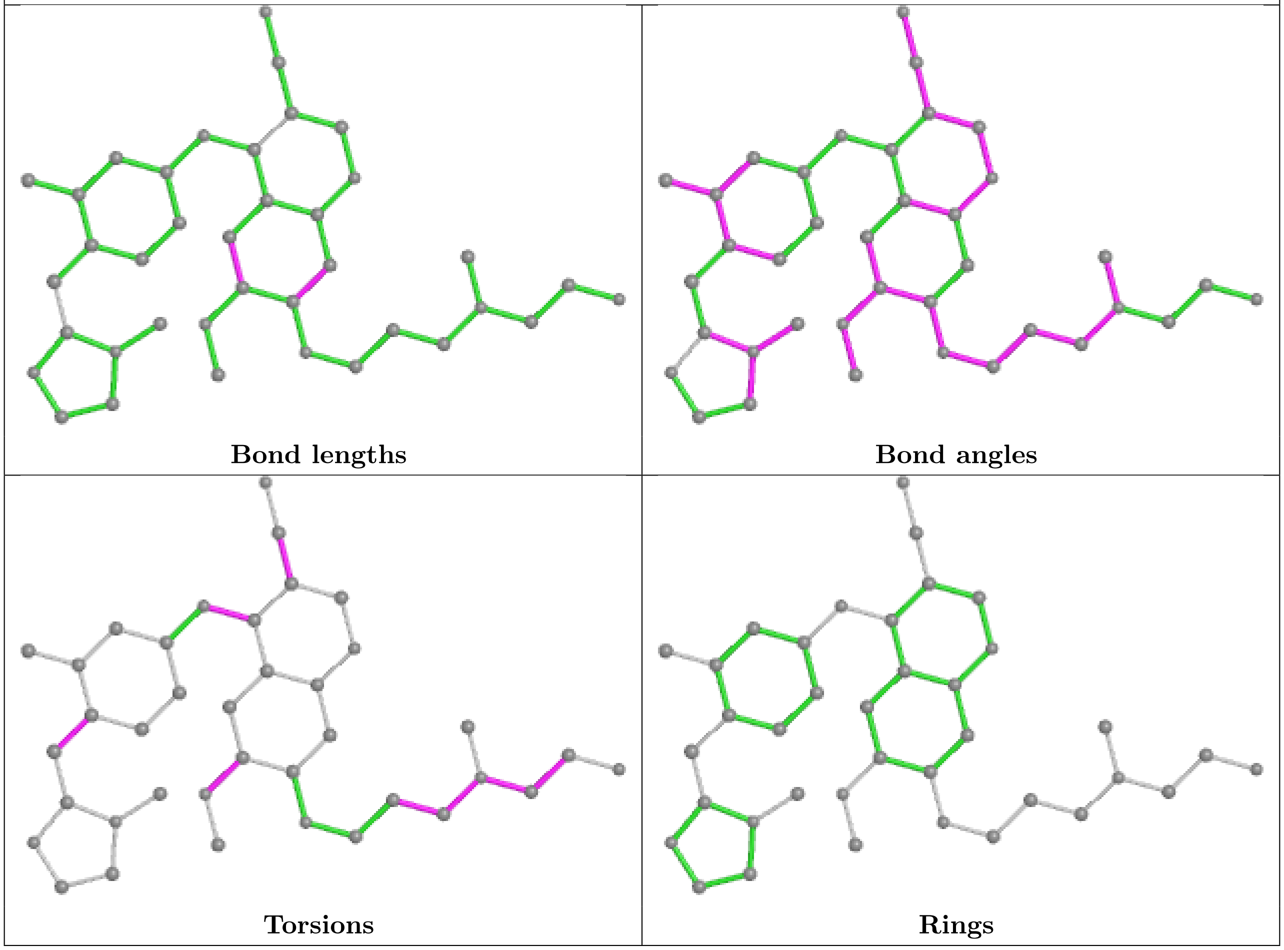
Bond angles



Torsions

Rings

Ligand 741 S 15



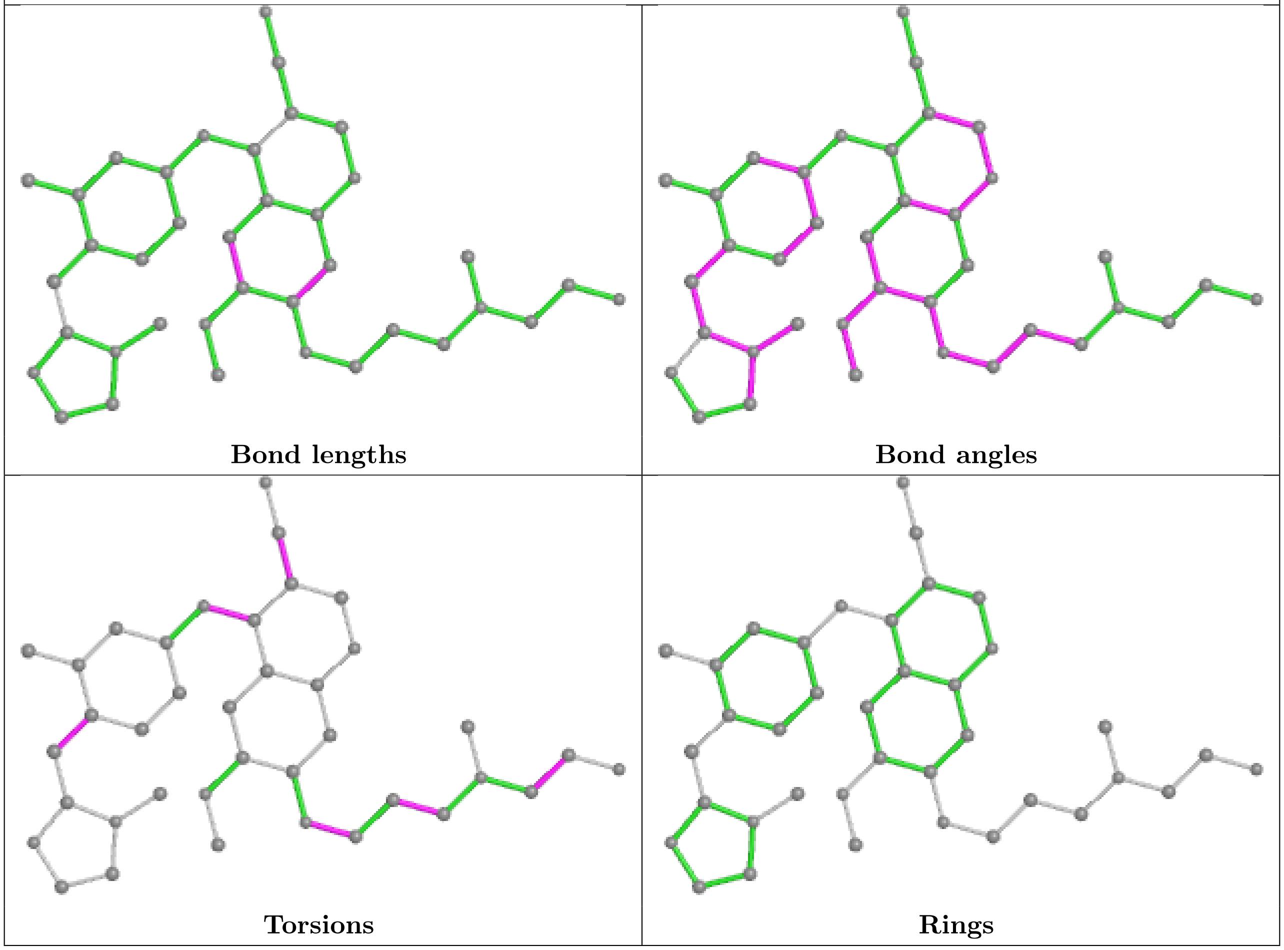
Bond lengths

Bond angles

Torsions

Rings

Ligand 741 E 5



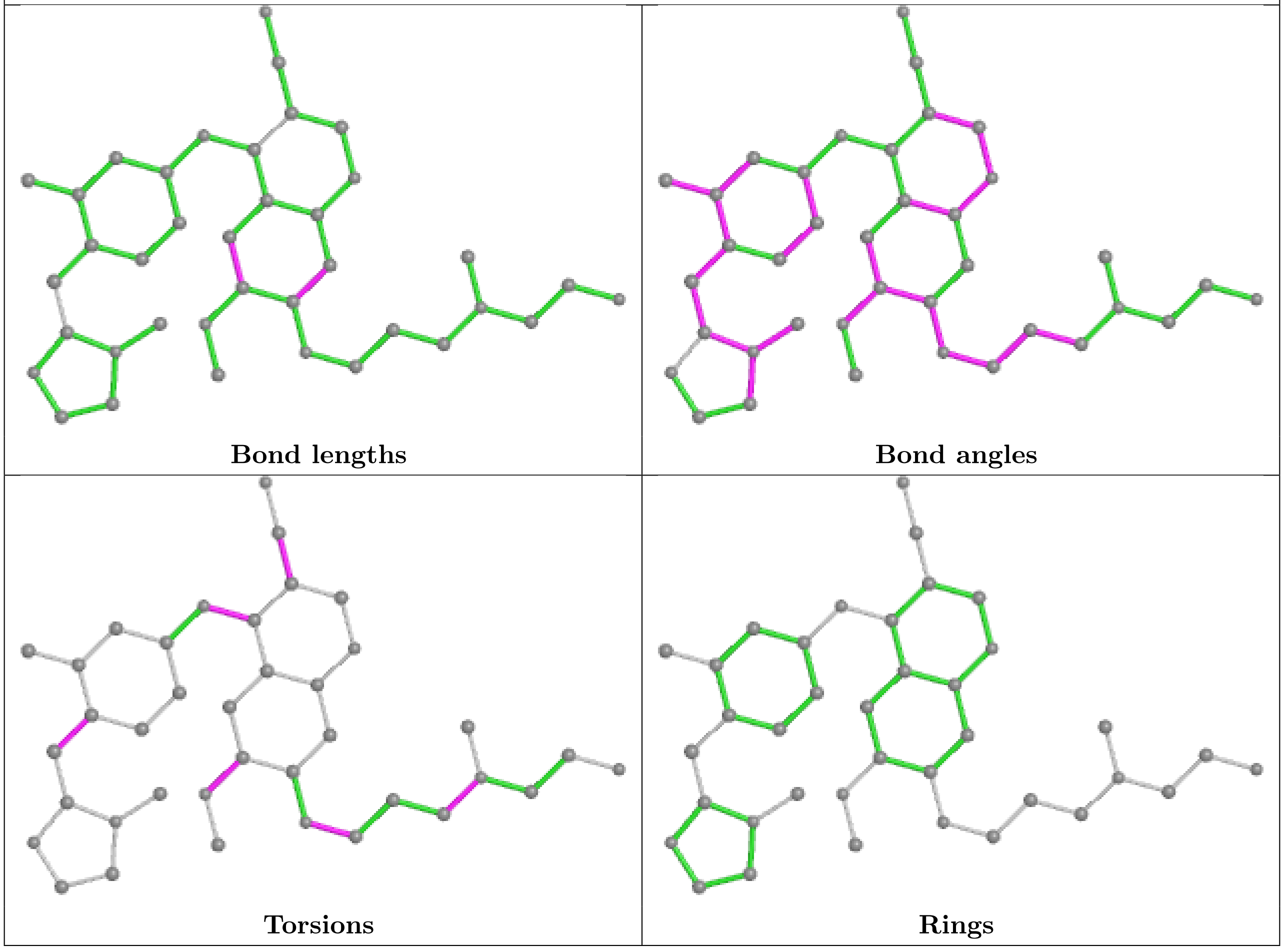
Bond lengths

Bond angles

Torsions

Rings

Ligand 741 T 16



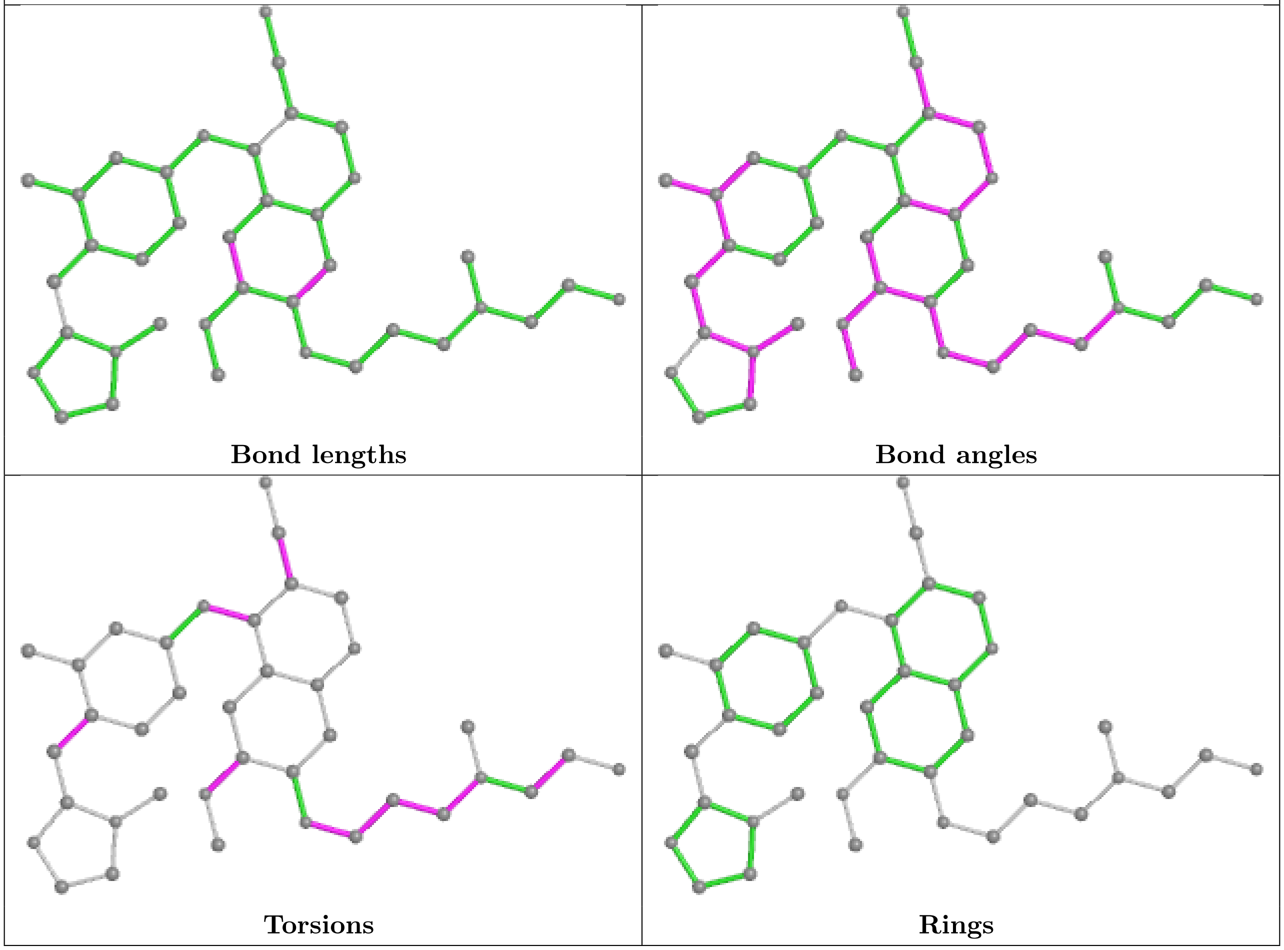
Bond lengths

Bond angles

Torsions

Rings

Ligand 741 G 7



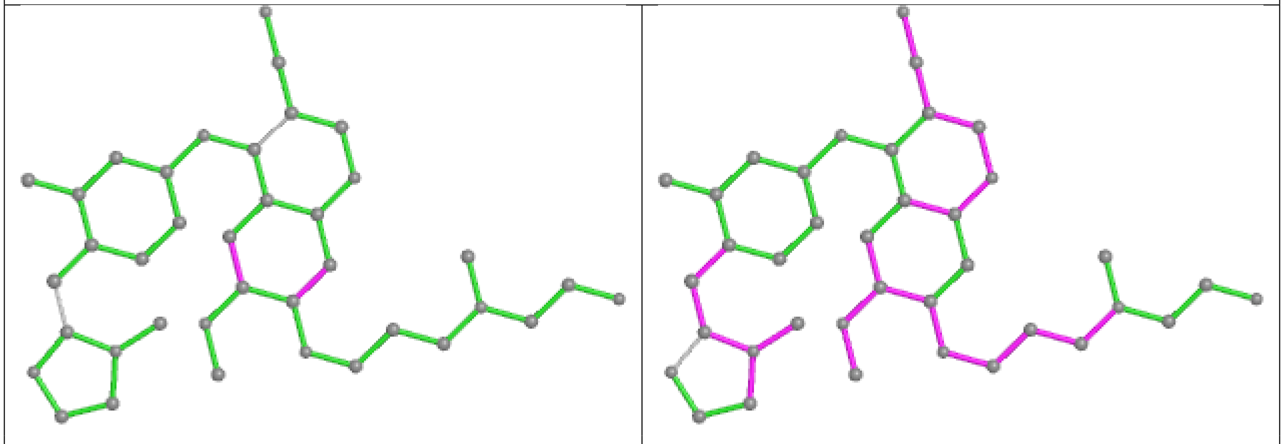
Bond lengths

Bond angles

Torsions

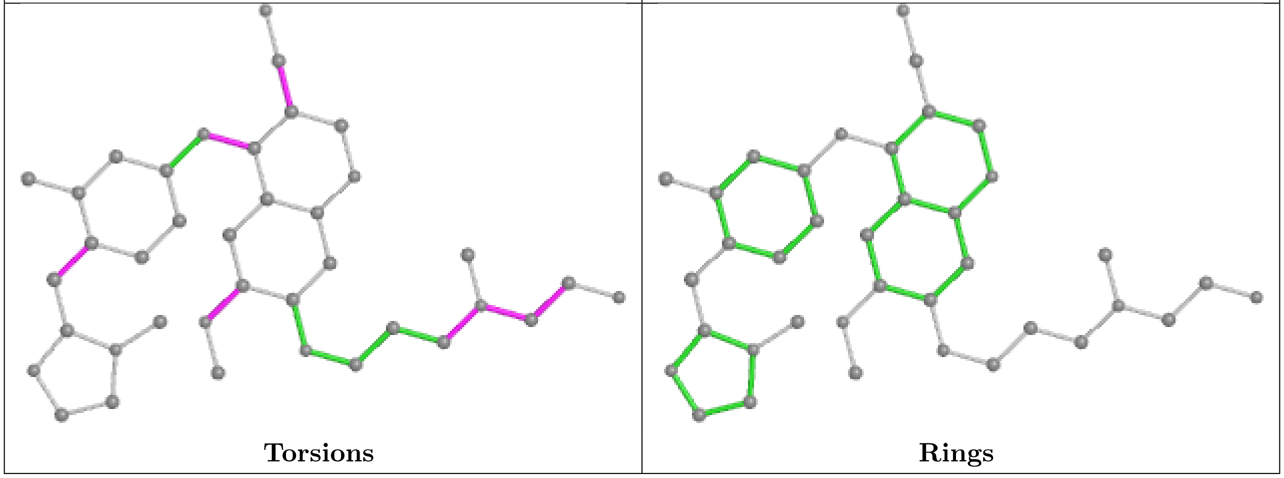
Rings

Ligand 741 B 2



Bond lengths

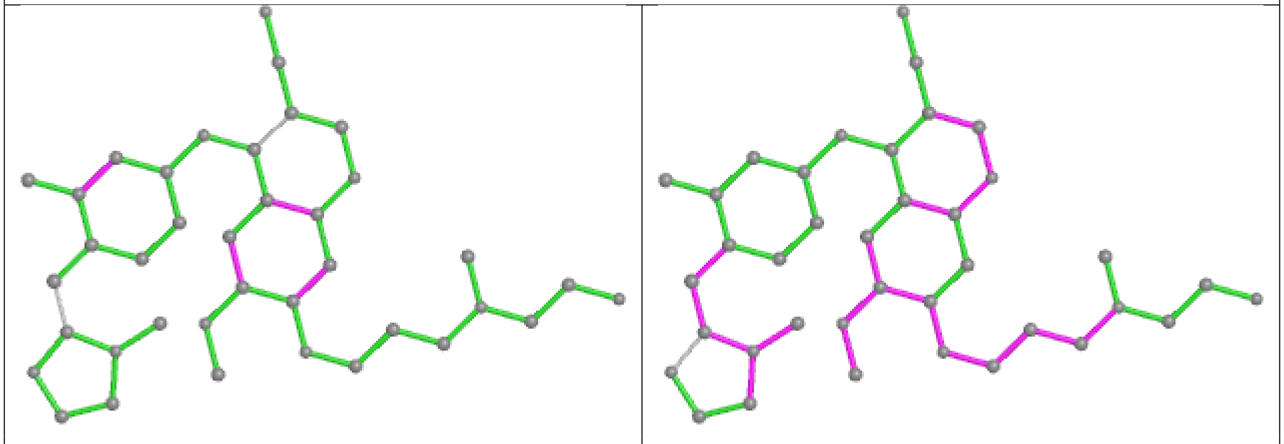
Bond angles



Torsions

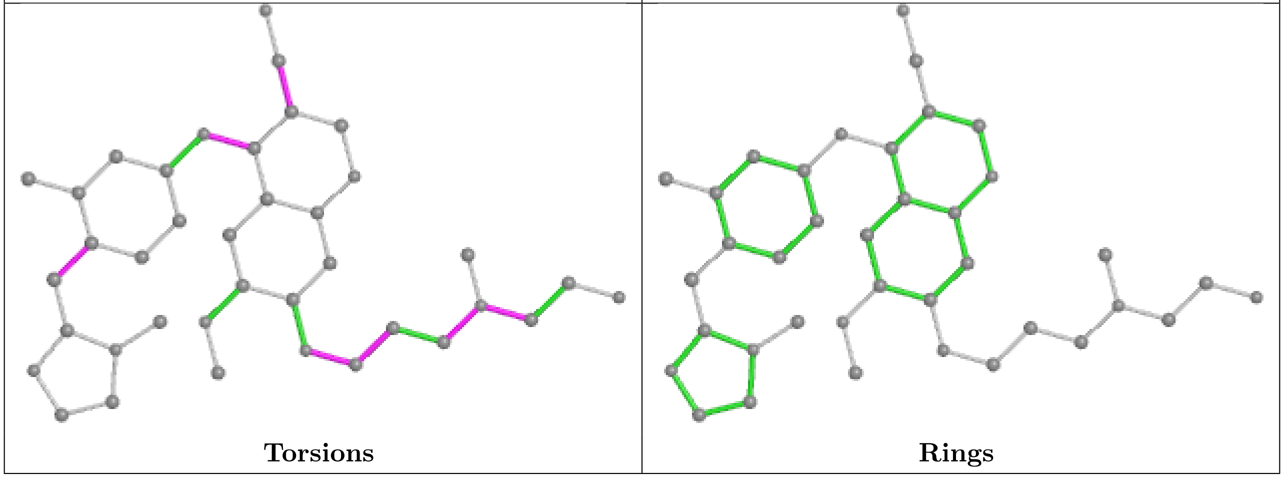
Rings

Ligand 741 R 14



Bond lengths

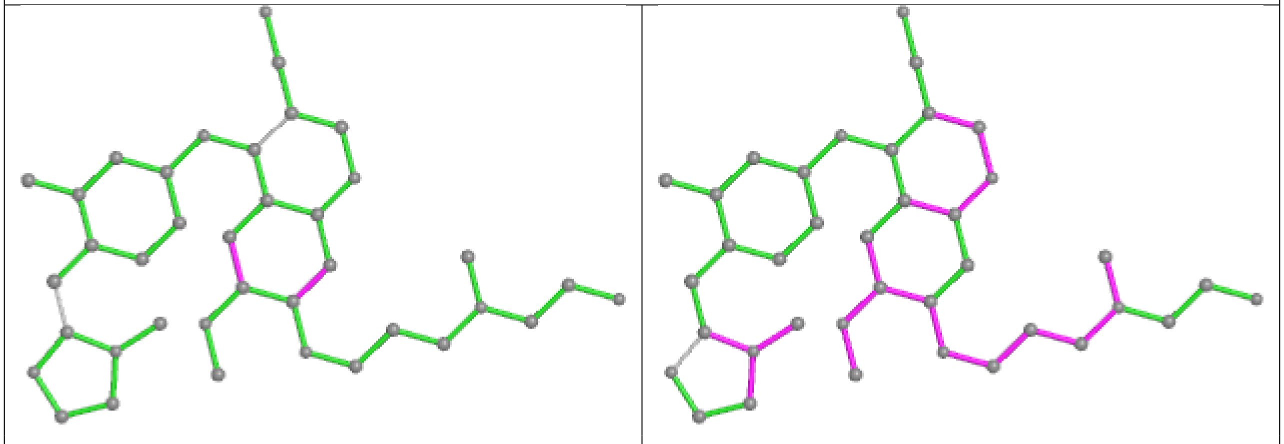
Bond angles



Torsions

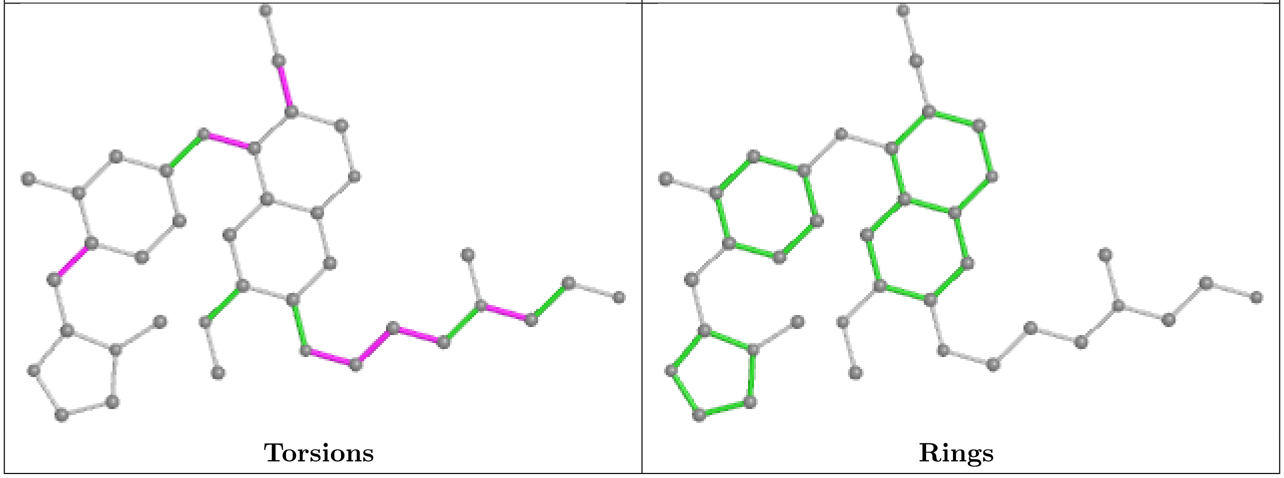
Rings

Ligand 741 C 3



Bond lengths

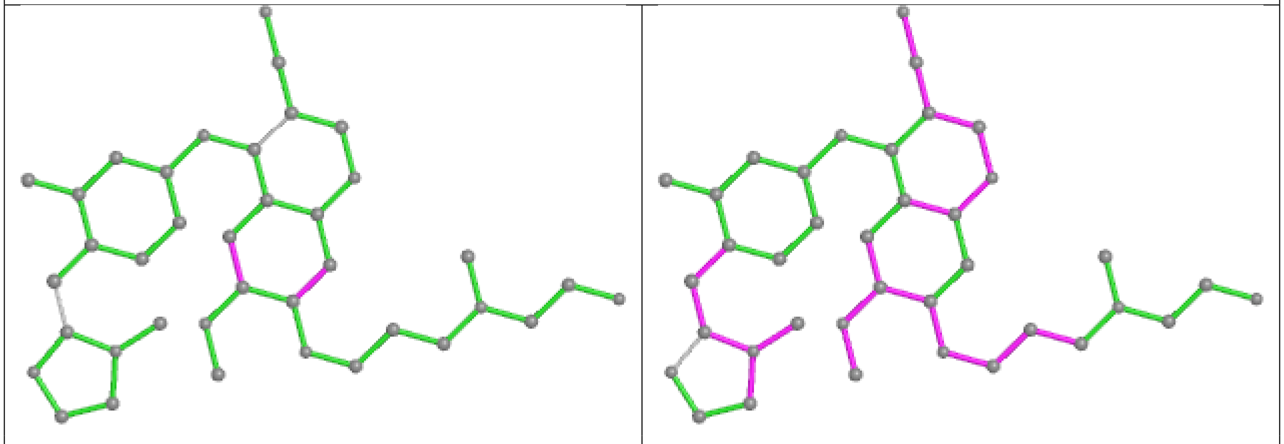
Bond angles



Torsions

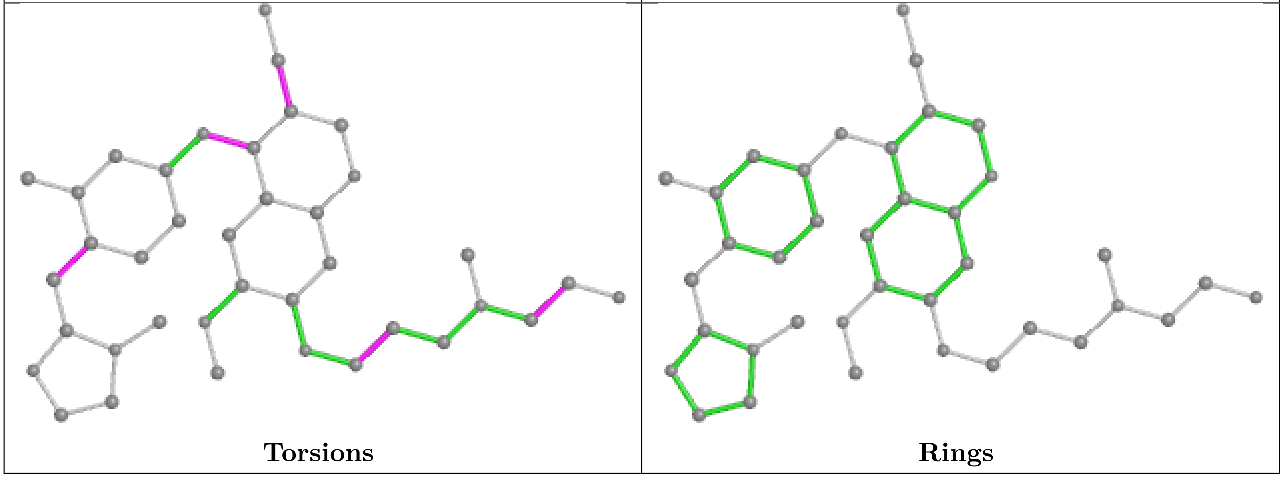
Rings

Ligand 741 I 9



Bond lengths

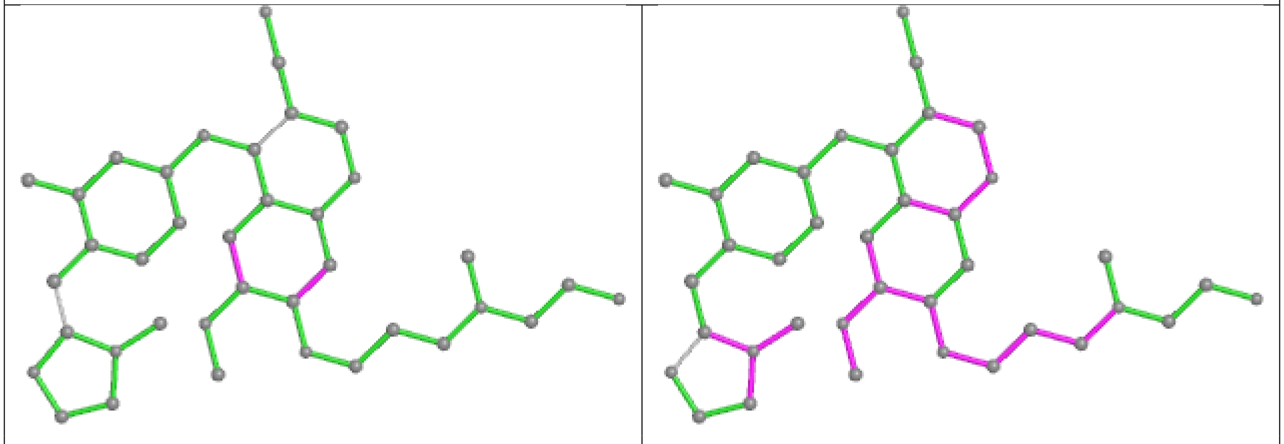
Bond angles



Torsions

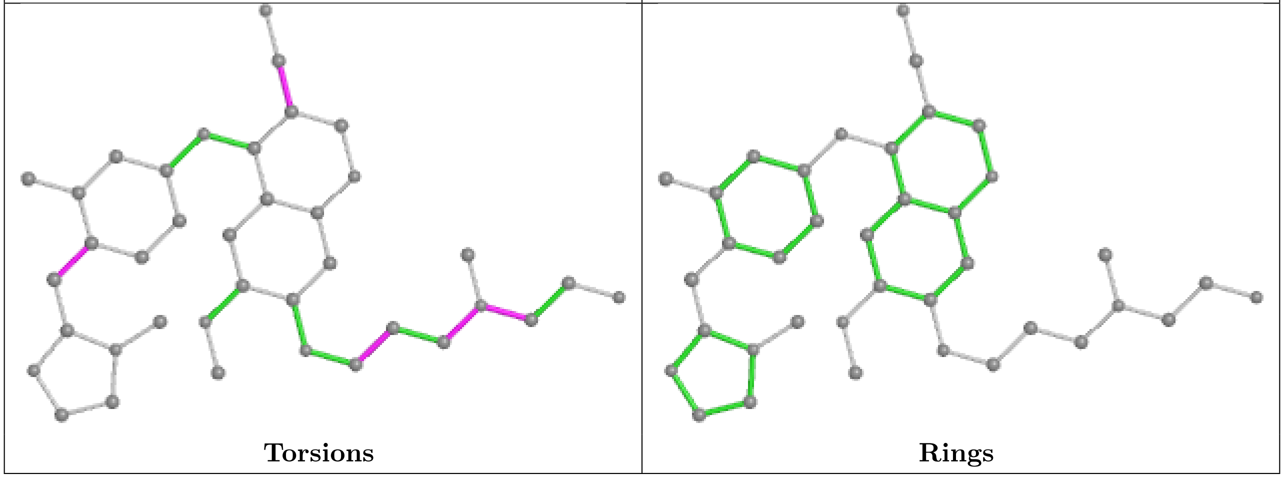
Rings

Ligand 741 M 12



Bond lengths

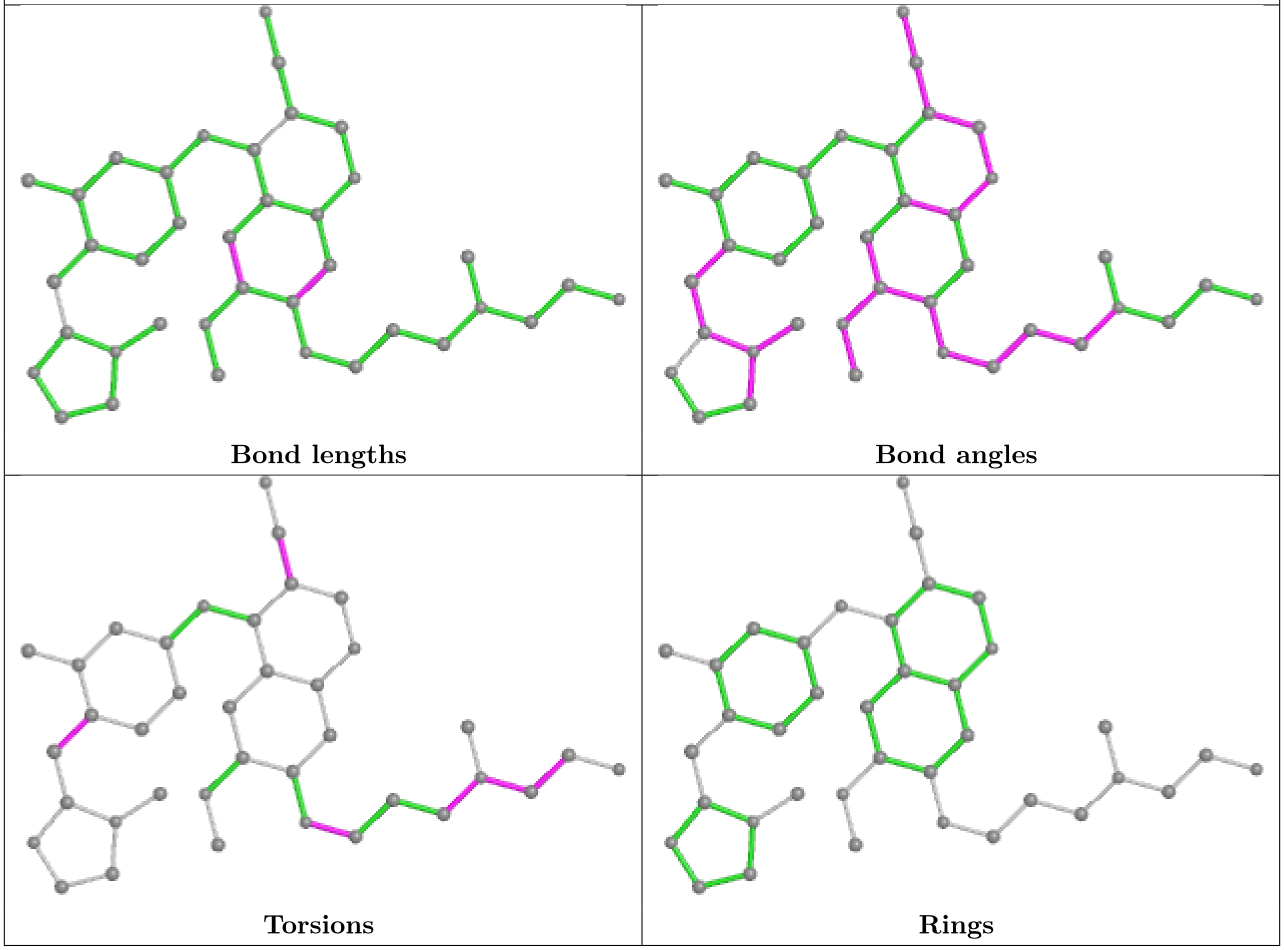
Bond angles



Torsions

Rings

Ligand 741 D 4



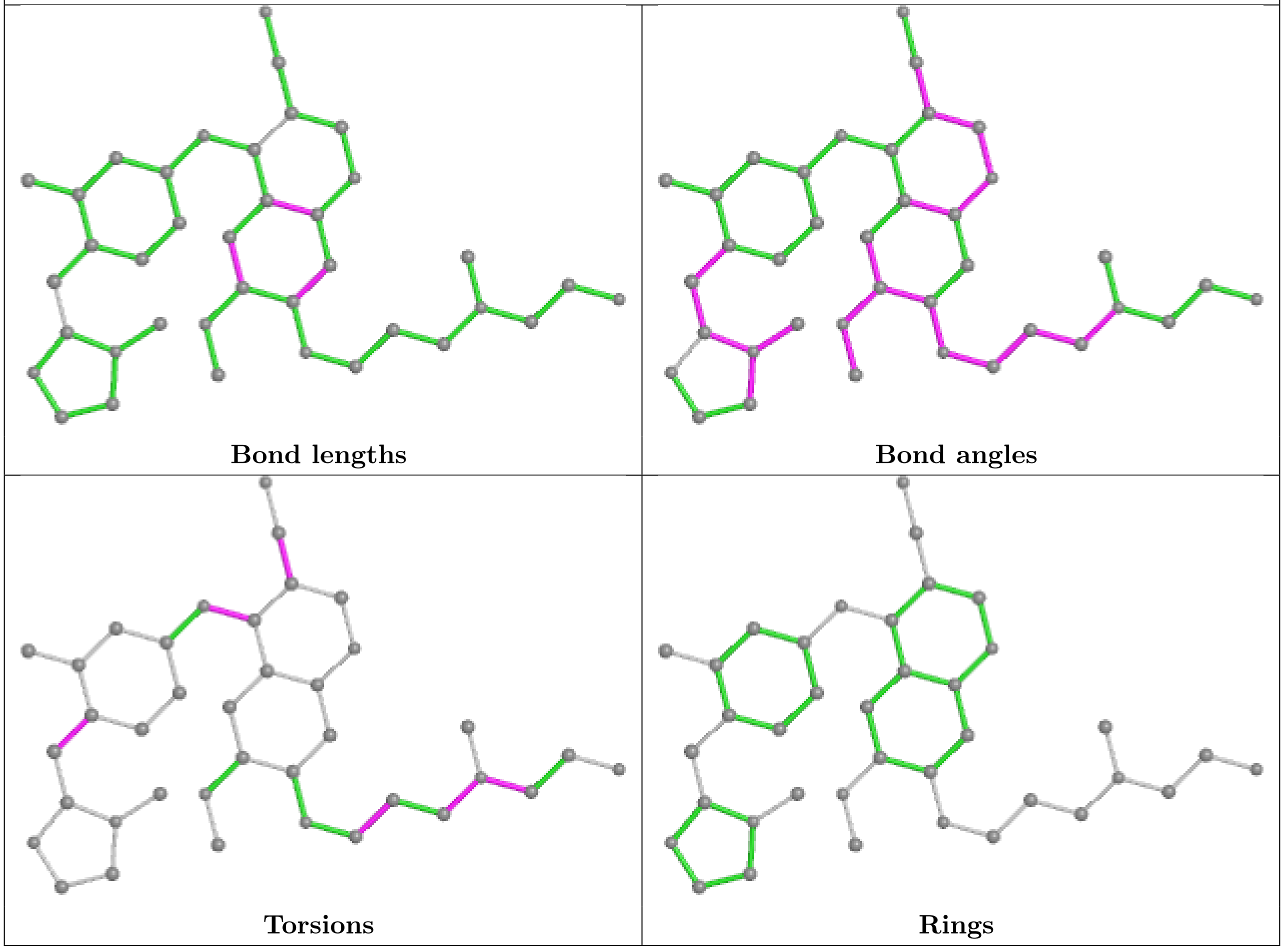
Bond lengths

Bond angles

Torsions

Rings

Ligand 741 J 10



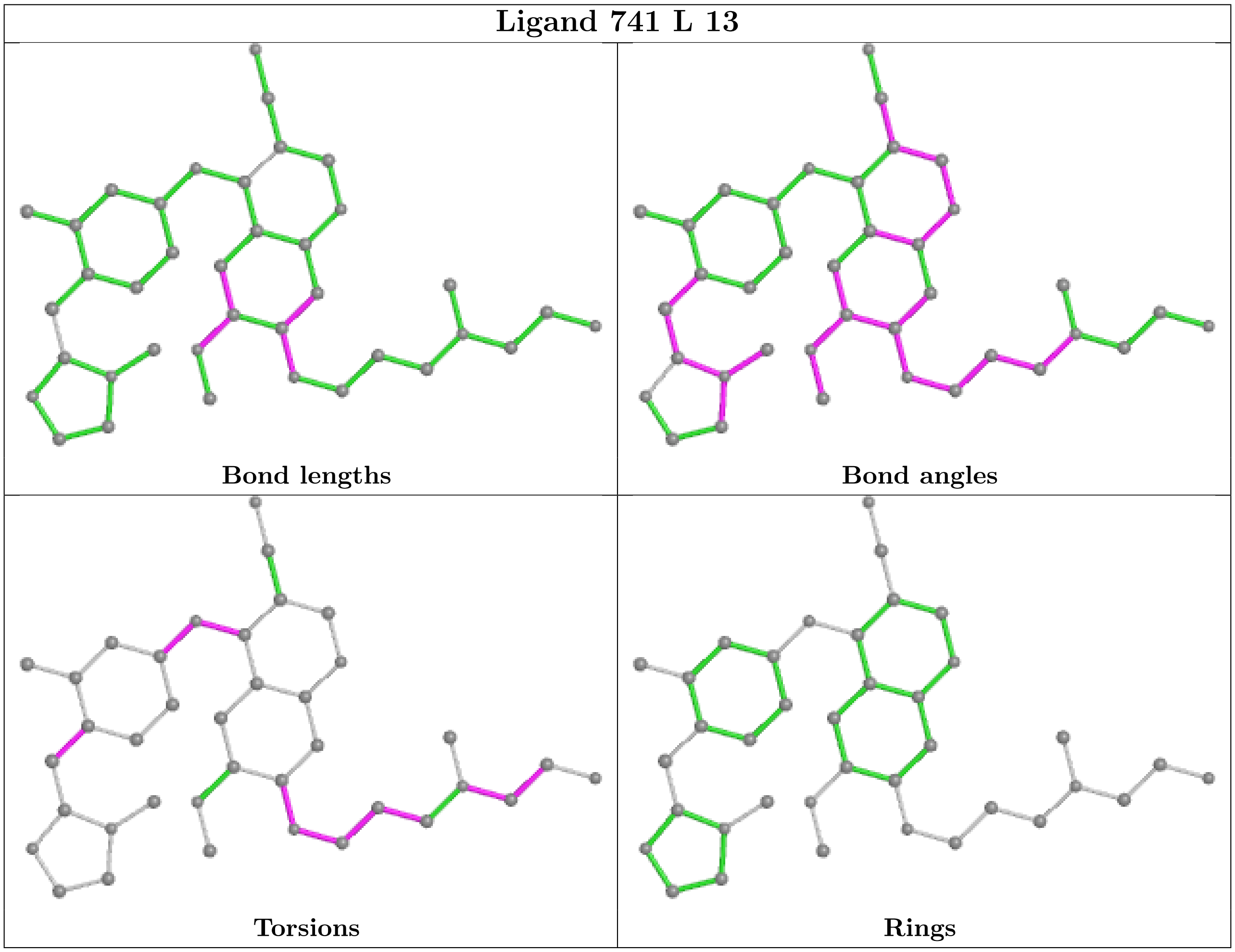
Bond lengths

Bond angles

Torsions

Rings

Ligand 741 L 13



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	299/308 (97%)	-0.24	5 (1%)	70	69	18, 36, 79, 100	0
1	B	298/308 (96%)	-0.23	4 (1%)	77	77	22, 39, 78, 98	0
1	C	301/308 (97%)	-0.16	9 (2%)	50	45	20, 42, 82, 108	0
1	D	297/308 (96%)	-0.18	6 (2%)	65	63	23, 41, 79, 106	0
1	E	299/308 (97%)	-0.05	11 (3%)	41	37	26, 45, 84, 105	0
1	F	299/308 (97%)	-0.11	11 (3%)	41	37	22, 43, 88, 108	0
1	G	299/308 (97%)	-0.23	4 (1%)	77	77	23, 41, 76, 100	0
1	H	299/308 (97%)	-0.13	10 (3%)	46	41	24, 43, 85, 107	0
1	I	294/308 (95%)	-0.31	4 (1%)	75	75	18, 31, 60, 84	0
1	J	293/308 (95%)	-0.29	3 (1%)	82	82	26, 39, 69, 92	0
1	K	293/308 (95%)	-0.19	3 (1%)	82	82	26, 41, 72, 93	0
1	L	293/308 (95%)	-0.23	7 (2%)	59	56	24, 41, 75, 92	0
1	M	295/308 (95%)	-0.24	2 (0%)	87	87	25, 40, 72, 88	0
1	R	294/308 (95%)	-0.29	2 (0%)	87	87	19, 38, 73, 94	0
1	S	295/308 (95%)	-0.07	8 (2%)	54	50	28, 46, 79, 110	0
1	T	295/308 (95%)	-0.17	6 (2%)	65	63	23, 40, 71, 86	0
All	All	4743/4928 (96%)	-0.19	95 (2%)	65	63	18, 41, 77, 110	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	1073	GLN	6.5
1	K	1073	GLN	6.1
1	D	1037	GLU	4.7
1	S	1073	GLN	4.5
1	E	1009	SER	4.3

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

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
1	PTR	K	1161	12/17	0.72	0.27	43,69,87,92	0
1	PTR	M	1161	12/17	0.75	0.26	49,64,81,84	0
1	PTR	L	1161	12/17	0.75	0.30	50,67,82,86	0
1	PTR	C	1161	12/17	0.77	0.37	50,67,81,88	0
1	PTR	B	1161	12/17	0.81	0.30	44,69,80,81	0
1	PTR	A	1161	16/17	0.82	0.30	46,81,114,234	0
1	PTR	D	1161	12/17	0.82	0.35	58,65,81,83	0
1	PTR	I	1161	12/17	0.82	0.24	39,64,80,83	0
1	PTR	T	1161	12/17	0.82	0.25	47,71,82,84	0
1	PTR	H	1161	12/17	0.84	0.27	53,70,78,81	0
1	PTR	F	1161	12/17	0.85	0.28	58,72,85,88	0
1	PTR	G	1161	12/17	0.85	0.31	49,60,71,73	0
1	PTR	R	1161	12/17	0.86	0.26	45,59,74,76	0
1	PTR	S	1161	12/17	0.86	0.20	51,61,68,68	0
1	PTR	J	1161	12/17	0.86	0.28	46,64,81,87	0
1	PTR	E	1161	12/17	0.88	0.23	53,68,76,81	0
1	PTR	F	1165	16/17	0.90	0.21	40,50,73,73	0
1	PTR	E	1165	16/17	0.91	0.19	38,46,51,61	0
1	PTR	B	1165	16/17	0.91	0.18	34,44,63,68	0
1	PTR	C	1165	16/17	0.91	0.19	32,46,60,63	0
1	PTR	M	1166	16/17	0.91	0.18	32,39,69,78	0
1	PTR	L	1165	16/17	0.92	0.20	40,47,66,72	0
1	PTR	M	1165	16/17	0.92	0.20	37,48,61,64	0
1	PTR	I	1165	16/17	0.92	0.20	32,44,64,66	0
1	PTR	S	1165	16/17	0.92	0.26	36,47,64,66	0
1	PTR	D	1165	16/17	0.92	0.19	42,51,63,63	0
1	PTR	T	1165	16/17	0.92	0.23	37,53,63,67	0
1	PTR	H	1165	16/17	0.93	0.20	40,48,55,56	0
1	PTR	K	1165	16/17	0.93	0.18	35,45,53,57	0
1	PTR	A	1165	16/17	0.93	0.20	37,44,59,61	0
1	PTR	J	1165	16/17	0.94	0.19	32,45,57,64	0
1	PTR	R	1165	16/17	0.94	0.18	33,44,64,64	0
1	PTR	G	1165	16/17	0.94	0.18	40,48,56,57	0
1	PTR	K	1166	16/17	0.96	0.14	29,38,47,48	0
1	PTR	F	1166	16/17	0.96	0.14	36,38,50,53	0
1	PTR	I	1166	16/17	0.96	0.15	27,33,45,48	0
1	PTR	B	1166	16/17	0.96	0.12	32,35,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	PTR	T	1166	16/17	0.96	0.14	38,44,54,55	0
1	PTR	D	1166	16/17	0.97	0.10	31,37,47,56	0
1	PTR	J	1166	16/17	0.97	0.13	26,31,44,44	0
1	PTR	S	1166	16/17	0.97	0.13	33,38,52,55	0
1	PTR	L	1166	16/17	0.97	0.14	36,39,55,56	0
1	PTR	H	1166	16/17	0.97	0.10	29,34,41,49	0
1	PTR	E	1166	16/17	0.97	0.11	27,31,39,43	0
1	PTR	A	1166	16/17	0.98	0.09	28,32,40,49	0
1	PTR	R	1166	16/17	0.98	0.11	29,34,44,48	0
1	PTR	G	1166	16/17	0.98	0.11	30,37,45,48	0
1	PTR	C	1166	16/17	0.98	0.10	30,33,38,42	0

6.3 Carbohydrates ⓘ

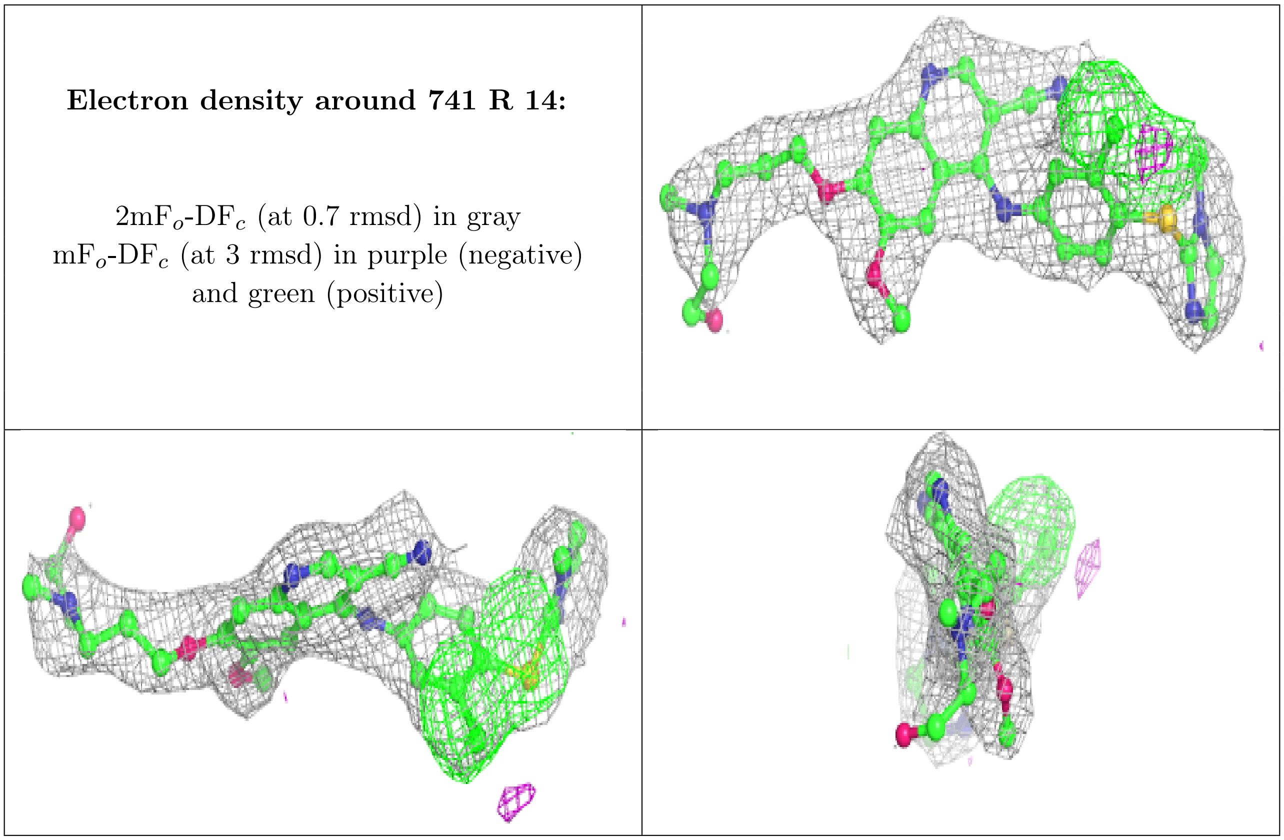
There are no monosaccharides in this entry.

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
2	741	R	14	38/38	0.84	0.22	24,34,59,304	0
2	741	E	5	38/38	0.88	0.20	40,45,57,58	0
2	741	D	4	38/38	0.90	0.21	31,41,57,78	0
2	741	H	8	38/38	0.91	0.20	33,44,53,60	0
2	741	B	2	38/38	0.92	0.19	31,36,59,84	0
2	741	G	7	38/38	0.93	0.17	31,38,48,54	0
2	741	A	1	38/38	0.94	0.18	24,33,51,60	0
2	741	C	3	38/38	0.94	0.17	32,39,55,84	0
2	741	J	10	38/38	0.94	0.17	20,30,48,69	0
2	741	K	11	38/38	0.94	0.15	29,36,52,59	0
2	741	F	6	38/38	0.94	0.17	33,41,55,58	0
2	741	S	15	38/38	0.94	0.15	27,42,67,77	0
2	741	L	13	38/38	0.95	0.14	24,30,44,51	0
2	741	I	9	38/38	0.95	0.14	17,21,34,53	0
2	741	M	12	38/38	0.95	0.15	23,27,58,64	0
2	741	T	16	38/38	0.95	0.14	22,28,43,56	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.

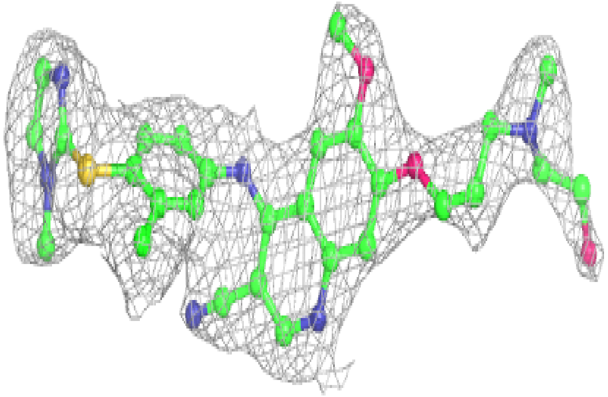


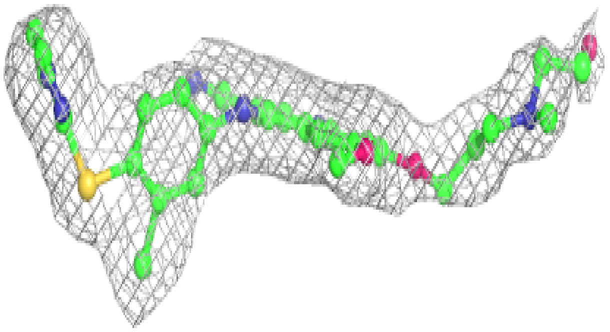
Electron density around 741 R 14:

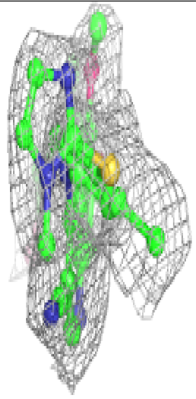
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 741 E 5:

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

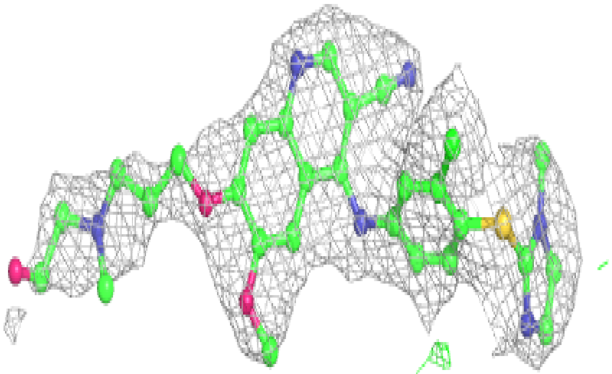


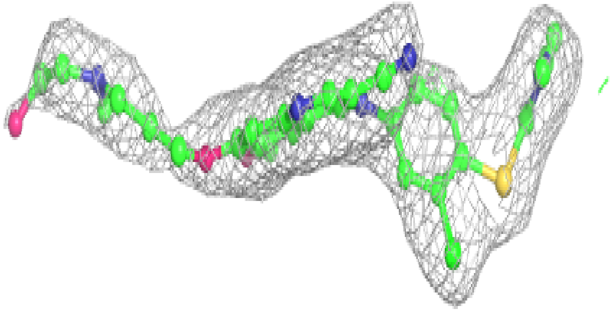


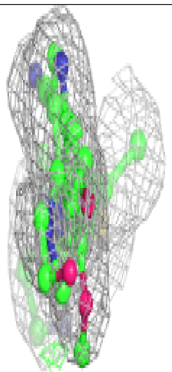


Electron density around 741 D 4:

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

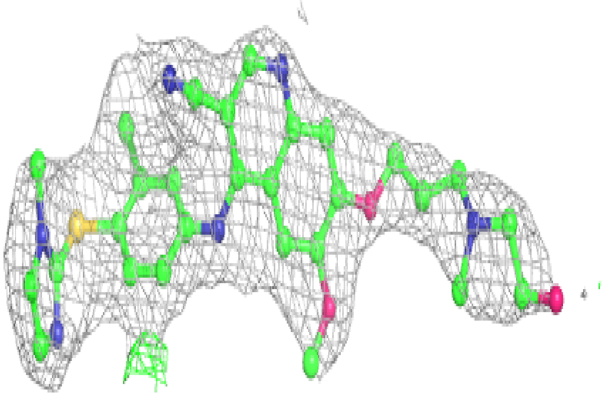


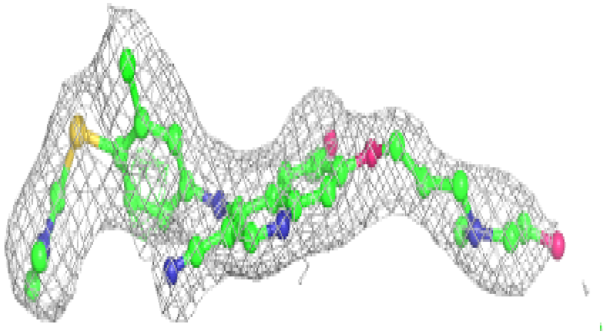


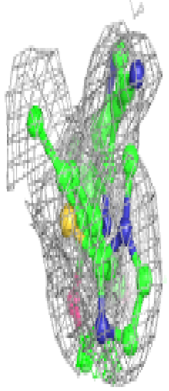


Electron density around 741 H 8:

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

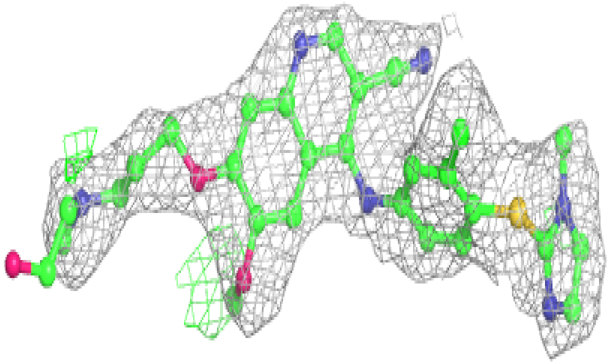


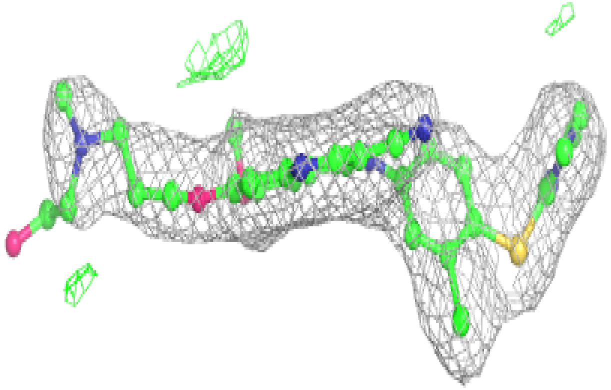




Electron density around 741 B 2:

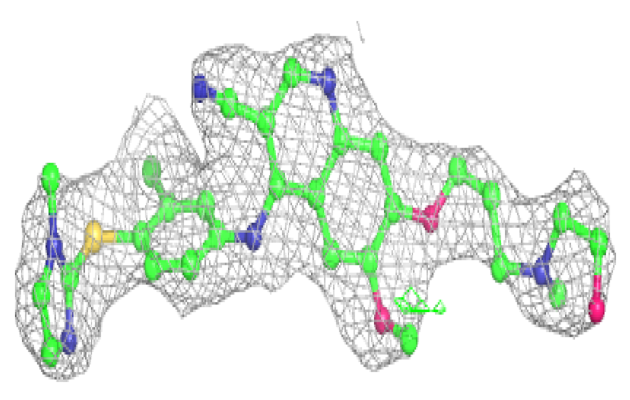
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

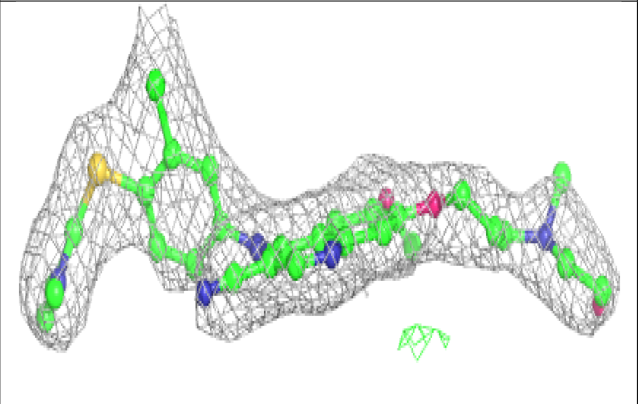


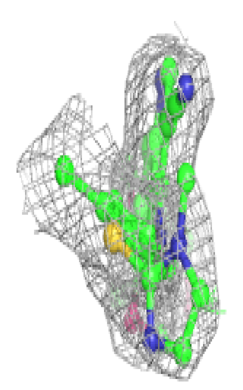


Electron density around 741 G 7:

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

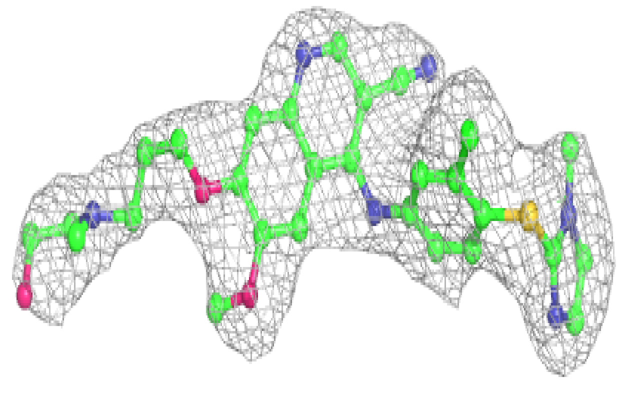


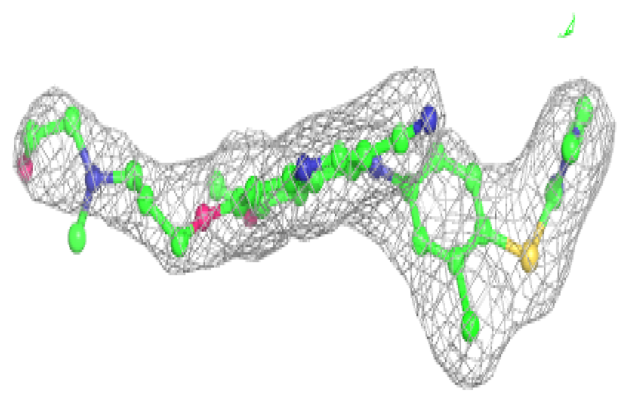


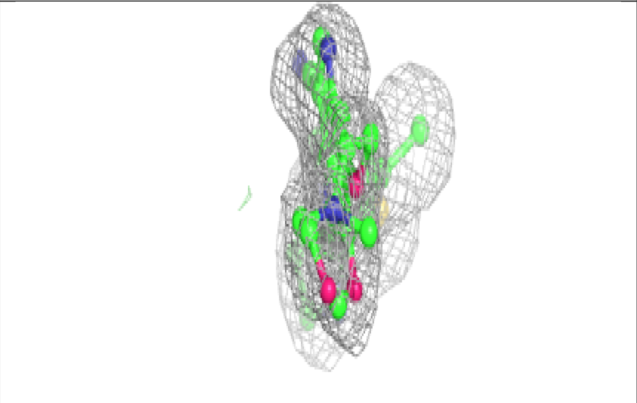


Electron density around 741 A 1:

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

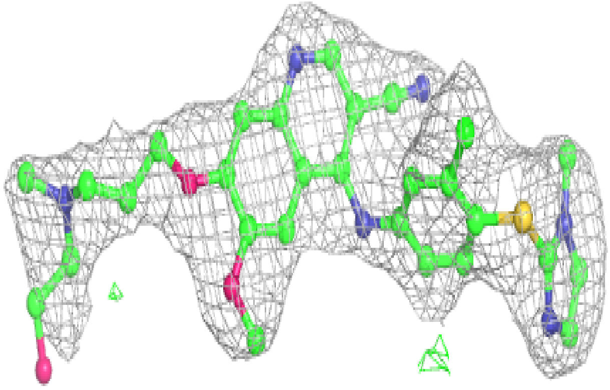


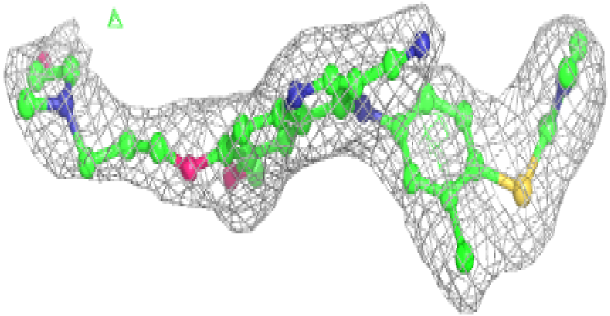


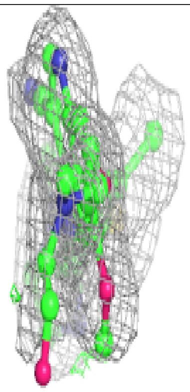


Electron density around 741 C 3:

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

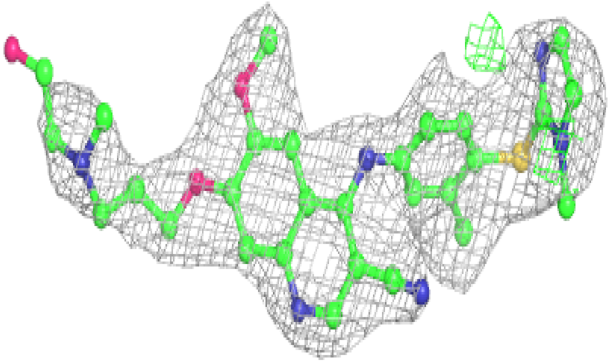


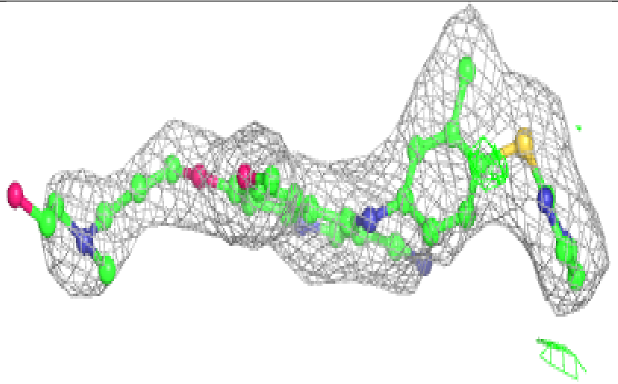


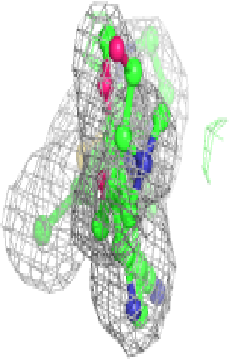


Electron density around 741 J 10:

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

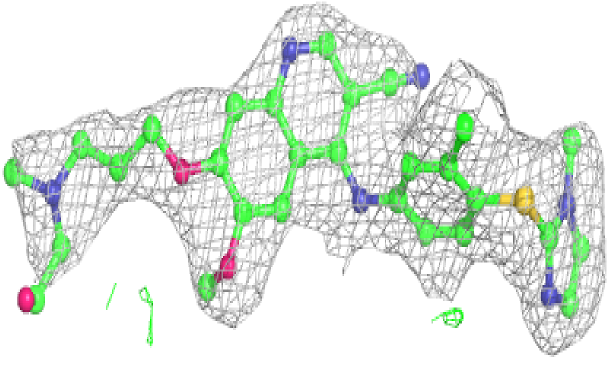


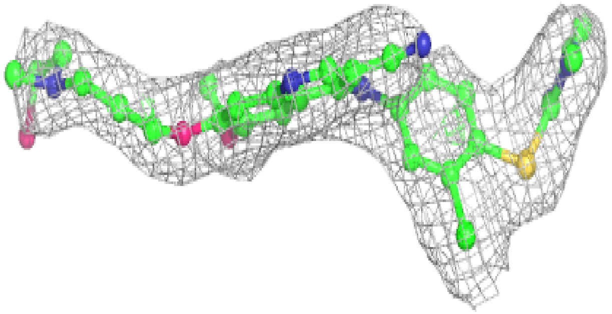


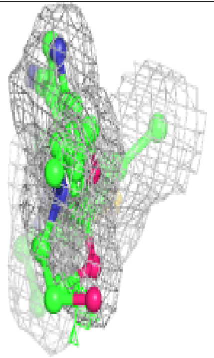


Electron density around 741 K 11:

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

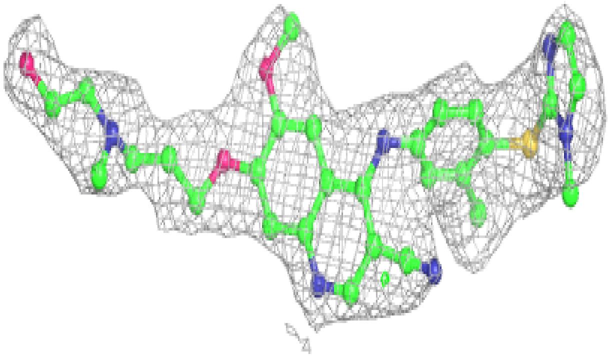


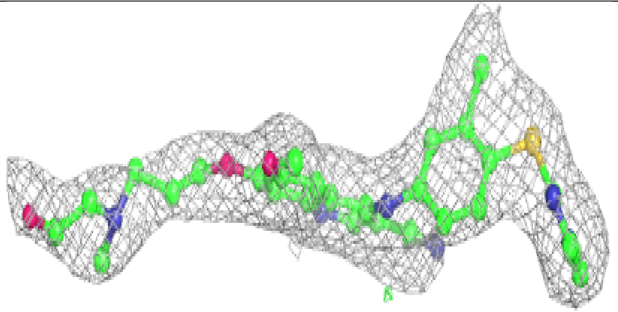


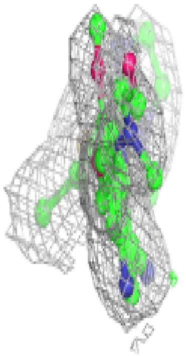


Electron density around 741 F 6:

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

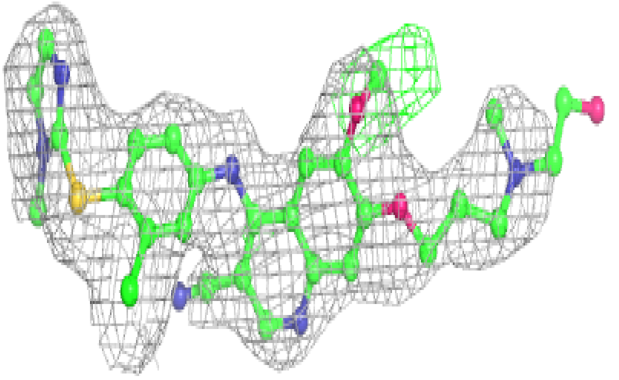


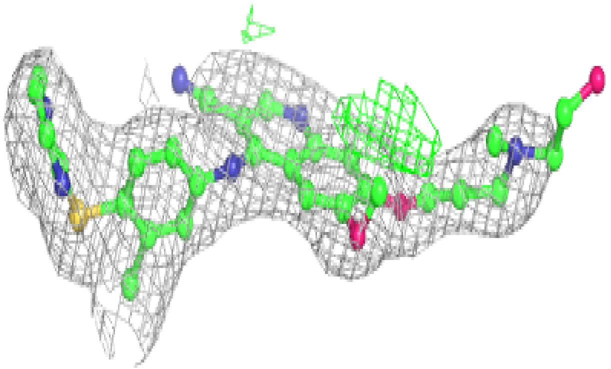


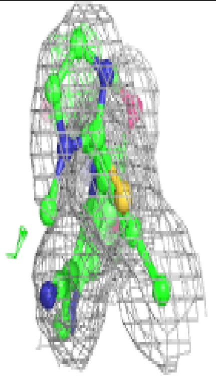


Electron density around 741 S 15:

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

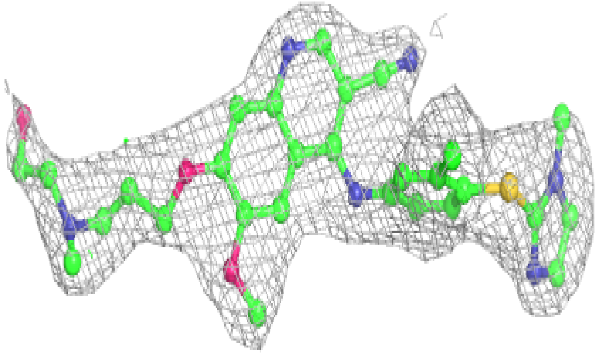


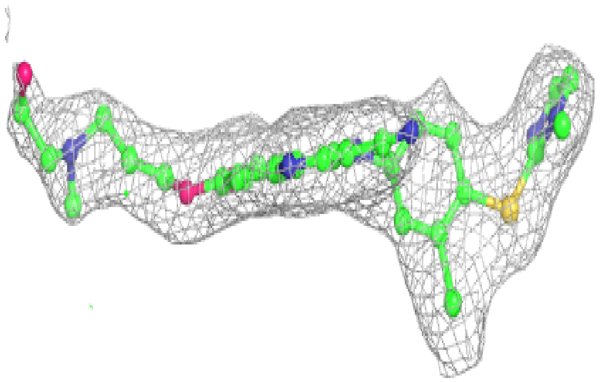


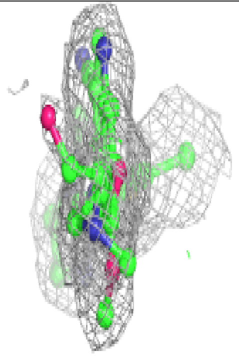


Electron density around 741 L 13:

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

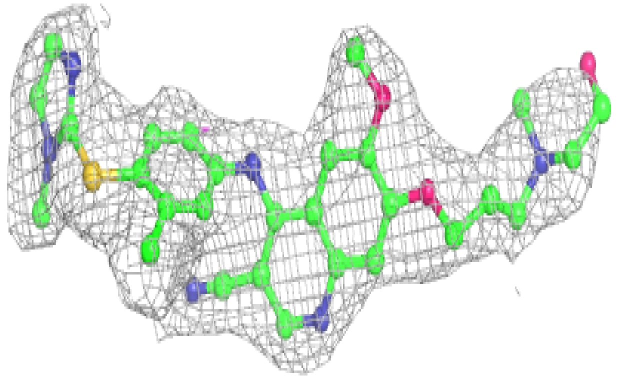


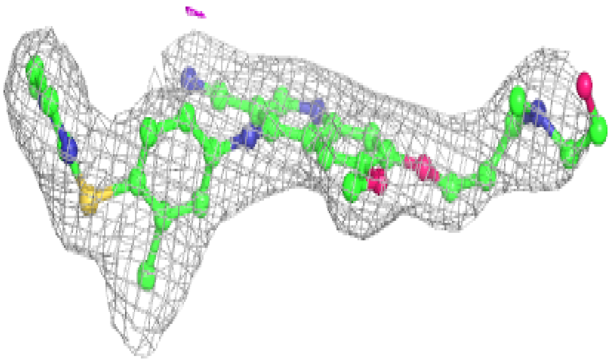


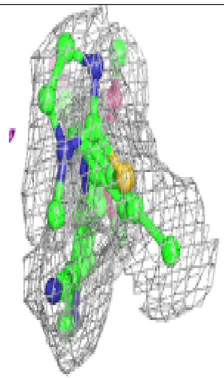


Electron density around 741 I 9:

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 741 M 12:

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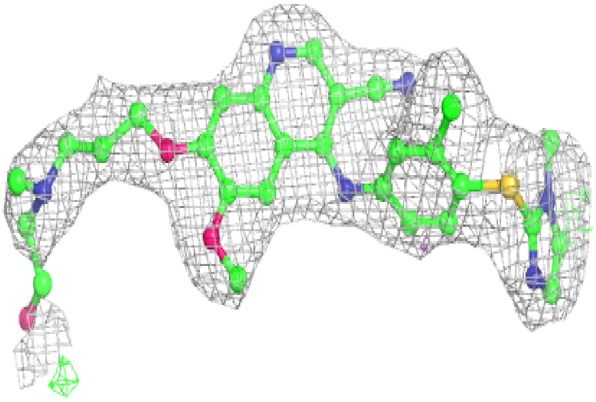
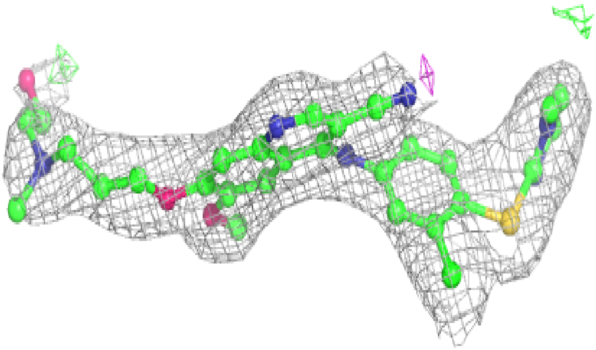
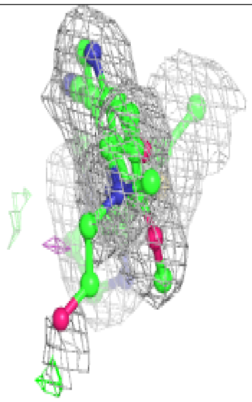
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

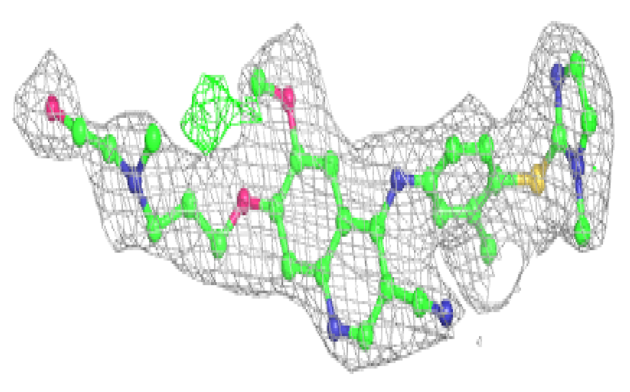


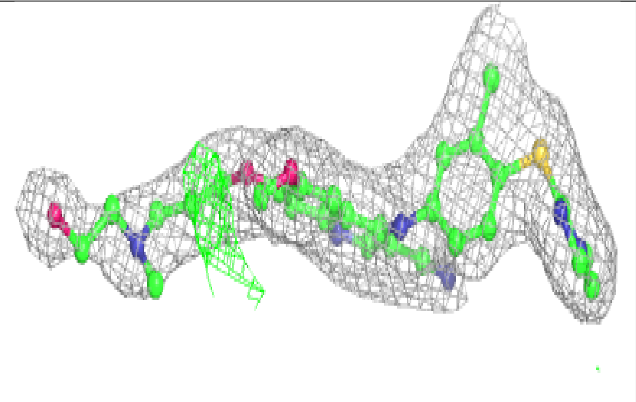


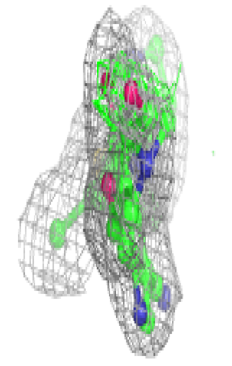


Electron density around 741 T 16:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.