wwPDB X-ray Structure Validation Summary Report (i)

Aug 14, 2023 – 11:22 PM EDT

PDB ID	:	1S64
Title	:	Rat protein geranylgeranyltransferase type-I complexed with L-778,123 and a sulfate anion
Authors	:	Reid, T.S.; Long, S.B.; Beese, L.S.
Deposited on	:	2004-01-22
Resolution	:	2.55 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:

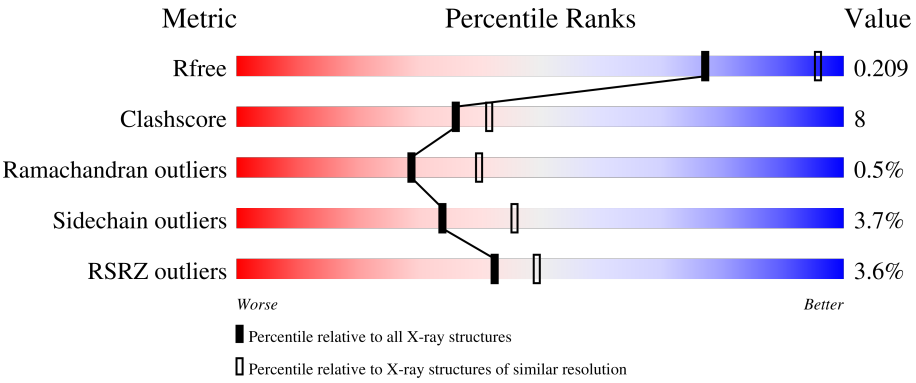
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.55 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.



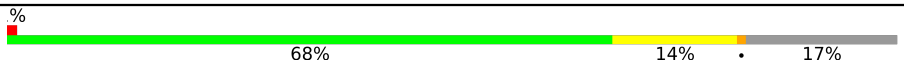
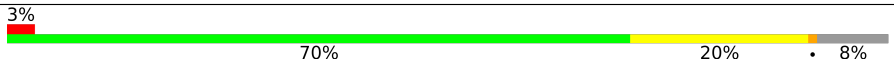
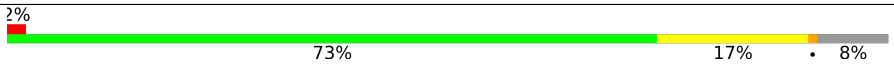
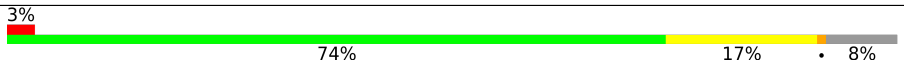
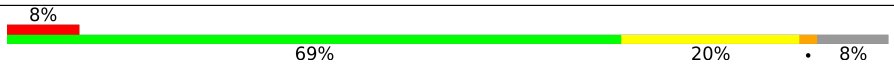
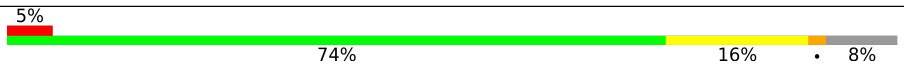
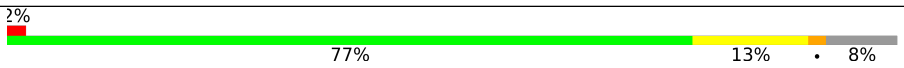
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	377	3% 67% 15% • 17%
1	C	377	3% 69% 14% • 17%
1	E	377	3% 65% 17% • 17%
1	G	377	5% 66% 18% 17%
1	I	377	2% 67% 15% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 33735 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 Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2626	1678	463	480	5			
1	C	314	Total	C	N	O	S	0	0	0
			2637	1686	458	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2651	1692	462	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

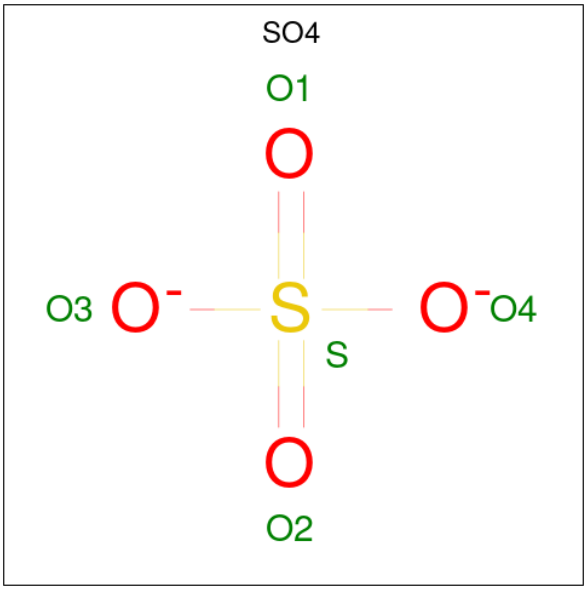
- Molecule 2 is a protein called Geranylgeranyl transferase type I beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2693	1704	467	498	24			
2	D	346	Total	C	N	O	S	0	0	0
			2690	1705	463	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2714	1714	474	502	24			
2	H	346	Total	C	N	O	S	0	0	0
			2688	1701	463	500	24			
2	J	346	Total	C	N	O	S	0	0	0
			2709	1711	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2719	1717	473	505	24			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

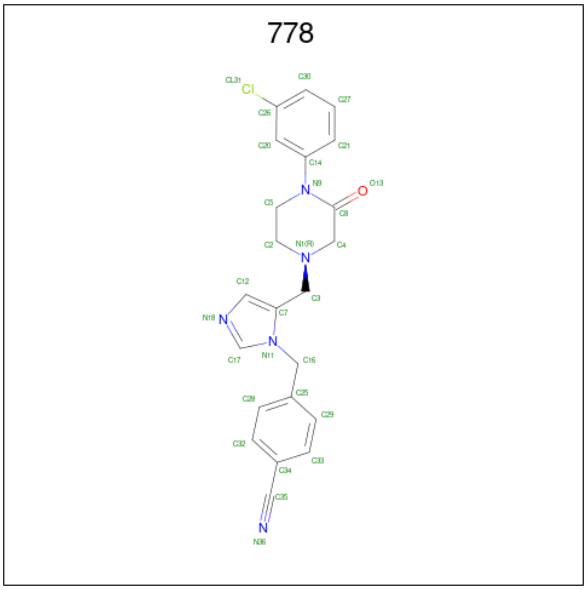
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



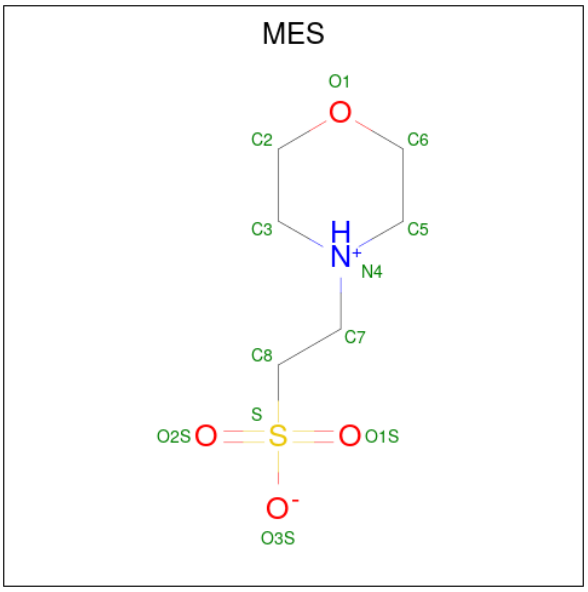
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

- Molecule 5 is 4-[(5-{[4-(3-CHLOROPHENYL)-3-OXOPIPERAZIN-1-YL]METHYL }-1H-IMIDAZOL-1-YL)METHYL]BENZONITRILE (three-letter code: 778) (formula: $C_{22}H_{20}ClN_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
5	D	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
5	F	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
5	H	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
5	J	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		
5	L	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O S 12 6 1 4 1	0	0
6	D	1	Total C N O S 12 6 1 4 1	0	0
6	F	1	Total C N O S 12 6 1 4 1	0	0
6	H	1	Total C N O S 12 6 1 4 1	0	0
6	J	1	Total C N O S 12 6 1 4 1	0	0
6	L	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Cl 1 1	0	0
7	D	1	Total Cl 1 1	0	0
7	F	1	Total Cl 1 1	0	0
7	G	1	Total Cl 1 1	0	0
7	H	1	Total Cl 1 1	0	0
7	I	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	1	Total Cl 1 1	0	0
7	K	1	Total Cl 1 1	0	0
7	L	1	Total Cl 1 1	0	0

- Molecule 8 is water.

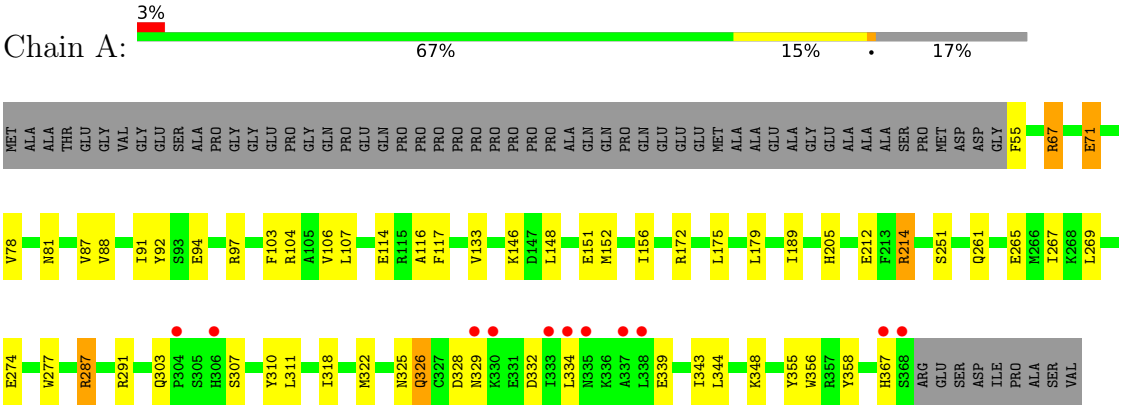
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	95	Total O 95 95	0	0
8	B	74	Total O 74 74	0	0
8	C	102	Total O 102 102	0	0
8	D	123	Total O 123 123	0	0
8	E	97	Total O 97 97	0	0
8	F	114	Total O 114 114	0	0
8	G	96	Total O 96 96	0	0
8	H	65	Total O 65 65	0	0
8	I	134	Total O 134 134	0	0
8	J	102	Total O 102 102	0	0
8	K	207	Total O 207 207	0	0
8	L	166	Total O 166 166	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.

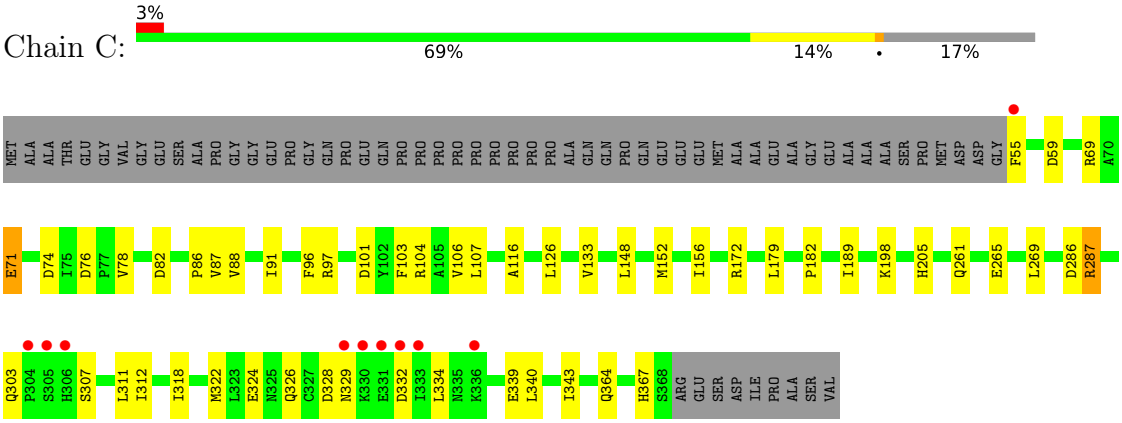
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit

Chain A:



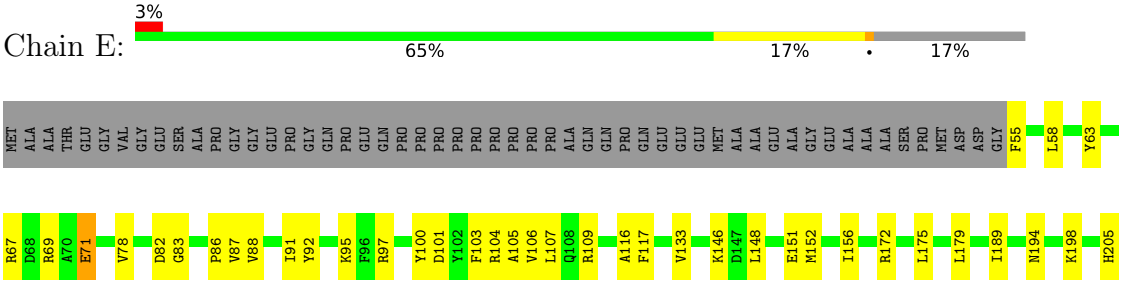
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit

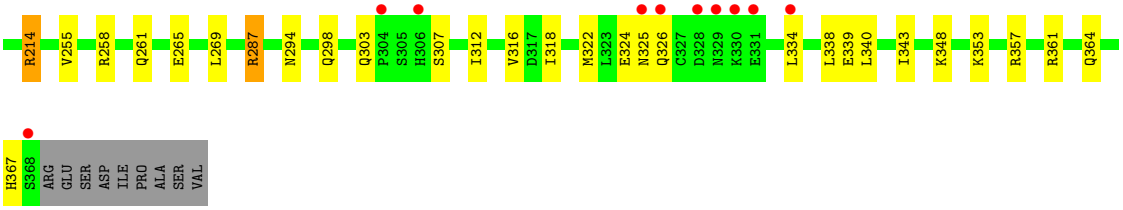
Chain C:



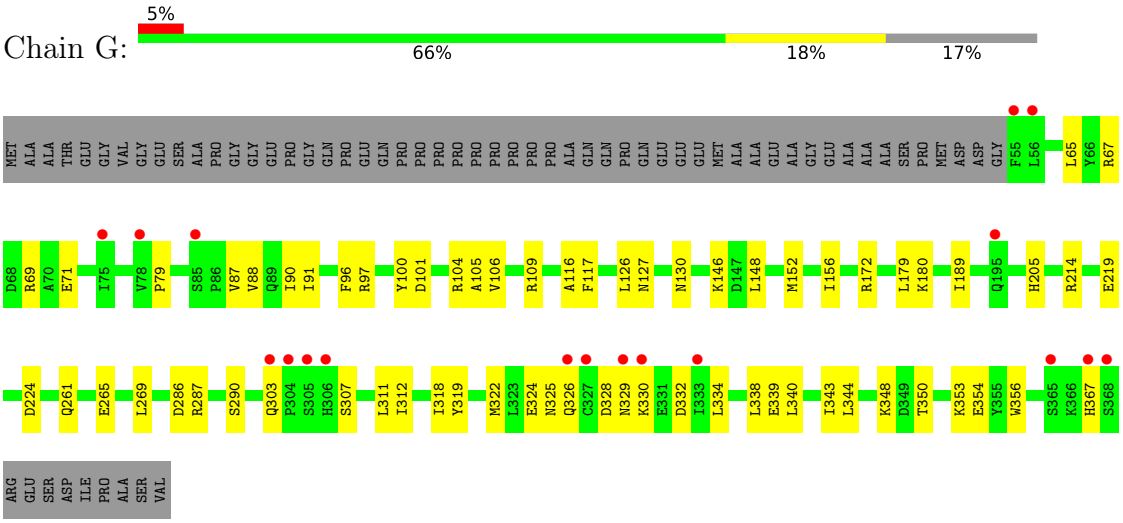
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit

Chain E:

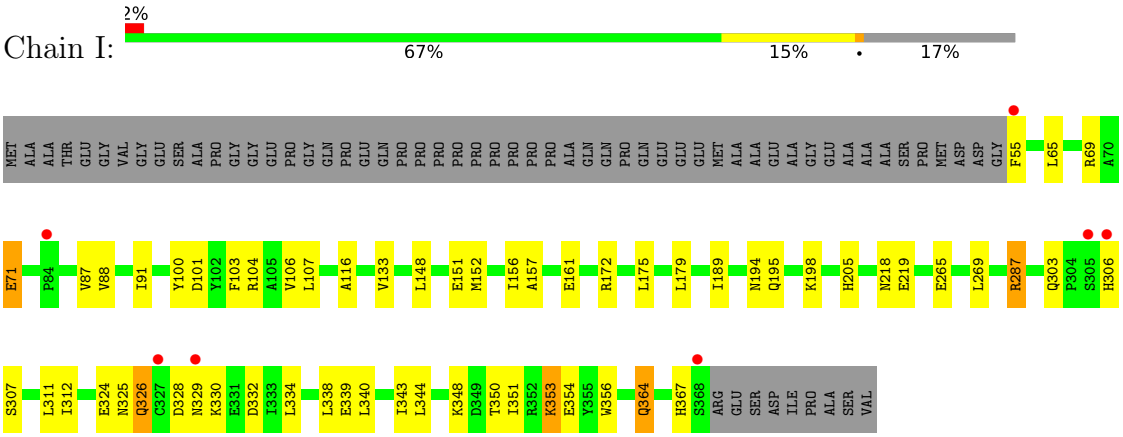




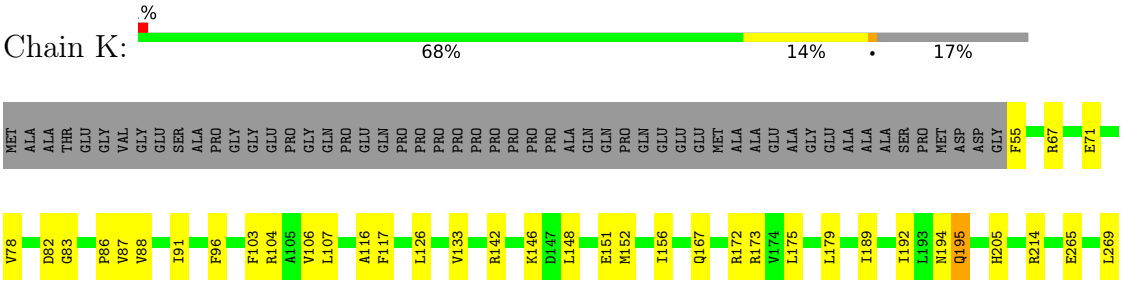
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit

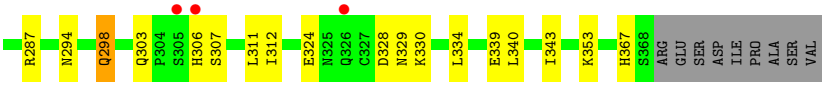


• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit

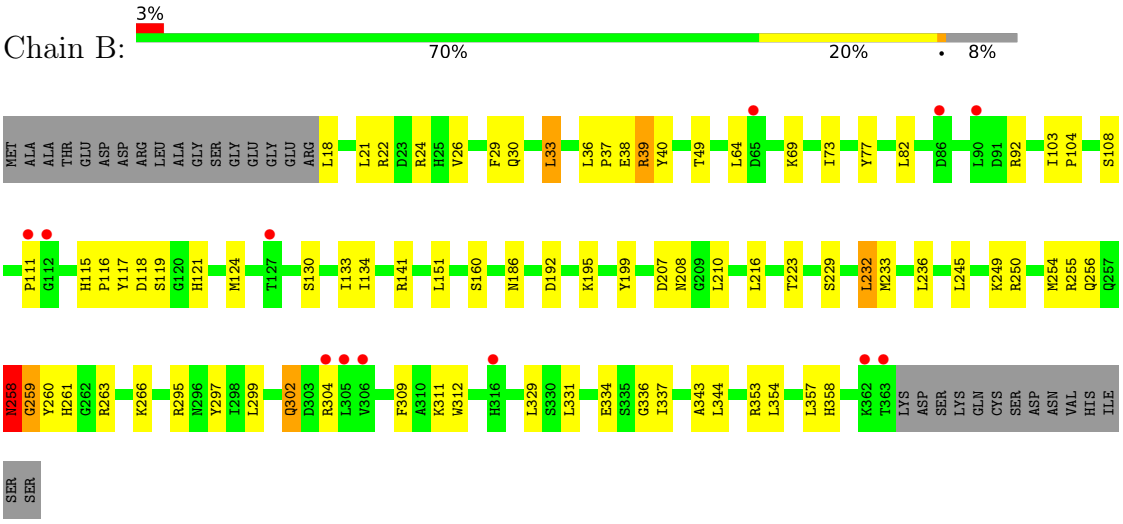


• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit

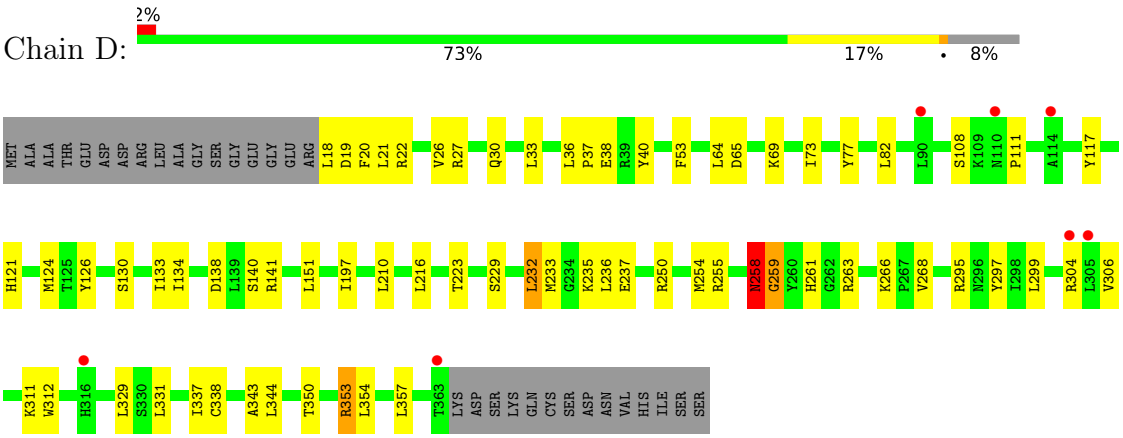




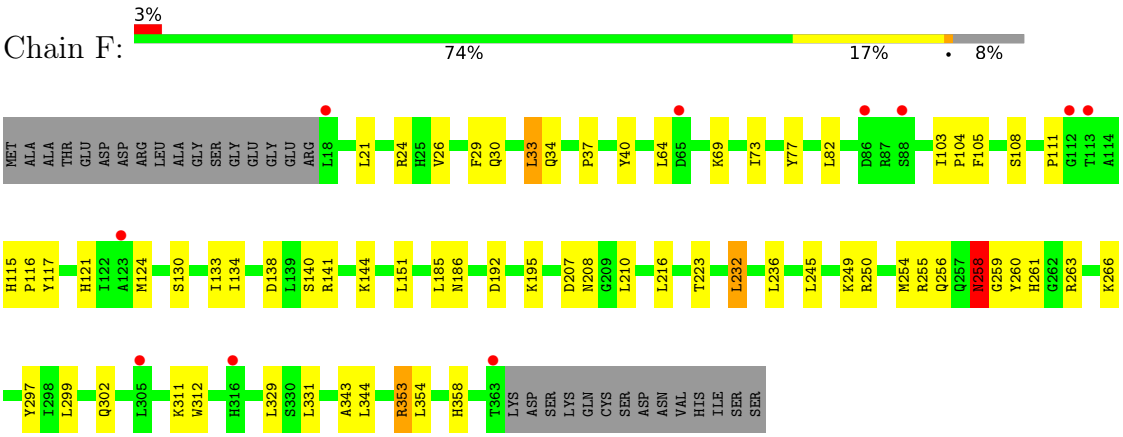
• Molecule 2: Geranylgeranyl transferase type I beta subunit



• Molecule 2: Geranylgeranyl transferase type I beta subunit

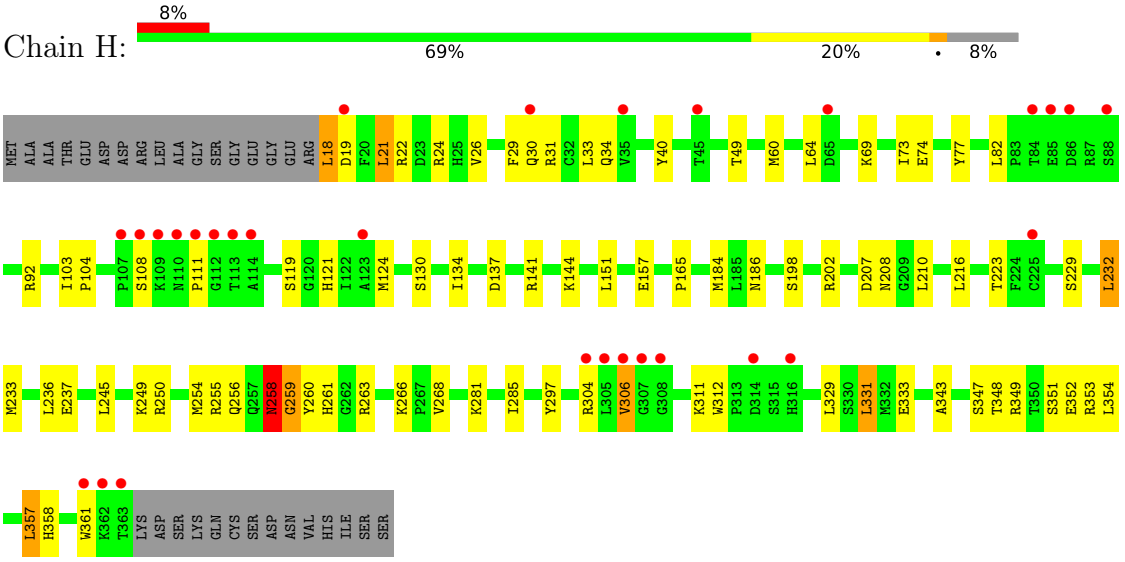


• Molecule 2: Geranylgeranyl transferase type I beta subunit



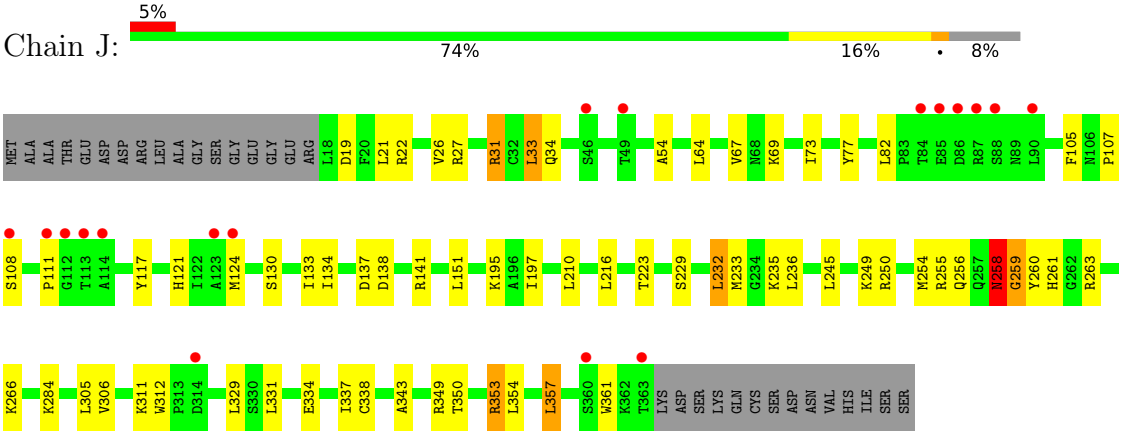
• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain H:



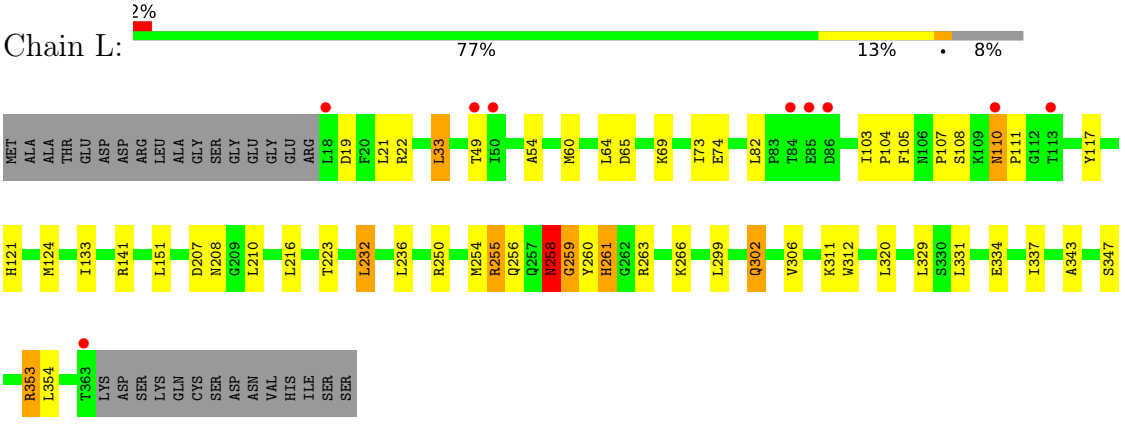
• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain J:



• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.15Å 268.68Å 184.62Å 90.00° 131.55° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 39.18 – 2.54	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-2.55) 93.1 (39.18-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.213 0.192 , 0.209	Depositor DCC
R_{free} test set	15041 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.086 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33735	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ZN, 778, MES, SO4

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	0.34	0/2692	0.51	0/3664
1	C	0.35	0/2703	0.52	0/3677
1	E	0.34	0/2708	0.53	0/3684
1	G	0.34	0/2699	0.51	0/3672
1	I	0.36	0/2717	0.52	0/3694
1	K	0.40	0/2733	0.54	0/3713
2	B	0.35	0/2754	0.59	2/3725 (0.1%)
2	D	0.36	0/2751	0.60	2/3720 (0.1%)
2	F	0.37	0/2775	0.60	2/3750 (0.1%)
2	H	0.34	0/2749	0.59	2/3720 (0.1%)
2	J	0.35	0/2770	0.60	2/3745 (0.1%)
2	L	0.39	0/2780	0.61	2/3756 (0.1%)
All	All	0.36	0/32831	0.56	12/44520 (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
2	B	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	259	GLY	N-CA-C	-6.06	97.95	113.10
2	H	259	GLY	N-CA-C	-5.96	98.21	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	259	GLY	N-CA-C	-5.90	98.34	113.10
2	D	259	GLY	N-CA-C	-5.87	98.44	113.10
2	L	259	GLY	N-CA-C	-5.84	98.50	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	F	297	TYR	Sidechain

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	2626	0	2518	43	0
1	C	2637	0	2529	36	0
1	E	2642	0	2534	48	0
1	G	2633	0	2524	49	0
1	I	2651	0	2551	40	0
1	K	2667	0	2577	36	0
2	B	2693	0	2589	57	0
2	D	2690	0	2588	39	0
2	F	2714	0	2624	39	0
2	H	2688	0	2573	60	0
2	J	2709	0	2610	40	0
2	L	2719	0	2632	33	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	5	0	0	0	0
4	L	5	0	0	0	0
5	B	29	0	20	0	0
5	D	29	0	20	0	0
5	F	29	0	20	0	0
5	H	29	0	20	0	0
5	J	29	0	20	0	0
5	L	29	0	20	0	0
6	B	12	0	13	0	0
6	D	12	0	13	2	0
6	F	12	0	13	0	0
6	H	12	0	13	0	0
6	J	12	0	13	0	0
6	L	12	0	13	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	1	0
7	H	1	0	0	0	0
7	I	1	0	0	1	0
7	J	1	0	0	0	0
7	K	1	0	0	1	0
7	L	1	0	0	0	0
8	A	95	0	0	2	0
8	B	74	0	0	2	0
8	C	102	0	0	2	0
8	D	123	0	0	3	0
8	E	97	0	0	1	0
8	F	114	0	0	1	0
8	G	96	0	0	3	0
8	H	65	0	0	3	0
8	I	134	0	0	3	0
8	J	102	0	0	2	0
8	K	207	0	0	5	0
8	L	166	0	0	0	0
All	All	33735	0	31047	504	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 8.

The worst 5 of 504 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:E:156:ILE:HG12	1:E:172:ARG:HH12	1.10	1.13
1:A:156:ILE:HG12	1:A:172:ARG:HH12	0.97	1.12
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.05	1.11
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.07
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.20	1.05

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	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	41	51
1	C	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	41	51
1	E	312/377 (83%)	288 (92%)	24 (8%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	I	312/377 (83%)	292 (94%)	18 (6%)	2 (1%)	25	34
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	41	51
2	B	344/377 (91%)	325 (94%)	17 (5%)	2 (1%)	25	34
2	D	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	25	34
2	F	344/377 (91%)	327 (95%)	15 (4%)	2 (1%)	25	34
2	H	344/377 (91%)	326 (95%)	15 (4%)	3 (1%)	17	24
2	J	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	17	24
2	L	344/377 (91%)	332 (96%)	10 (3%)	2 (1%)	25	34
All	All	3936/4524 (87%)	3716 (94%)	201 (5%)	19 (0%)	29	40

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	258	ASN
1	C	326	GLN
2	D	258	ASN
2	H	258	ASN

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	279/338 (82%)	273 (98%)	6 (2%)	52	66
1	C	282/338 (83%)	274 (97%)	8 (3%)	43	58
1	E	284/338 (84%)	277 (98%)	7 (2%)	47	62
1	G	281/338 (83%)	276 (98%)	5 (2%)	59	74
1	I	286/338 (85%)	278 (97%)	8 (3%)	43	58
1	K	290/338 (86%)	281 (97%)	9 (3%)	40	54
2	B	287/326 (88%)	275 (96%)	12 (4%)	30	40
2	D	286/326 (88%)	273 (96%)	13 (4%)	27	37
2	F	292/326 (90%)	279 (96%)	13 (4%)	27	37
2	H	286/326 (88%)	272 (95%)	14 (5%)	25	34
2	J	291/326 (89%)	276 (95%)	15 (5%)	23	30
2	L	294/326 (90%)	278 (95%)	16 (5%)	22	29
All	All	3438/3984 (86%)	3312 (96%)	126 (4%)	34	46

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	331	LEU
2	L	21	LEU
2	H	255	ARG
1	K	324	GLU
2	L	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	364	GLN
2	J	30	GLN
1	K	81	ASN
2	D	246	ASN
2	D	30	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 15 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
4	SO4	L	380	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	H	380	-	4,4,4	0.27	0	6,6,6	0.18	0
5	778	L	381	3	29,32,32	2.43	15 (51%)	39,44,44	2.18	11 (28%)
5	778	H	381	3	29,32,32	2.37	15 (51%)	39,44,44	2.17	12 (30%)
6	MES	H	382	-	12,12,12	9.52	8 (66%)	14,16,16	2.43	6 (42%)
6	MES	J	382	-	12,12,12	9.46	8 (66%)	14,16,16	2.60	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MES	D	382	-	12,12,12	9.53	8 (66%)	14,16,16	2.52	6 (42%)
6	MES	B	381	-	12,12,12	9.37	8 (66%)	14,16,16	2.60	7 (50%)
5	778	J	381	3	29,32,32	2.38	13 (44%)	39,44,44	2.16	11 (28%)
5	778	B	380	3	29,32,32	2.48	16 (55%)	39,44,44	2.17	12 (30%)
6	MES	L	382	-	12,12,12	9.70	9 (75%)	14,16,16	2.66	7 (50%)
5	778	F	381	3	29,32,32	2.44	14 (48%)	39,44,44	2.20	12 (30%)
6	MES	F	382	-	12,12,12	9.28	8 (66%)	14,16,16	2.63	7 (50%)
4	SO4	J	380	-	4,4,4	0.23	0	6,6,6	0.22	0
5	778	D	381	3	29,32,32	2.40	16 (55%)	39,44,44	2.16	11 (28%)
4	SO4	F	380	-	4,4,4	0.22	0	6,6,6	0.25	0
4	SO4	D	380	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	B	379	-	4,4,4	0.26	0	6,6,6	0.06	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
5	778	L	381	3	-	2/14/27/27	0/4/4/4
5	778	H	381	3	-	2/14/27/27	0/4/4/4
6	MES	H	382	-	-	0/6/14/14	0/1/1/1
6	MES	J	382	-	-	0/6/14/14	0/1/1/1
6	MES	D	382	-	-	0/6/14/14	0/1/1/1
6	MES	B	381	-	-	0/6/14/14	0/1/1/1
5	778	J	381	3	-	2/14/27/27	0/4/4/4
5	778	B	380	3	-	2/14/27/27	0/4/4/4
6	MES	L	382	-	-	0/6/14/14	0/1/1/1
5	778	F	381	3	-	3/14/27/27	0/4/4/4
6	MES	F	382	-	-	0/6/14/14	0/1/1/1
5	778	D	381	3	-	2/14/27/27	0/4/4/4

The worst 5 of 138 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	382	MES	C8-S	-25.41	1.41	1.77
6	D	382	MES	C8-S	-24.85	1.42	1.77
6	H	382	MES	C8-S	-24.74	1.42	1.77
6	J	382	MES	C8-S	-24.47	1.42	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	381	MES	C8-S	-23.98	1.43	1.77

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	382	MES	O3S-S-C8	6.52	116.31	105.77
6	J	382	MES	O3S-S-C8	6.03	115.53	105.77
6	D	382	MES	O3S-S-C8	5.95	115.39	105.77
6	B	381	MES	O3S-S-C8	5.90	115.31	105.77
5	L	381	778	C2-C5-N9	5.83	120.66	110.88

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	381	778	N11-C16-C25-C29
5	D	381	778	N11-C16-C25-C28
5	F	381	778	N11-C16-C25-C29
5	J	381	778	N11-C16-C25-C29
5	F	381	778	N11-C16-C25-C28

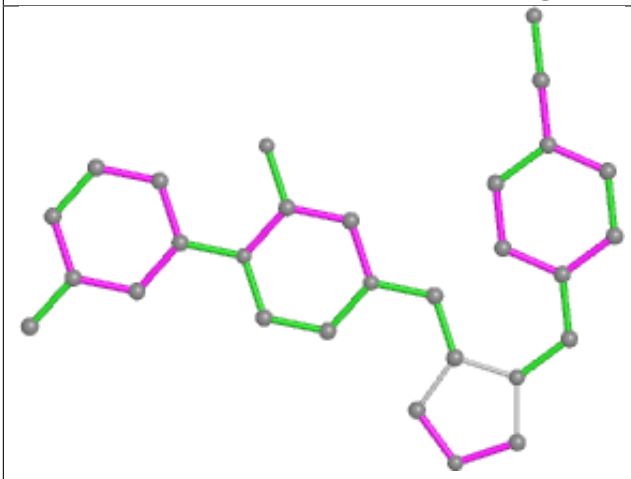
There are no ring outliers.

1 monomer is involved in 2 short contacts:

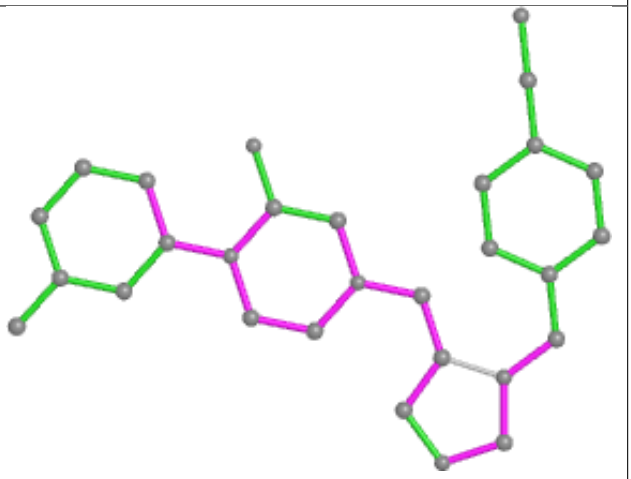
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	382	MES	2	0

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

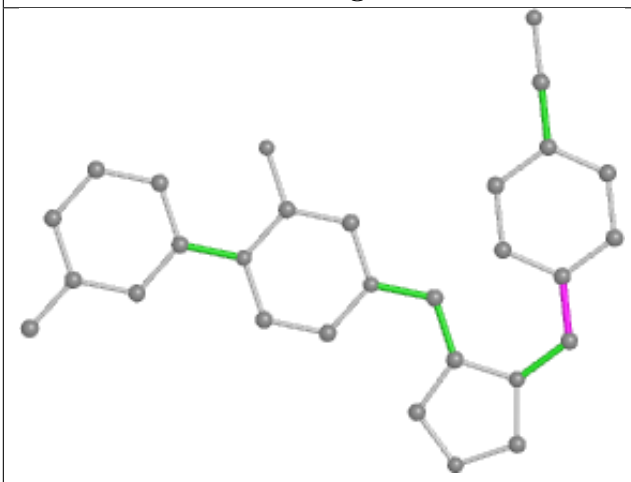
Ligand 778 L 381



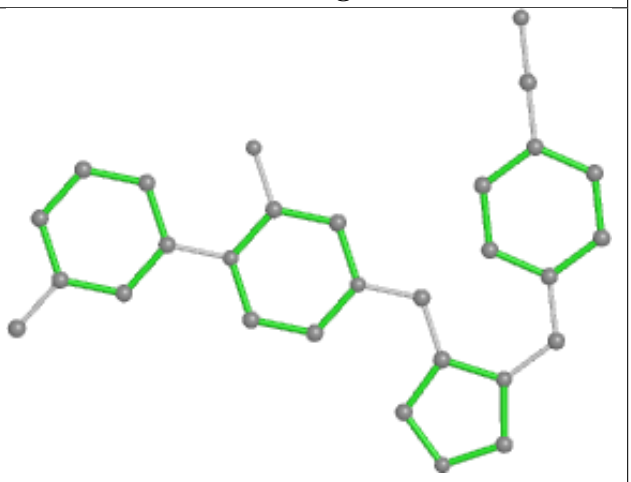
Bond lengths



Bond angles

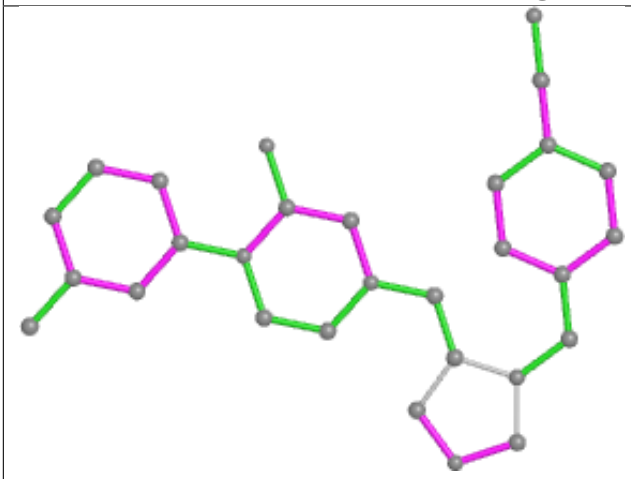


Torsions

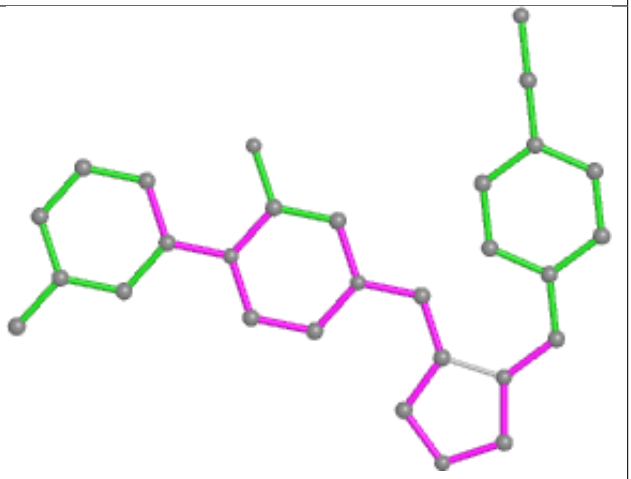


Rings

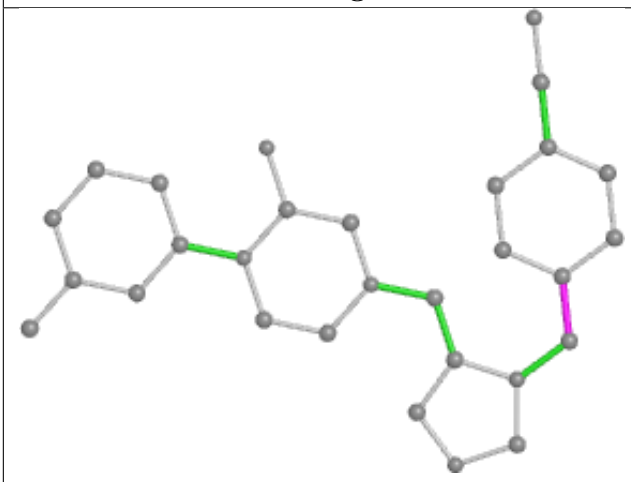
Ligand 778 H 381



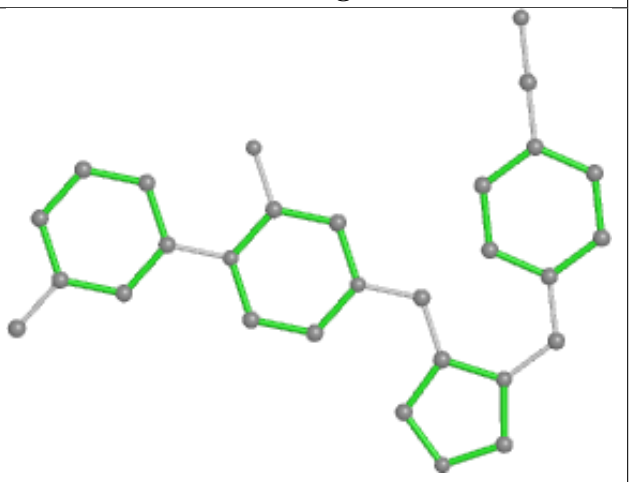
Bond lengths



Bond angles

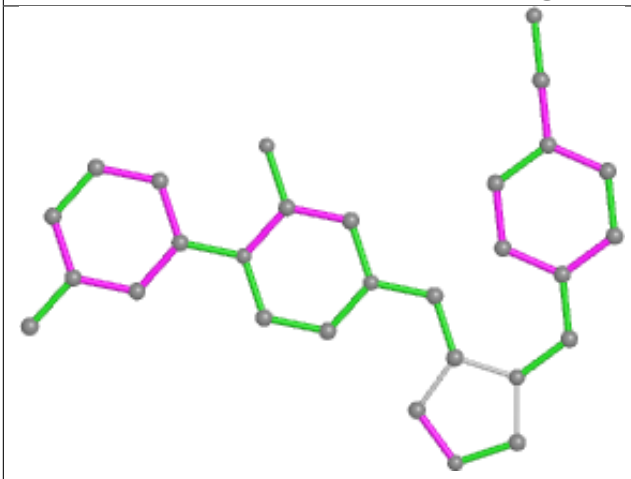


Torsions

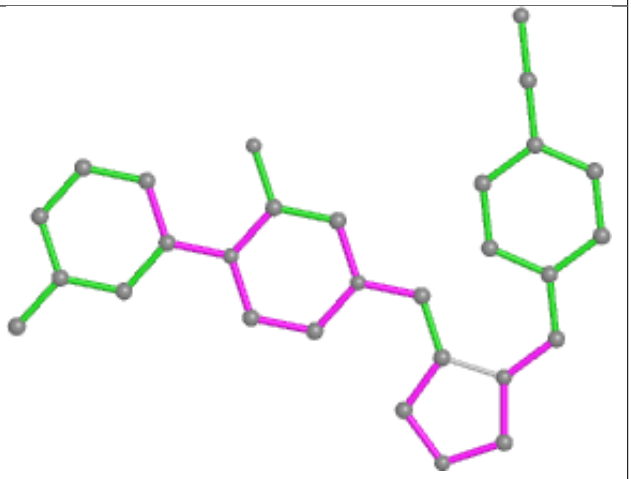


Rings

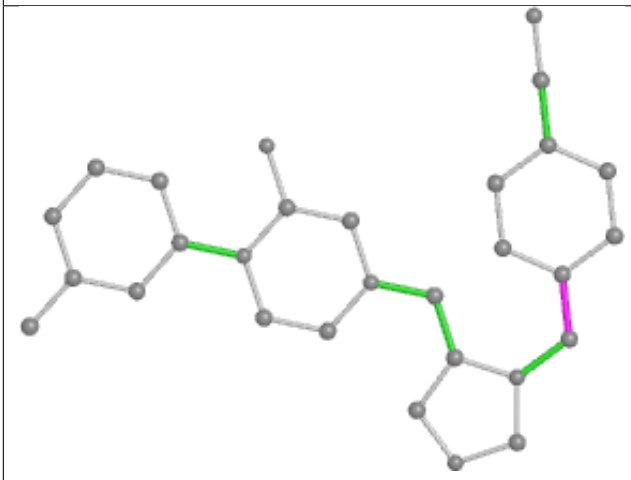
Ligand 778 J 381



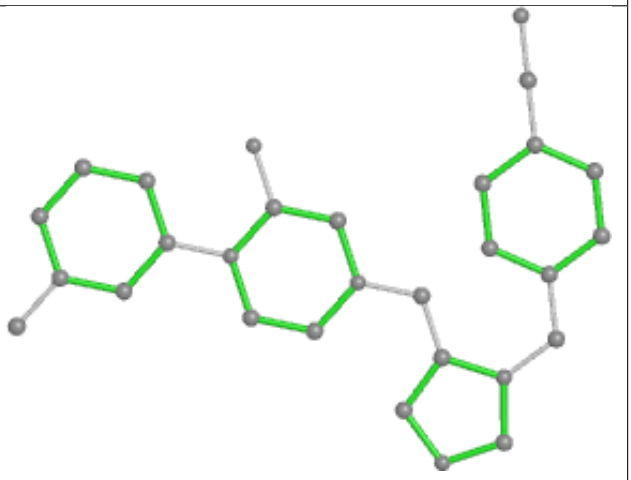
Bond lengths



Bond angles

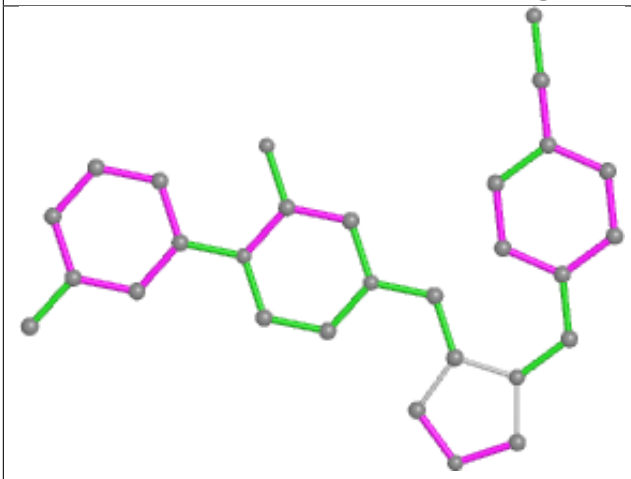


Torsions

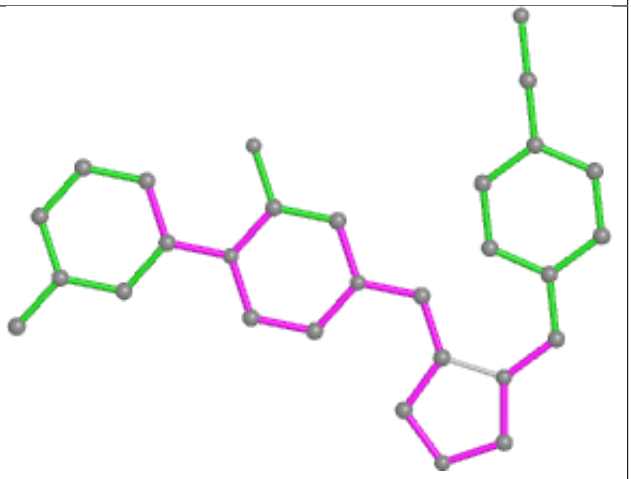


Rings

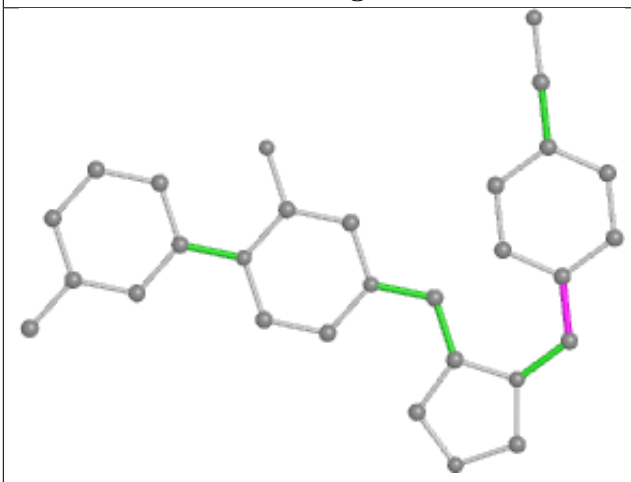
Ligand 778 B 380



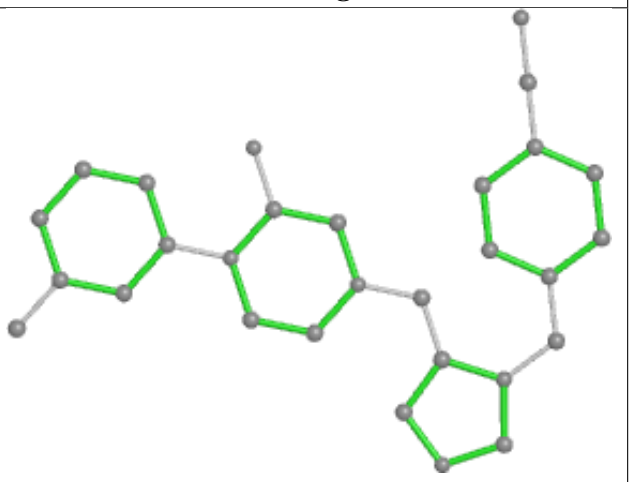
Bond lengths



Bond angles

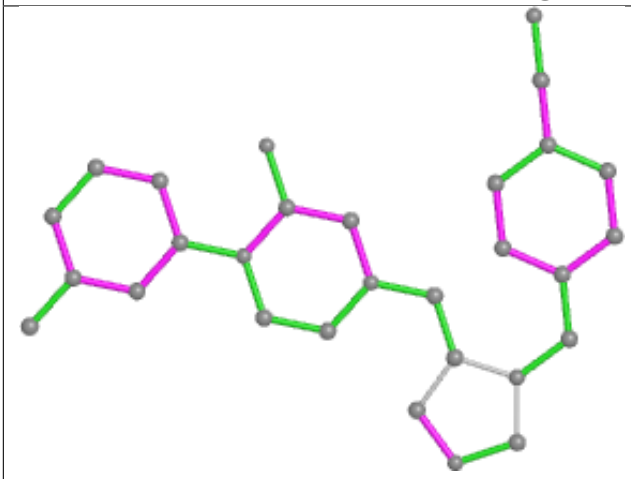


Torsions

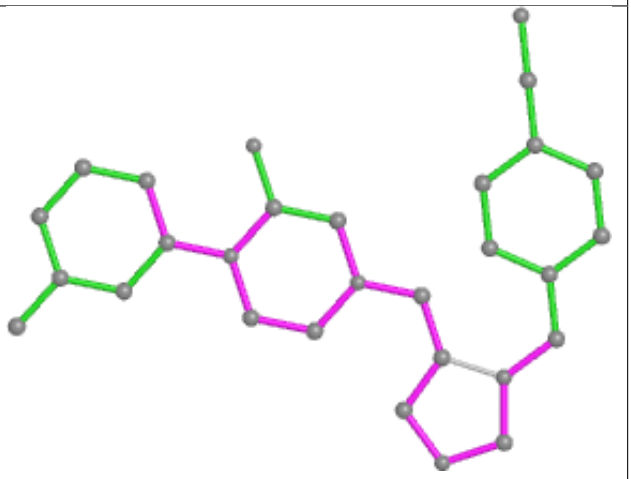


Rings

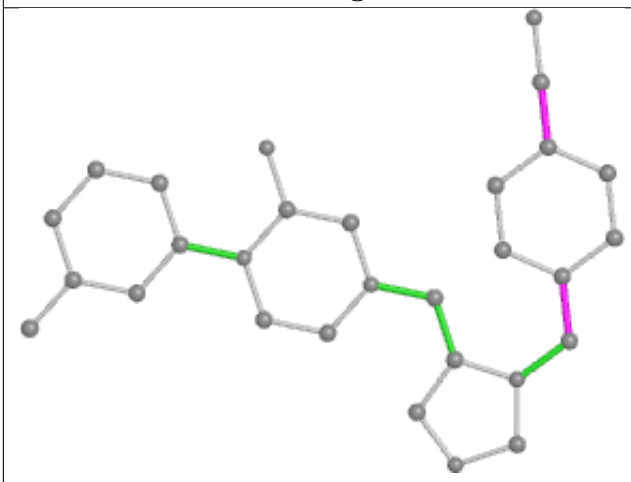
Ligand 778 F 381



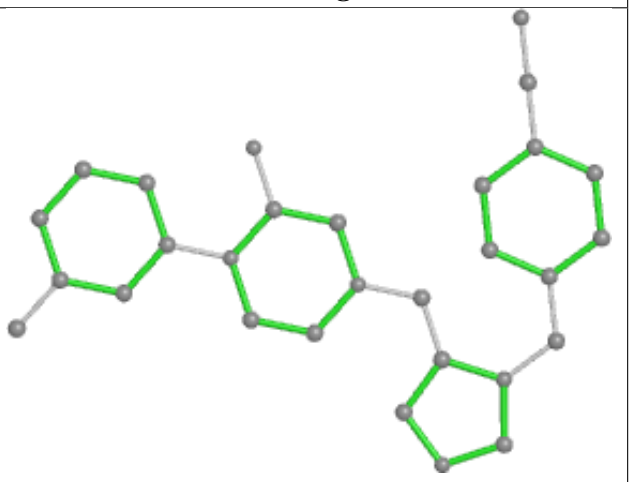
Bond lengths



Bond angles

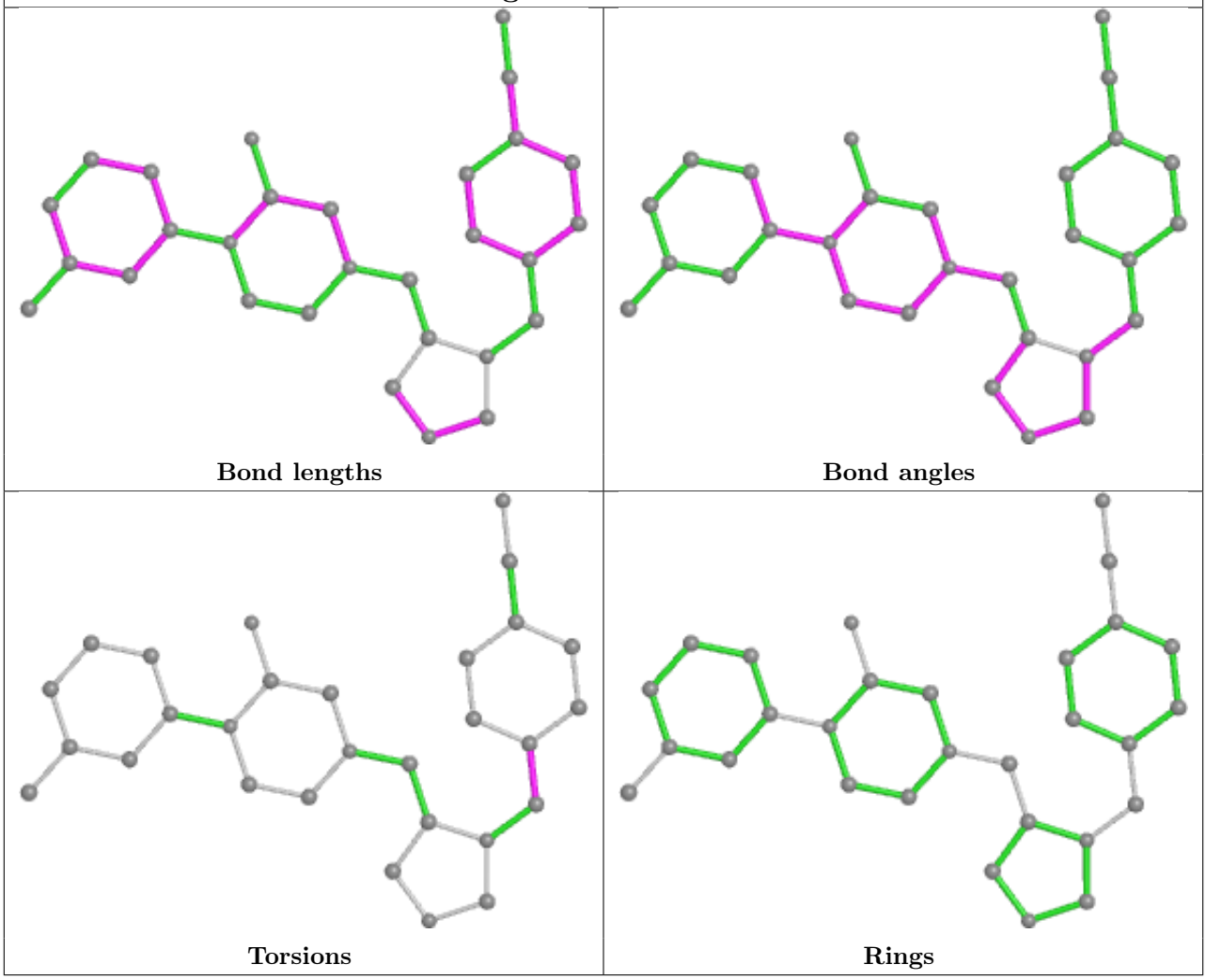


Torsions



Rings

Ligand 778 D 381



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	314/377 (83%)	0.01	11 (3%)	44	51	41, 63, 97, 108	0
1	C	314/377 (83%)	-0.03	10 (3%)	47	55	41, 59, 87, 108	0
1	E	314/377 (83%)	0.02	10 (3%)	47	55	44, 63, 91, 106	0
1	G	314/377 (83%)	0.14	18 (5%)	23	28	41, 64, 94, 110	0
1	I	314/377 (83%)	-0.10	7 (2%)	62	68	34, 57, 87, 96	0
1	K	314/377 (83%)	-0.25	3 (0%)	82	86	31, 47, 72, 87	0
2	B	346/377 (91%)	0.09	12 (3%)	44	51	42, 57, 82, 102	0
2	D	346/377 (91%)	0.07	7 (2%)	65	72	35, 51, 77, 91	0
2	F	346/377 (91%)	0.02	10 (2%)	51	59	36, 51, 77, 101	0
2	H	346/377 (91%)	0.54	29 (8%)	11	13	40, 71, 97, 114	0
2	J	346/377 (91%)	0.15	18 (5%)	27	32	35, 55, 84, 104	0
2	L	346/377 (91%)	0.03	9 (2%)	56	62	29, 44, 71, 95	0
All	All	3960/4524 (87%)	0.06	144 (3%)	42	49	29, 57, 88, 114	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	304	ARG	6.3
1	G	306	HIS	5.9
1	C	306	HIS	5.9
2	H	305	LEU	5.9
1	G	55	PHE	5.5

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	778	J	381	29/29	0.89	0.25	29,39,42,42	0
5	778	F	381	29/29	0.91	0.24	36,45,52,52	0
5	778	B	380	29/29	0.91	0.25	39,46,53,56	0
5	778	L	381	29/29	0.91	0.26	27,33,36,39	0
5	778	D	381	29/29	0.92	0.24	35,45,47,51	0
5	778	H	381	29/29	0.92	0.24	42,48,51,54	0
6	MES	H	382	12/12	0.93	0.26	74,75,84,84	0
6	MES	B	381	12/12	0.94	0.30	69,71,81,83	0
6	MES	J	382	12/12	0.94	0.38	70,72,81,81	0
6	MES	L	382	12/12	0.94	0.36	69,71,76,77	0
6	MES	F	382	12/12	0.95	0.31	72,73,85,86	0
6	MES	D	382	12/12	0.95	0.28	71,72,78,78	0
7	CL	G	378	1/1	0.96	0.16	61,61,61,61	0
7	CL	H	379	1/1	0.96	0.10	68,68,68,68	0
7	CL	I	378	1/1	0.96	0.18	75,75,75,75	0
7	CL	J	379	1/1	0.97	0.11	63,63,63,63	0
7	CL	C	378	1/1	0.98	0.21	61,61,61,61	0
7	CL	D	379	1/1	0.98	0.15	52,52,52,52	0
7	CL	K	378	1/1	0.98	0.14	67,67,67,67	0
4	SO4	J	380	5/5	0.99	0.16	45,45,47,48	0
4	SO4	L	380	5/5	0.99	0.19	41,44,45,47	0
7	CL	F	379	1/1	0.99	0.17	53,53,53,53	0
3	ZN	H	378	1/1	0.99	0.11	55,55,55,55	0
4	SO4	B	379	5/5	0.99	0.18	56,56,58,59	0
4	SO4	D	380	5/5	0.99	0.16	51,52,54,55	0
4	SO4	F	380	5/5	0.99	0.19	53,54,58,58	0
4	SO4	H	380	5/5	0.99	0.14	60,61,62,62	0
7	CL	L	379	1/1	0.99	0.12	53,53,53,53	0
3	ZN	B	378	1/1	1.00	0.14	45,45,45,45	0
3	ZN	J	378	1/1	1.00	0.15	39,39,39,39	0
3	ZN	L	378	1/1	1.00	0.16	35,35,35,35	0
3	ZN	D	378	1/1	1.00	0.15	43,43,43,43	0

Continued on next page...

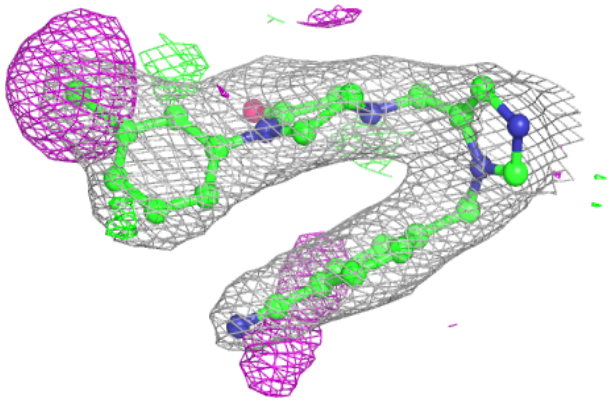
Continued from previous page...

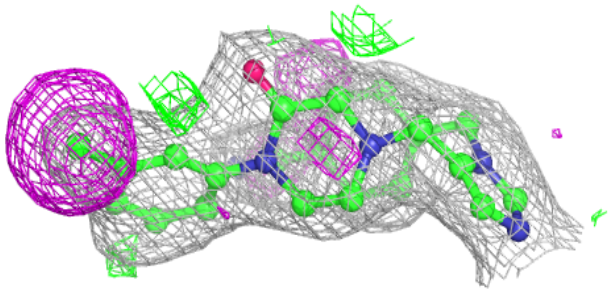
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	F	378	1/1	1.00	0.14	45,45,45,45	0

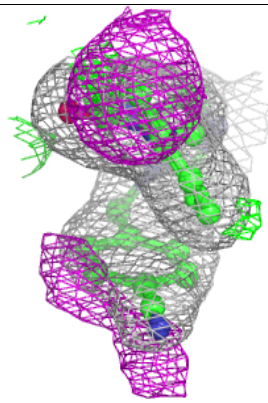
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 778 J 381:

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

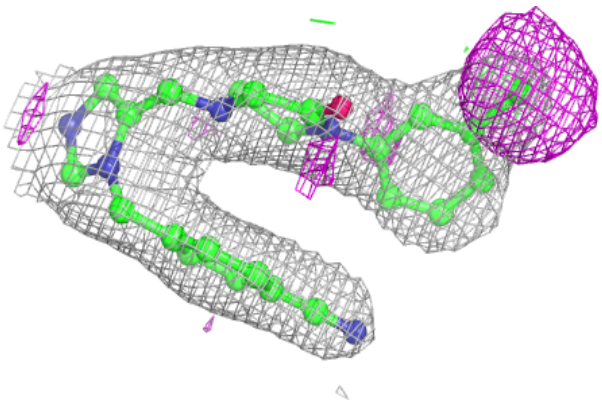


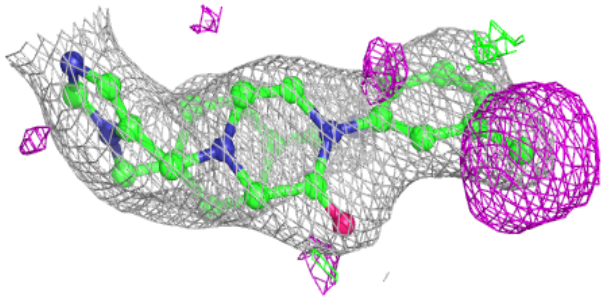


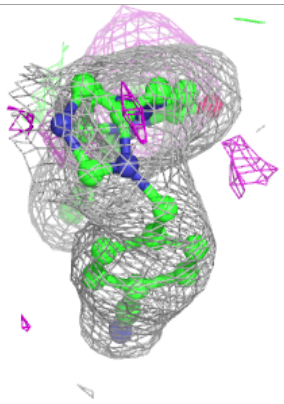


Electron density around 778 F 381:

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

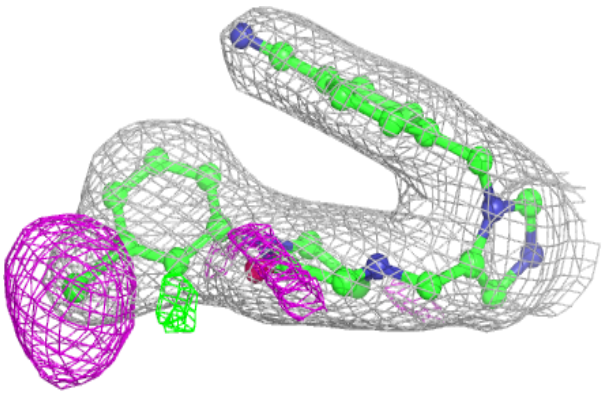


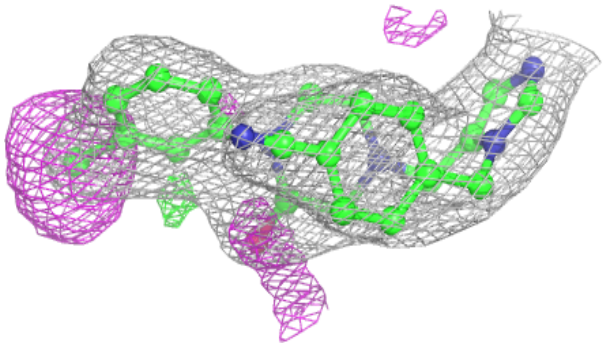


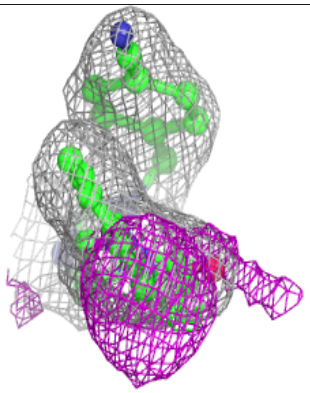


Electron density around 778 B 380:

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

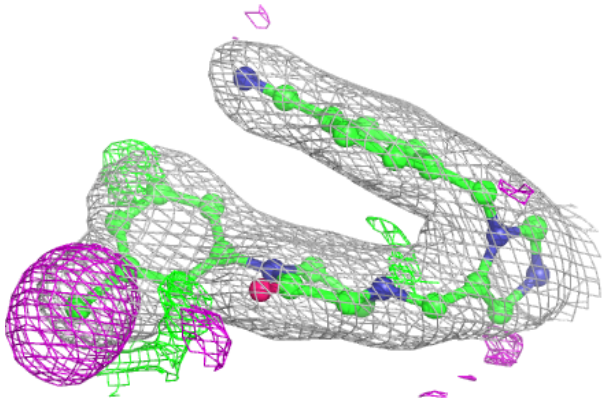


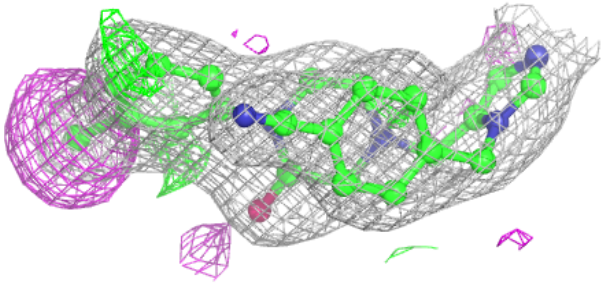


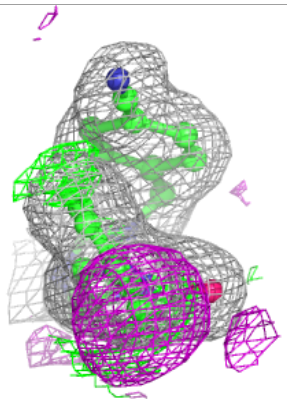


Electron density around 778 L 381:

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

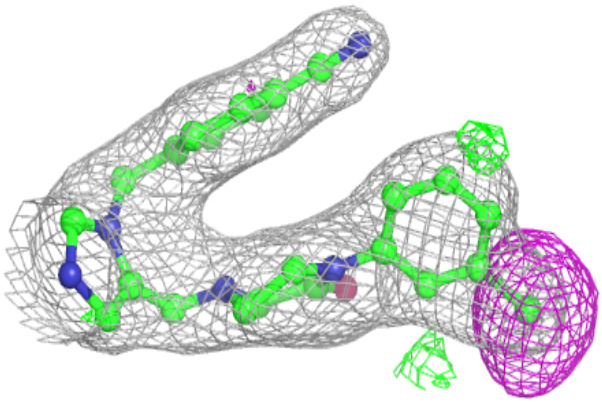


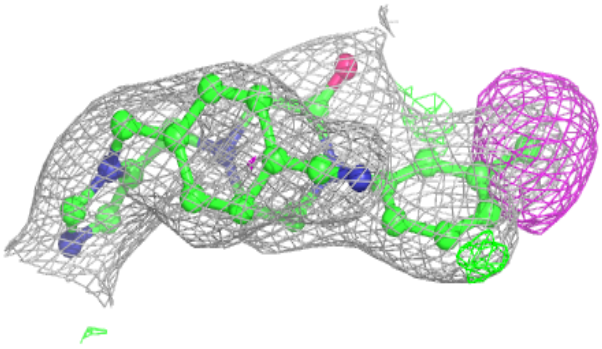


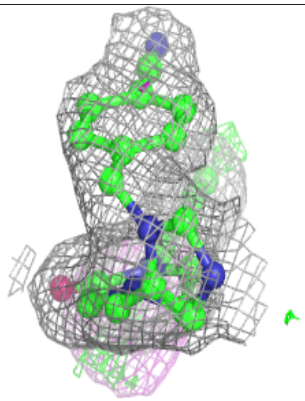


Electron density around 778 D 381:

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

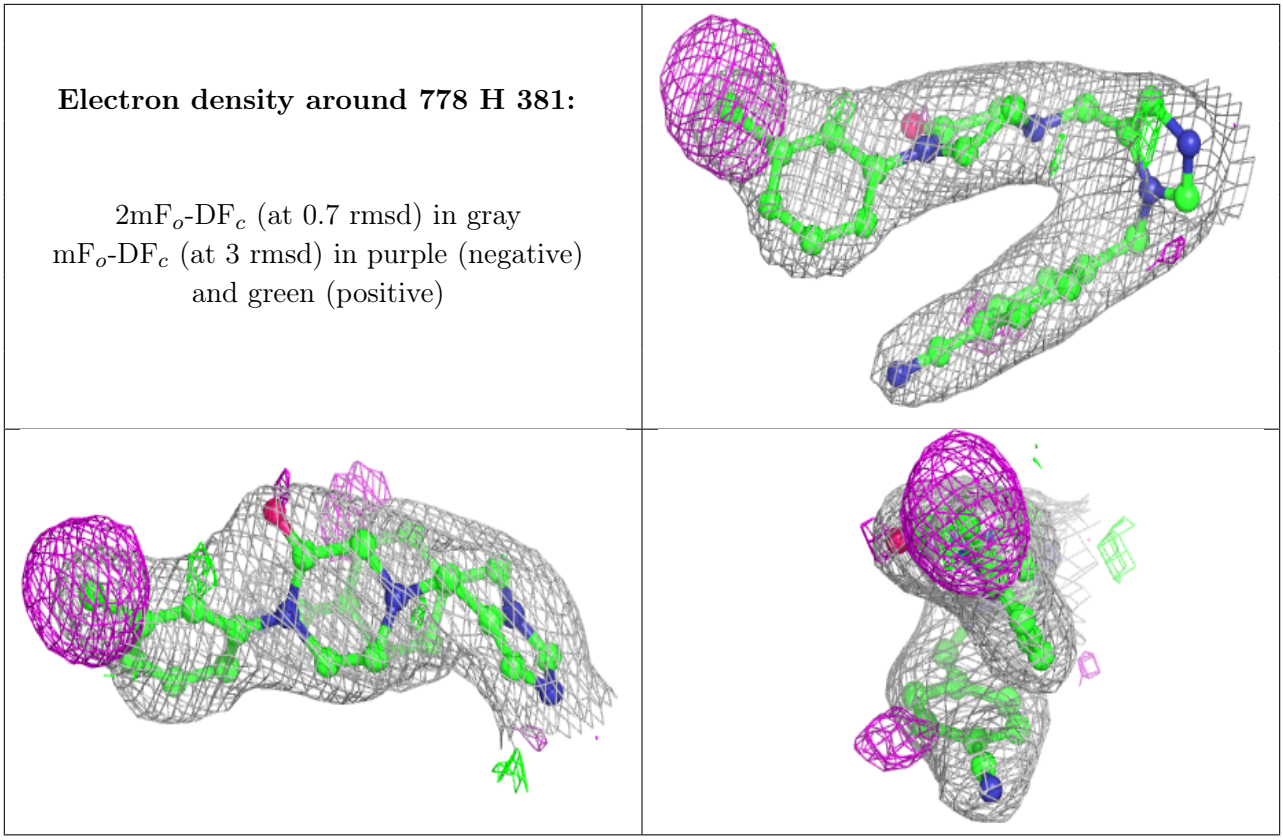






Electron density around 778 H 381:

$2mF_o$-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.