



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 12:09 am BST

PDB ID : 1TNO  
Title : Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a KKKSKTKCVIM Peptide Derived from K-Ras4B  
Authors : Reid, T.S.; Terry, K.L.; Casey, P.J.; Beese, L.S.  
Deposited on : 2004-06-11  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

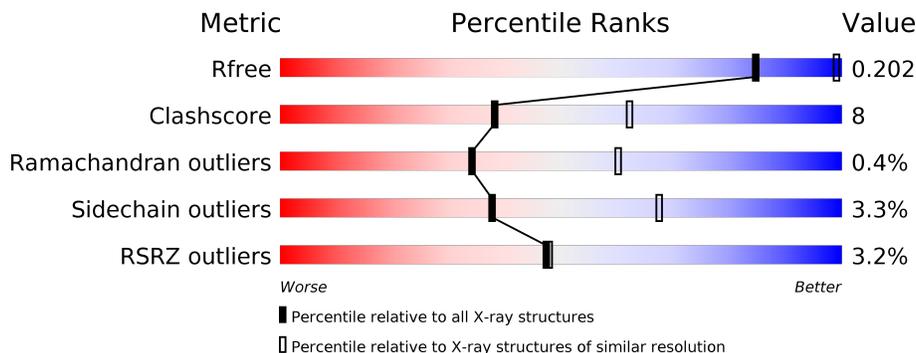
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	 2% 68% 15% 17%
1	E	377	 2% 67% 15% 17%
1	G	377	 2% 68% 14% 17%
1	I	377	 4% 67% 15% 17%
1	K	377	 % 70% 12% 17%

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Mol	Chain	Length	Quality of chain
2	B	377	<p>2% 74% 16% 8%</p>
2	D	377	<p>4% 77% 13% 8%</p>
2	F	377	<p>3% 77% 13% 8%</p>
2	H	377	<p>6% 72% 18% 8%</p>
2	J	377	<p>3% 72% 19% 8%</p>
2	L	377	<p>0% 78% 12% 8%</p>
3	M	11	<p>9% 55% 45%</p>
3	N	11	<p>0% 55% 45%</p>
3	O	11	<p>9% 27% 27% 45%</p>
3	P	11	<p>9% 55% 45%</p>
3	Q	11	<p>9% 55% 45%</p>
3	R	11	<p>9% 55% 45%</p>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33292 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 geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	Total 2629	C 1679	N 463	O 482	S 5	0	0	0
1	C	314	Total 2643	C 1689	N 461	O 488	S 5	0	0	0
1	E	314	Total 2642	C 1686	N 461	O 490	S 5	0	0	0
1	G	314	Total 2633	C 1683	N 459	O 486	S 5	0	0	0
1	I	314	Total 2656	C 1694	N 465	O 492	S 5	0	0	0
1	K	314	Total 2671	C 1703	N 467	O 496	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	346	Total 2697	C 1707	N 467	O 499	S 24	0	0	0
2	D	346	Total 2713	C 1715	N 472	O 502	S 24	0	0	0
2	F	346	Total 2718	C 1717	N 474	O 503	S 24	0	0	0
2	H	346	Total 2694	C 1706	N 464	O 500	S 24	0	0	0
2	J	346	Total 2711	C 1713	N 471	O 503	S 24	0	0	0
2	L	346	Total 2723	C 1720	N 473	O 506	S 24	0	0	0

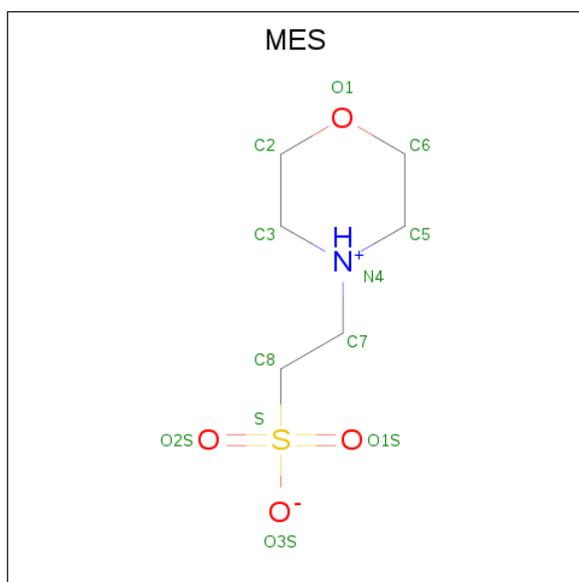
- Molecule 3 is a protein called c-K-ras2 protein isoform b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	N	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	O	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	P	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	Q	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	R	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

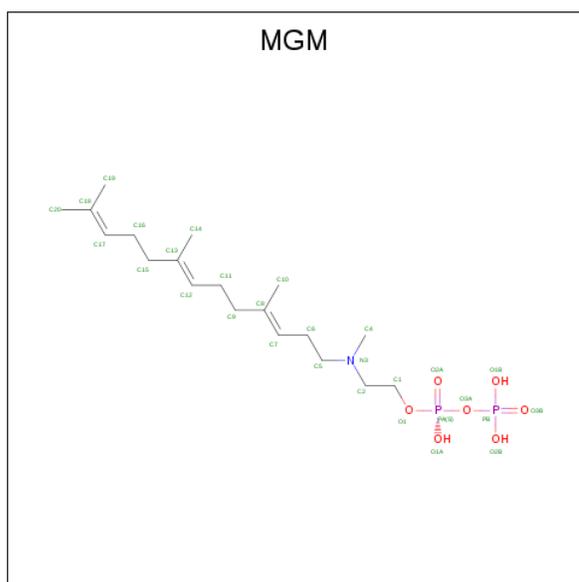
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0
5	F	1	12	6	1	4	1	0	0

- Molecule 6 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (three-letter code: MGM) (formula:  $C_{19}H_{37}NO_7P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	29	19	1	7	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
6	F	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
6	H	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
6	J	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
6	L	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Cl	0	0
			1	1		
7	L	1	Total	Cl	0	0
			1	1		
7	D	1	Total	Cl	0	0
			1	1		
7	F	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

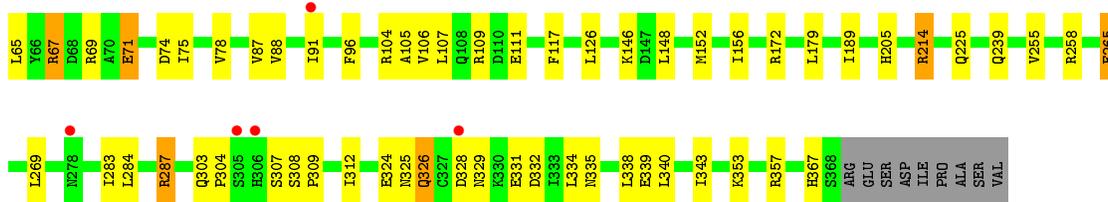
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	0
			44	44		
8	B	34	Total	O	0	0
			34	34		
8	C	41	Total	O	0	0
			41	41		
8	D	51	Total	O	0	0
			51	51		
8	E	50	Total	O	0	0
			50	50		
8	F	58	Total	O	0	0
			58	58		
8	G	40	Total	O	0	0
			40	40		
8	H	31	Total	O	0	0
			31	31		

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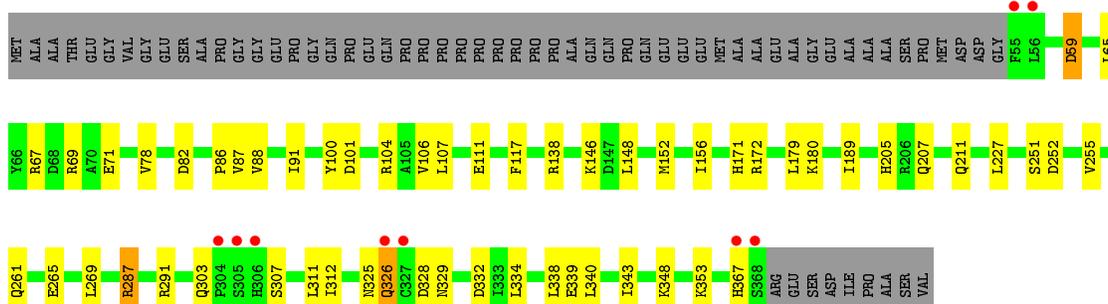
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	I	52	Total 52	O 52	0	0
8	J	47	Total 47	O 47	0	0
8	K	123	Total 123	O 123	0	0
8	L	93	Total 93	O 93	0	0
8	N	2	Total 2	O 2	0	0
8	O	2	Total 2	O 2	0	0
8	P	4	Total 4	O 4	0	0
8	Q	2	Total 2	O 2	0	0
8	R	4	Total 4	O 4	0	0

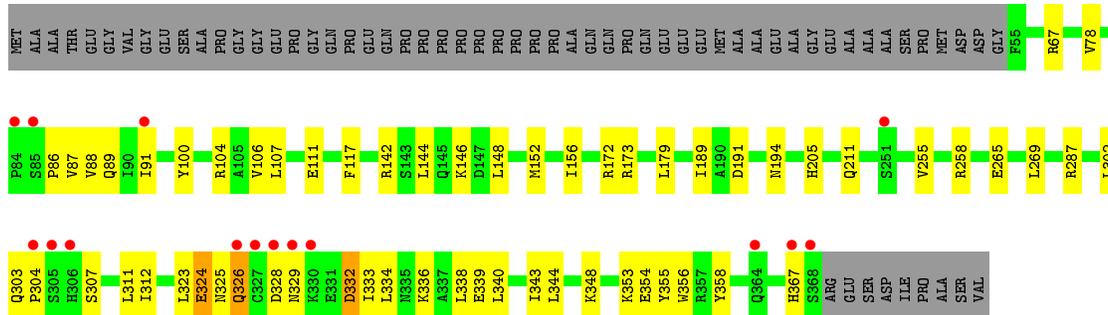




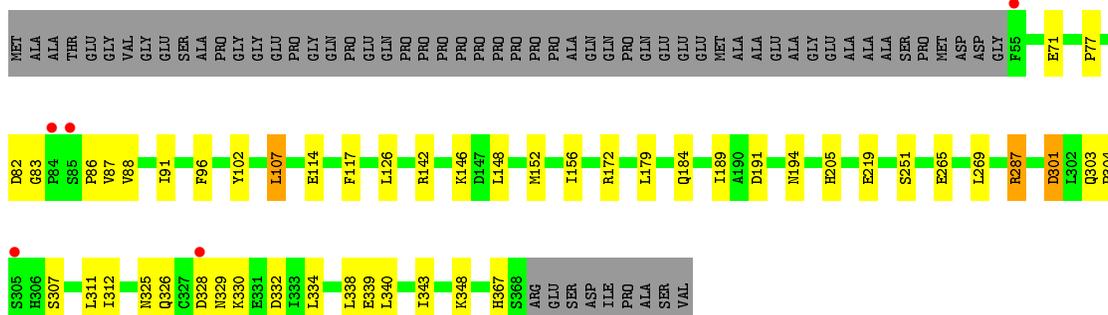
• Molecule 1: geranylgeranyltransferase type I alpha subunit



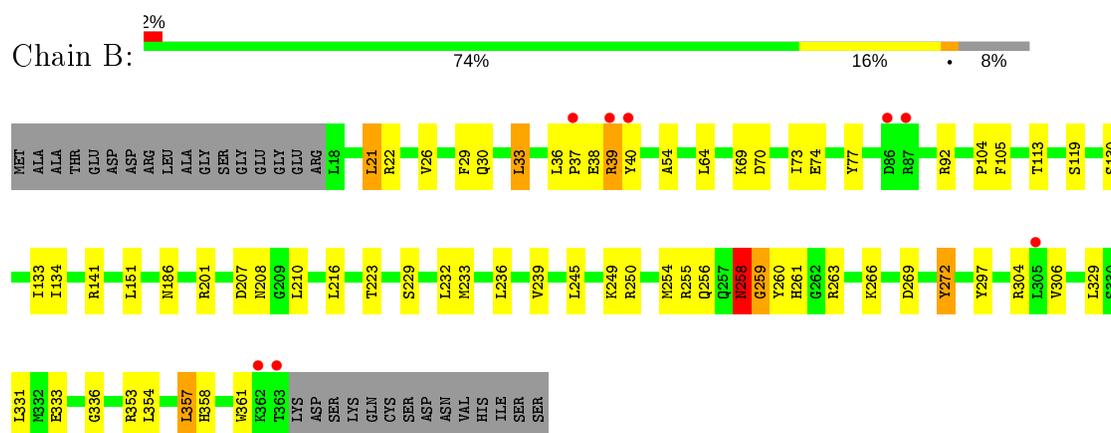
• Molecule 1: geranylgeranyltransferase type I alpha subunit



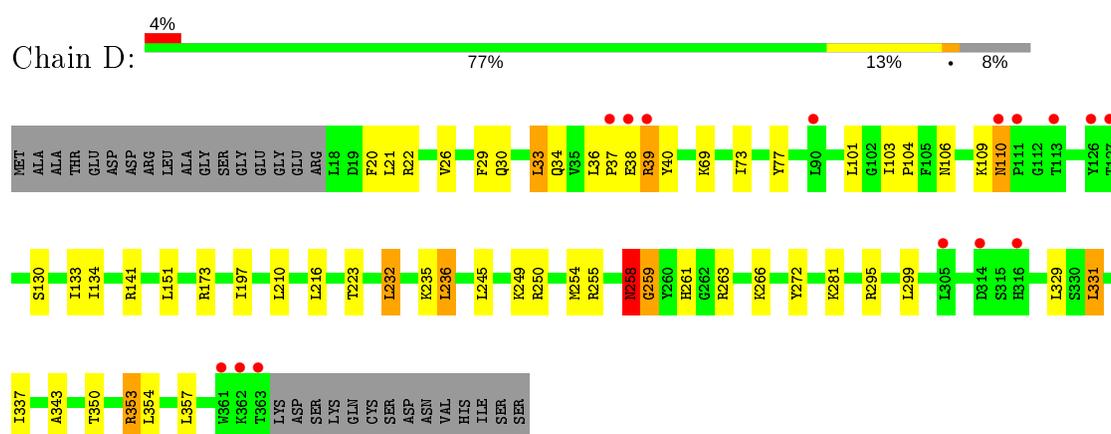
• Molecule 1: geranylgeranyltransferase type I alpha subunit



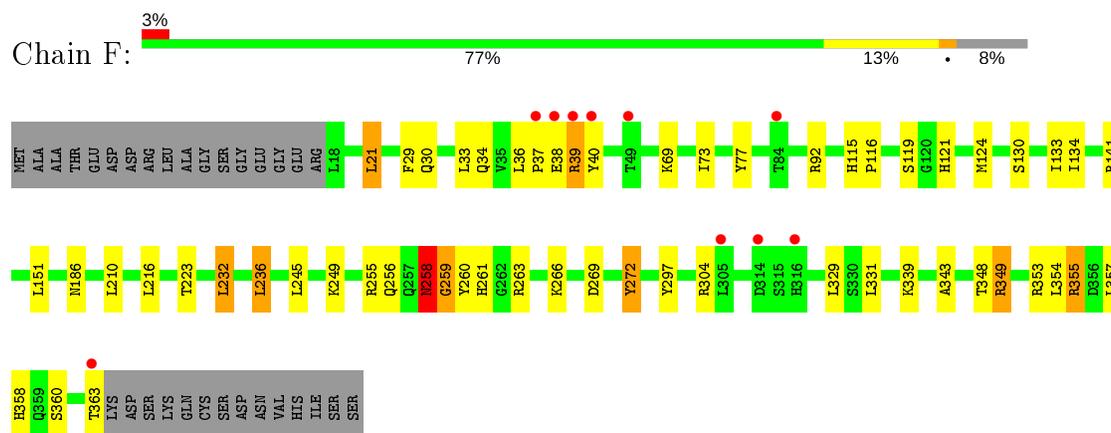
• Molecule 2: Geranylgeranyl transferase type I beta subunit



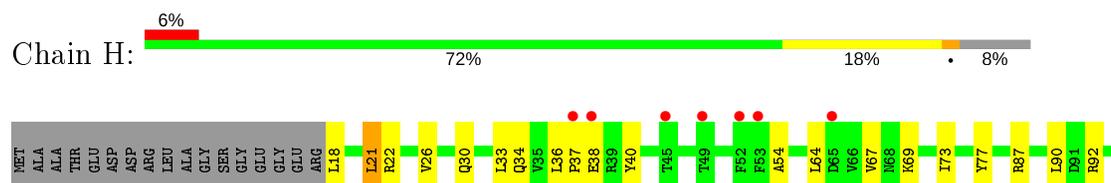
- Molecule 2: Geranylgeranyl transferase type I beta subunit

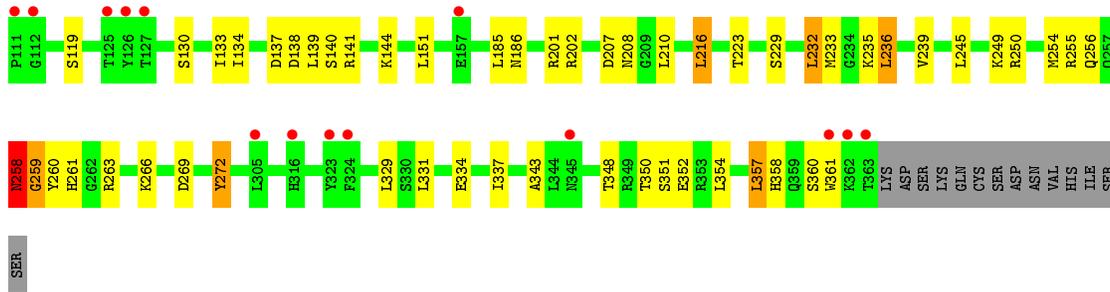


- Molecule 2: Geranylgeranyl transferase type I beta subunit

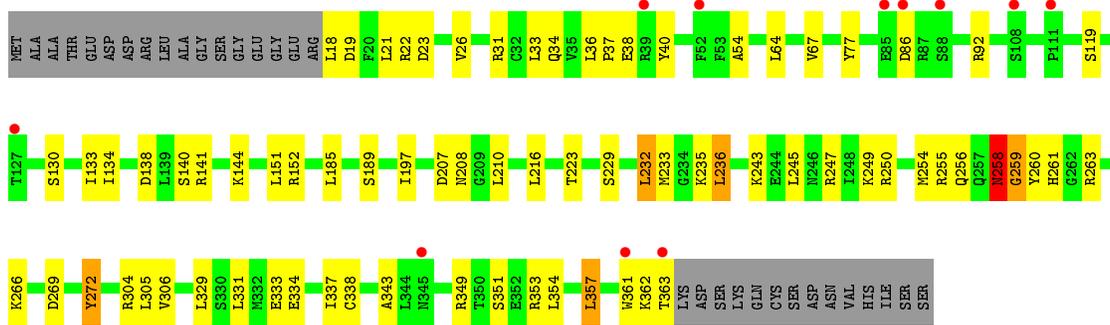


- Molecule 2: Geranylgeranyl transferase type I beta subunit





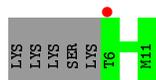
• Molecule 2: Geranylgeranyl transferase type I beta subunit



• Molecule 2: Geranylgeranyl transferase type I beta subunit

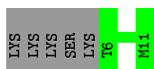


• Molecule 3: c-K-ras2 protein isoform b

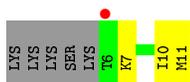


• Molecule 3: c-K-ras2 protein isoform b

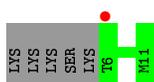




- Molecule 3: c-K-ras2 protein isoform b



- Molecule 3: c-K-ras2 protein isoform b



- Molecule 3: c-K-ras2 protein isoform b



- Molecule 3: c-K-ras2 protein isoform b



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	272.53Å 268.48Å 185.94Å 90.00° 131.48° 90.00°	Depositor
Resolution (Å)	29.98 – 2.70 29.98 – 2.54	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.98-2.70) 85.5 (29.98-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.54Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.194 , 0.211 0.185 , 0.202	Depositor DCC
$R_{free}$ test set	12637 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.089 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	33292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.35	0/2695	0.52	0/3668
1	C	0.38	0/2709	0.54	0/3684
1	E	0.37	0/2708	0.54	0/3684
1	G	0.39	0/2699	0.54	0/3672
1	I	0.38	0/2722	0.53	0/3700
1	K	0.40	0/2737	0.55	0/3717
2	B	0.38	0/2759	0.59	2/3733 (0.1%)
2	D	0.38	0/2775	0.59	2/3752 (0.1%)
2	F	0.40	0/2780	0.61	2/3758 (0.1%)
2	H	0.36	0/2756	0.59	2/3729 (0.1%)
2	J	0.37	0/2773	0.59	2/3750 (0.1%)
2	L	0.41	0/2785	0.61	2/3764 (0.1%)
3	M	0.51	0/45	0.68	0/57
3	N	0.53	0/45	0.69	0/57
3	O	0.51	0/45	0.79	0/57
3	P	0.49	0/45	0.67	0/57
3	Q	0.57	0/45	0.73	0/57
3	R	0.55	0/45	0.70	0/57
All	All	0.38	0/33168	0.57	12/44953 (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	2
2	D	0	1
2	F	0	2
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-5.91	98.33	113.10
2	L	259	GLY	N-CA-C	-5.89	98.37	113.10
2	F	259	GLY	N-CA-C	-5.76	98.69	113.10
2	H	259	GLY	N-CA-C	-5.76	98.71	113.10
2	B	259	GLY	N-CA-C	-5.68	98.90	113.10

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	TYR	Sidechain
2	B	297	TYR	Sidechain
2	D	272	TYR	Sidechain
2	F	272	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	2629	0	2520	52	0
1	C	2643	0	2540	39	0
1	E	2642	0	2534	40	0
1	G	2633	0	2524	45	0
1	I	2656	0	2560	42	0
1	K	2671	0	2588	38	0
2	B	2697	0	2600	45	0
2	D	2713	0	2628	43	0
2	F	2718	0	2635	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2694	0	2590	49	0
2	J	2711	0	2616	47	0
2	L	2723	0	2643	27	0
3	M	46	0	52	0	0
3	N	46	0	52	0	0
3	O	46	0	52	1	0
3	P	46	0	52	0	0
3	Q	46	0	52	0	0
3	R	46	0	52	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	B	12	0	13	0	0
5	F	12	0	13	0	0
6	B	29	0	34	0	0
6	D	29	0	34	1	0
6	F	29	0	34	0	0
6	H	29	0	34	1	0
6	J	29	0	34	0	0
6	L	29	0	34	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	A	44	0	0	1	0
8	B	34	0	0	0	0
8	C	41	0	0	2	0
8	D	51	0	0	0	0
8	E	50	0	0	0	0
8	F	58	0	0	0	0
8	G	40	0	0	0	0
8	H	31	0	0	0	0
8	I	52	0	0	1	0
8	J	47	0	0	0	0
8	K	123	0	0	2	0
8	L	93	0	0	0	0
8	N	2	0	0	0	0
8	O	2	0	0	0	0
8	P	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Q	2	0	0	0	0
8	R	4	0	0	0	0
All	All	33292	0	31520	485	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 485 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:K:156:ILE:HG12	1:K:172:ARG:HH12	1.02	1.10
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.09	1.09
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.18	1.07
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.10	1.05
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.15	1.04

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 66
1	C	312/377 (83%)	293 (94%)	18 (6%)	1 (0%)	41 66
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	41 66
1	G	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	41 66
1	I	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	41 66
1	K	312/377 (83%)	293 (94%)	19 (6%)	0	100 100
2	B	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	41 66
2	D	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	41 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	41	66
2	H	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	41	66
2	J	344/377 (91%)	329 (96%)	11 (3%)	4 (1%)	13	32
2	L	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	41	66
3	M	4/11 (36%)	4 (100%)	0	0	100	100
3	N	4/11 (36%)	4 (100%)	0	0	100	100
3	O	4/11 (36%)	4 (100%)	0	0	100	100
3	P	4/11 (36%)	4 (100%)	0	0	100	100
3	Q	4/11 (36%)	4 (100%)	0	0	100	100
3	R	4/11 (36%)	4 (100%)	0	0	100	100
All	All	3960/4590 (86%)	3761 (95%)	185 (5%)	14 (0%)	34	60

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
1	E	326	GLN
1	G	326	GLN
2	J	333	GLU
2	J	362	LYS

### 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	280/338 (83%)	273 (98%)	7 (2%)	47	76
1	C	283/338 (84%)	275 (97%)	8 (3%)	43	73
1	E	284/338 (84%)	276 (97%)	8 (3%)	43	73
1	G	281/338 (83%)	277 (99%)	4 (1%)	67	86
1	I	287/338 (85%)	280 (98%)	7 (2%)	49	77
1	K	291/338 (86%)	286 (98%)	5 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	289/326 (89%)	275 (95%)	14 (5%)	25	53
2	D	293/326 (90%)	279 (95%)	14 (5%)	25	53
2	F	294/326 (90%)	281 (96%)	13 (4%)	28	56
2	H	288/326 (88%)	278 (96%)	10 (4%)	36	65
2	J	292/326 (90%)	280 (96%)	12 (4%)	30	59
2	L	296/326 (91%)	283 (96%)	13 (4%)	28	56
3	M	6/11 (54%)	6 (100%)	0	100	100
3	N	6/11 (54%)	6 (100%)	0	100	100
3	O	6/11 (54%)	5 (83%)	1 (17%)	2	5
3	P	6/11 (54%)	6 (100%)	0	100	100
3	Q	6/11 (54%)	6 (100%)	0	100	100
3	R	6/11 (54%)	6 (100%)	0	100	100
All	All	3494/4050 (86%)	3378 (97%)	116 (3%)	38	67

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	39	ARG
1	G	59	ASP
2	L	232	LEU
2	F	216	LEU
2	F	261	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	225	GLN
1	G	81	ASN
2	J	246	ASN
1	E	325	ASN
1	E	335	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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
6	MGM	B	380	-	26,28,28	0.95	2 (7%)	33,37,37	2.03	5 (15%)
6	MGM	L	380	-	26,28,28	0.99	2 (7%)	33,37,37	2.03	5 (15%)
5	MES	F	380	-	12,12,12	9.13	8 (66%)	14,16,16	2.47	5 (35%)
6	MGM	H	380	-	26,28,28	0.91	2 (7%)	33,37,37	1.96	5 (15%)
6	MGM	J	379	-	26,28,28	0.98	2 (7%)	33,37,37	2.03	6 (18%)
5	MES	B	379	-	12,12,12	8.94	8 (66%)	14,16,16	2.44	5 (35%)
6	MGM	F	381	-	26,28,28	0.99	2 (7%)	33,37,37	2.03	6 (18%)
6	MGM	D	380	-	26,28,28	0.97	2 (7%)	33,37,37	2.05	5 (15%)

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
6	MGM	B	380	-	-	9/31/31/31	-
6	MGM	L	380	-	-	8/31/31/31	-
5	MES	F	380	-	-	3/6/14/14	0/1/1/1
6	MGM	H	380	-	-	9/31/31/31	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MGM	J	379	-	-	9/31/31/31	-
5	MES	B	379	-	-	1/6/14/14	0/1/1/1
6	MGM	F	381	-	-	9/31/31/31	-
6	MGM	D	380	-	-	8/31/31/31	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	380	MES	C8-S	-24.08	1.43	1.77
5	B	379	MES	C8-S	-22.34	1.45	1.77
5	B	379	MES	O2S-S	12.99	1.83	1.45
5	F	380	MES	O2S-S	12.46	1.81	1.45
5	B	379	MES	O1S-S	12.45	1.81	1.45

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	380	MGM	C1-C2-N3	7.36	131.26	113.31
6	F	381	MGM	C1-C2-N3	7.27	131.04	113.31
6	D	380	MGM	C1-C2-N3	7.24	130.95	113.31
6	L	380	MGM	C1-C2-N3	7.15	130.73	113.31
6	J	379	MGM	C1-C2-N3	7.12	130.65	113.31

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

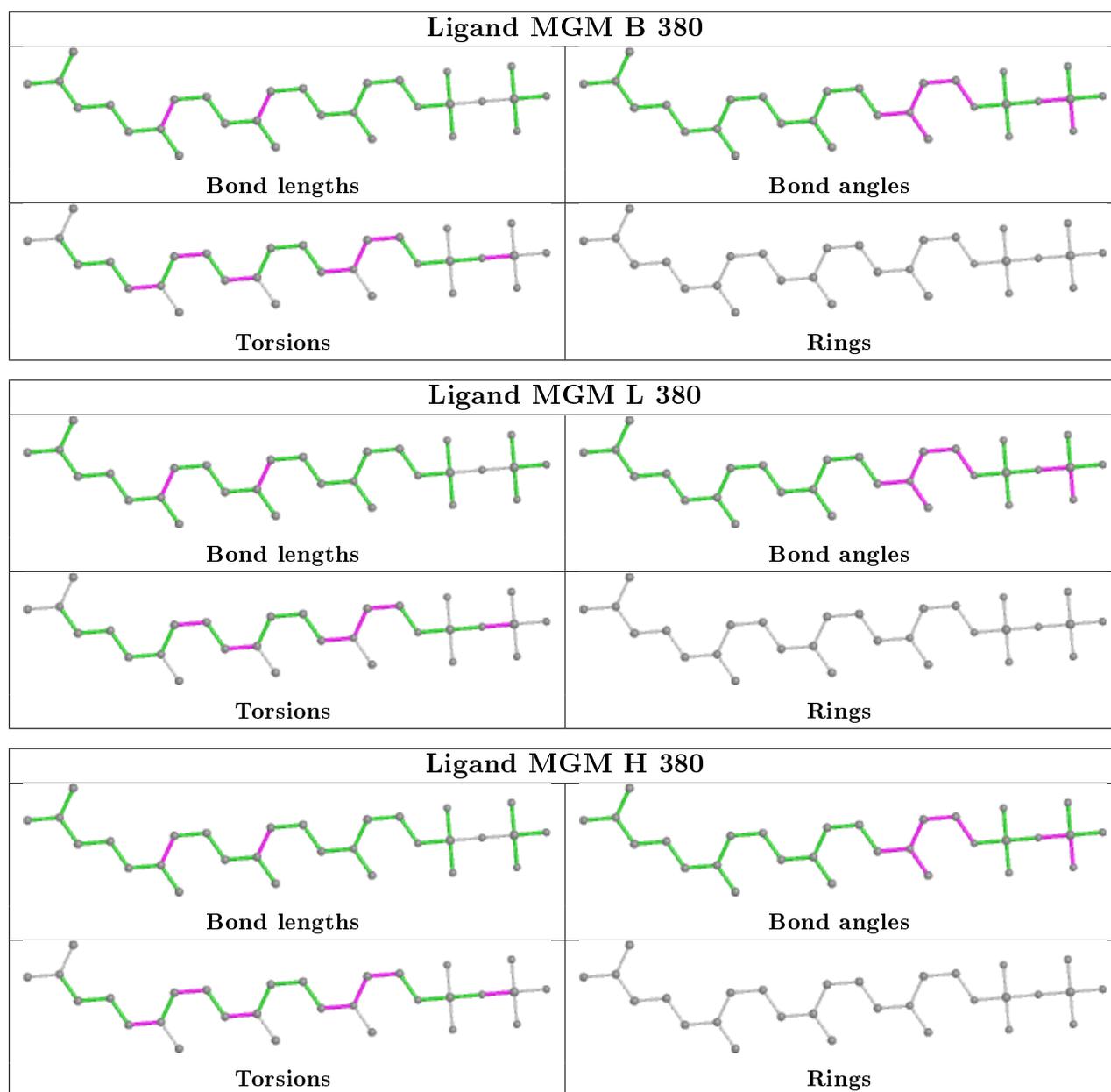
Mol	Chain	Res	Type	Atoms
6	B	380	MGM	C1-C2-N3-C4
6	B	380	MGM	O1-C1-C2-N3
6	B	380	MGM	PA-O3A-PB-O1B
6	L	380	MGM	C1-C2-N3-C4
6	L	380	MGM	O1-C1-C2-N3

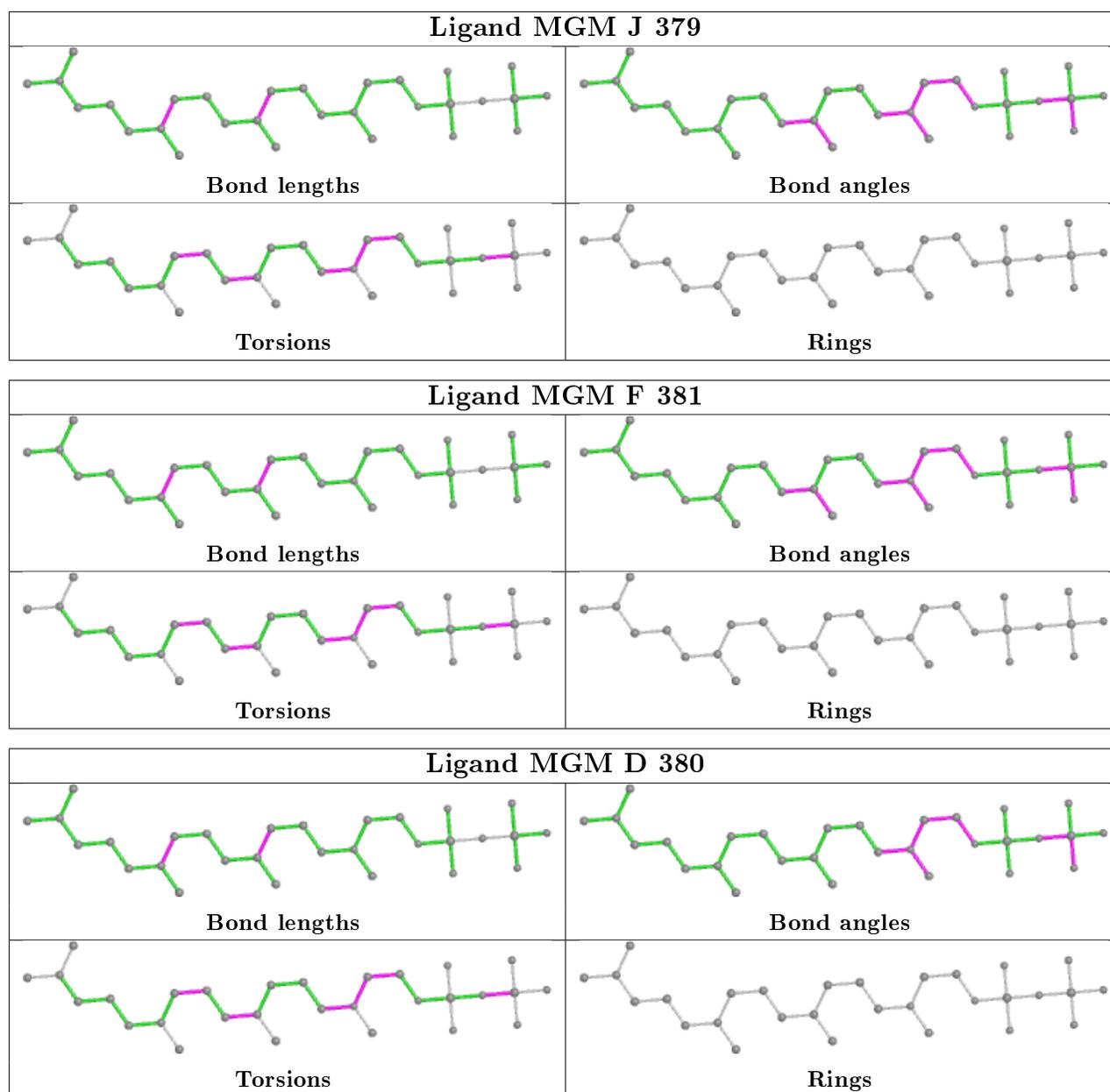
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	380	MGM	1	0
6	D	380	MGM	1	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 than 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.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	314/377 (83%)	-0.06	13 (4%) 37 36	47, 69, 103, 119	0
1	C	314/377 (83%)	-0.16	7 (2%) 62 63	44, 66, 94, 111	0
1	E	314/377 (83%)	-0.09	6 (1%) 66 69	42, 67, 96, 113	0
1	G	314/377 (83%)	-0.16	9 (2%) 51 52	43, 65, 96, 109	0
1	I	314/377 (83%)	-0.06	15 (4%) 30 28	43, 68, 98, 109	0
1	K	314/377 (83%)	-0.32	5 (1%) 72 74	35, 55, 80, 94	0
2	B	346/377 (91%)	-0.07	8 (2%) 60 62	48, 63, 89, 112	0
2	D	346/377 (91%)	-0.05	15 (4%) 35 33	43, 59, 86, 103	0
2	F	346/377 (91%)	-0.12	10 (2%) 51 52	42, 56, 84, 108	0
2	H	346/377 (91%)	0.11	21 (6%) 21 20	44, 72, 102, 119	0
2	J	346/377 (91%)	-0.03	11 (3%) 47 48	45, 65, 92, 117	0
2	L	346/377 (91%)	-0.14	4 (1%) 79 80	39, 53, 77, 106	0
3	M	6/11 (54%)	0.03	1 (16%) 1 1	53, 57, 78, 88	0
3	N	6/11 (54%)	0.00	0 100 100	53, 59, 78, 83	0
3	O	6/11 (54%)	0.23	1 (16%) 1 1	50, 58, 77, 85	0
3	P	6/11 (54%)	0.37	1 (16%) 1 1	60, 69, 86, 92	0
3	Q	6/11 (54%)	0.42	1 (16%) 1 1	51, 63, 82, 91	0
3	R	6/11 (54%)	0.35	1 (16%) 1 1	47, 58, 76, 84	0
All	All	3996/4590 (87%)	-0.09	129 (3%) 47 48	35, 63, 93, 119	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	5.3
2	B	363	THR	5.0
1	C	55	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
3	P	6	THR	4.0
1	C	306	HIS	4.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

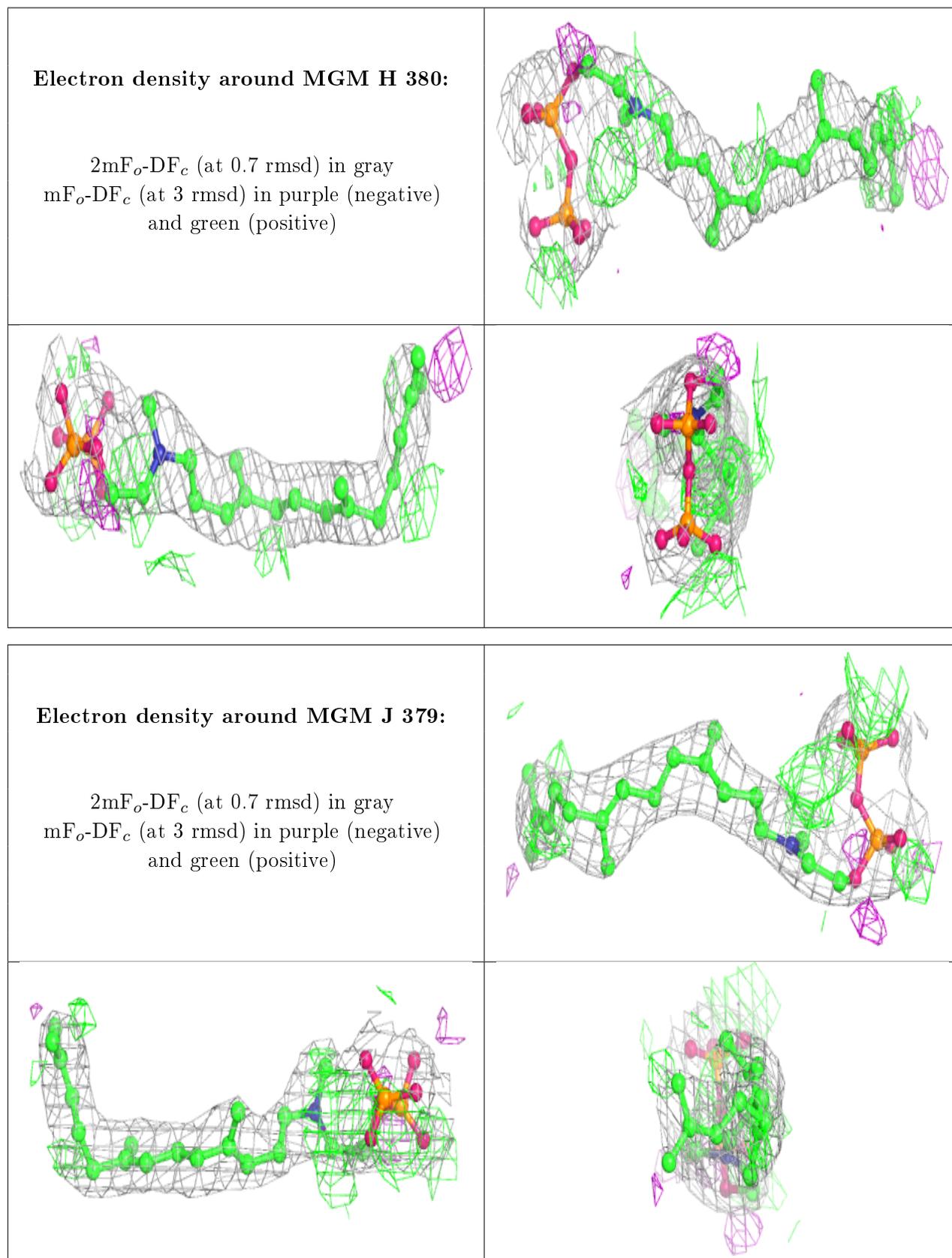
## 6.4 Ligands [i](#)

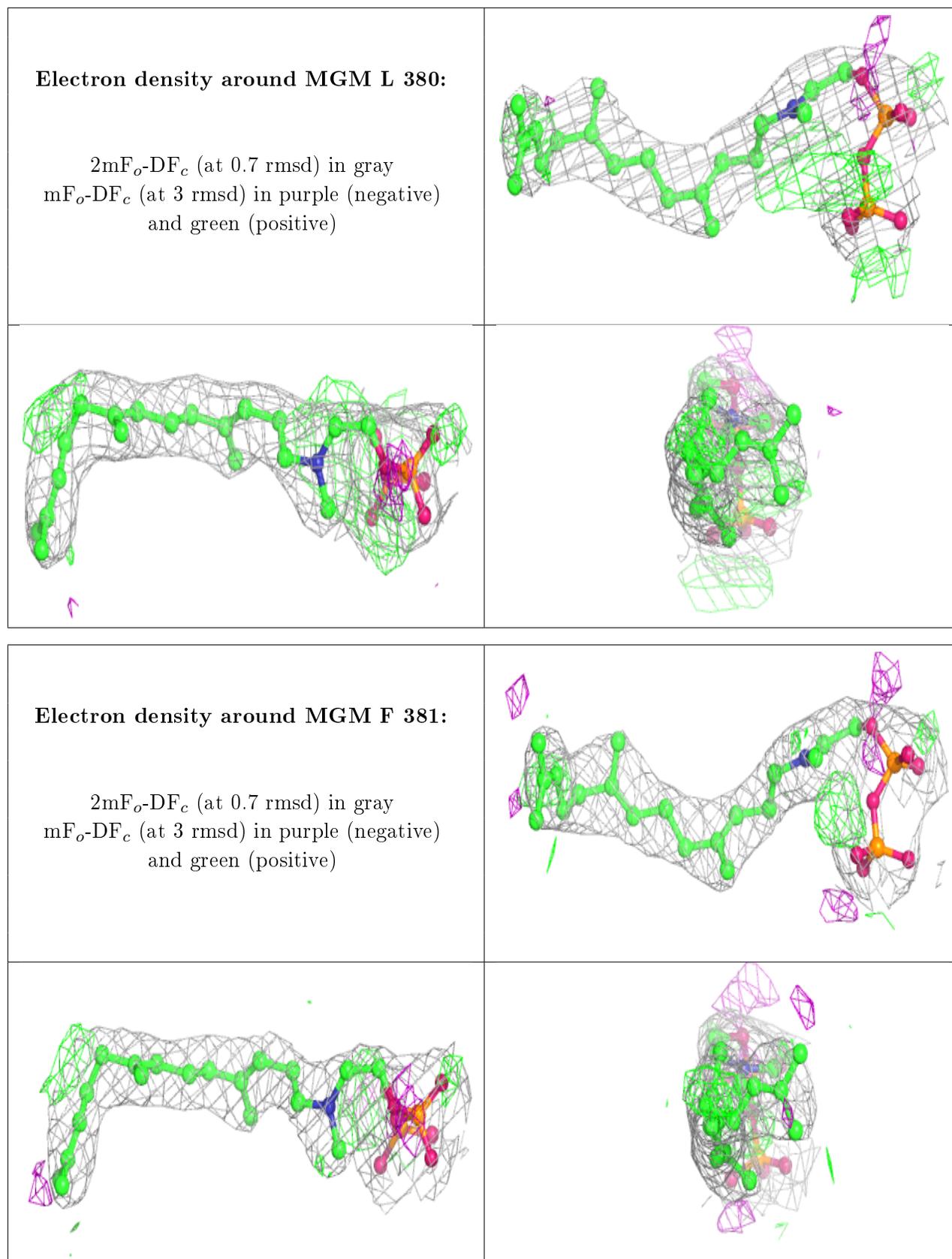
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MES	B	379	12/12	0.88	0.25	99,108,110,110	0
6	MGM	H	380	29/29	0.95	0.19	56,65,74,75	0
6	MGM	J	379	29/29	0.95	0.23	50,58,70,71	0
5	MES	F	380	12/12	0.96	0.22	86,94,97,97	0
6	MGM	L	380	29/29	0.96	0.22	41,54,65,67	0
7	CL	D	379	1/1	0.96	0.08	62,62,62,62	0
6	MGM	F	381	29/29	0.96	0.19	49,56,66,69	0
6	MGM	D	380	29/29	0.96	0.17	50,59,67,69	0
6	MGM	B	380	29/29	0.97	0.19	52,59,69,72	0
7	CL	L	379	1/1	0.98	0.04	59,59,59,59	0
7	CL	H	379	1/1	0.98	0.07	69,69,69,69	0
4	ZN	L	378	1/1	0.99	0.09	46,46,46,46	0
4	ZN	F	378	1/1	0.99	0.08	48,48,48,48	0
4	ZN	H	378	1/1	0.99	0.09	60,60,60,60	0
7	CL	F	379	1/1	0.99	0.10	55,55,55,55	0
4	ZN	B	378	1/1	0.99	0.08	51,51,51,51	0
4	ZN	J	378	1/1	0.99	0.08	53,53,53,53	0
4	ZN	D	378	1/1	1.00	0.09	53,53,53,53	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

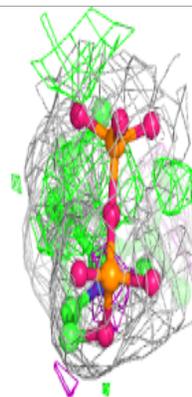
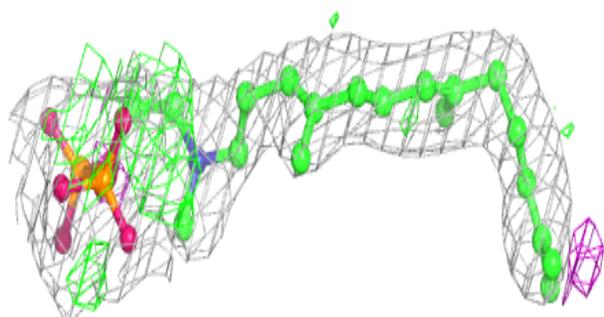
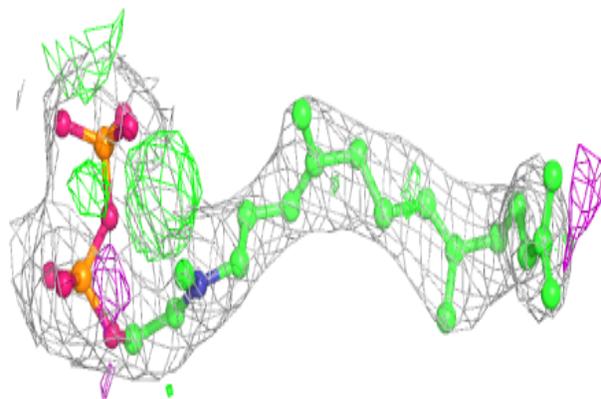
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



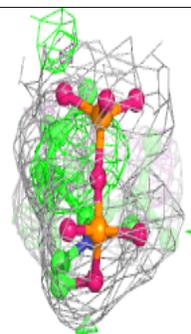
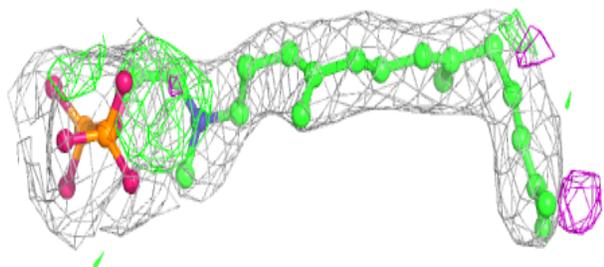
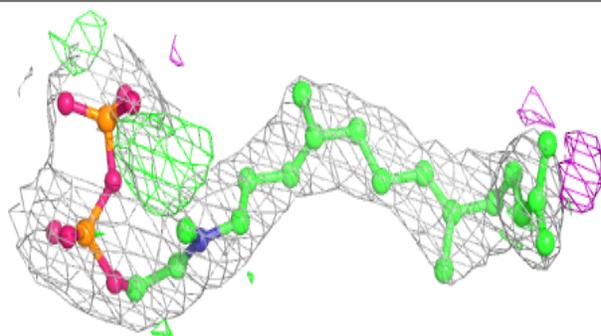


**Electron density around MGM D 380:**

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

**Electron density around MGM 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)



## 6.5 Other polymers

There are no such residues in this entry.