WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 01:25 AM EDT

PDB ID	:	1TNY
Title	:	Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a FREKKFFCAIL Peptide Derived from the Heterotrimeric G Protein Gamma-2 Subunit
Authors	:	S Reid, T.; Terry, K.L.; Casey, P.J.; Beese, L.S.
Deposited on	:	2004-06-11
Resolution	:	2.70 Å(reported)

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

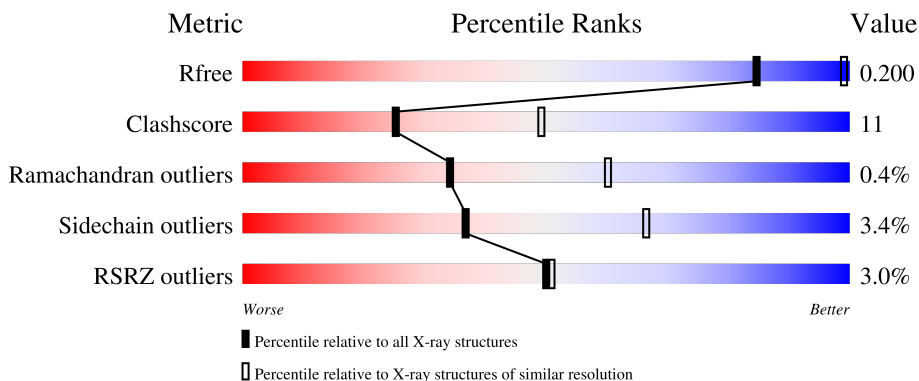|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.200
Clashscore		11
Ramachandran outliers		0.4%
Sidechain outliers		3.4%
RSRZ outliers		3.0%

Worse ⟶ *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 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% / 62% 19% • 17%
1	C	377	3% / 63% 19% • 17%
1	E	377	2% / 59% 23% • 17%
1	G	377	3% / 62% 20% • 17%

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Mol	Chain	Length	Quality of chain
1	I	377	3% 66% 16% • 17%
1	K	377	% 66% 16% • 17%
2	B	377	2% 70% 19% • 8%
2	D	377	3% 71% 18% • 8%
2	F	377	3% 73% 17% • 8%
2	H	377	6% 67% 22% • 8%
2	J	377	3% 71% 19% • 8%
2	L	377	% 72% 18% • 8%
3	M	11	45% 55%
3	N	11	36% 9% 55%
3	O	11	45% 55%
3	P	11	9% 36% 9% 55%
3	Q	11	36% 9% 55%
3	R	11	36% 9% 55%

2   Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 33566 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
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
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 guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total 38	C 27	N 4	O 6	S 1	0	0	0
3	N	5	Total 39	C 27	N 5	O 6	S 1	0	0	0
3	O	5	Total 39	C 27	N 5	O 6	S 1	0	0	0
3	P	5	Total 39	C 27	N 5	O 6	S 1	0	0	0
3	Q	5	Total 39	C 27	N 5	O 6	S 1	0	0	0
3	R	5	Total 39	C 27	N 5	O 6	S 1	0	0	0

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

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	F	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0
5	J	1	Total 1	Cl 1	0	0
5	L	1	Total 1	Cl 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
6	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
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 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

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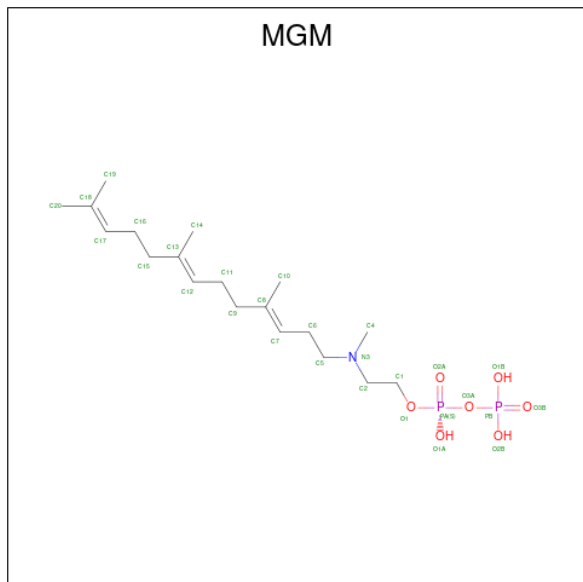
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	F	1	12	6	1	4	1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	66	Total 66	O 66	0	0
8	B	54	Total 54	O 54	0	0
8	C	69	Total 69	O 69	0	0
8	D	79	Total 79	O 79	0	0
8	E	63	Total 63	O 63	0	0
8	F	84	Total 84	O 84	0	0
8	G	70	Total 70	O 70	0	0
8	H	58	Total 58	O 58	0	0
8	I	80	Total 80	O 80	0	0
8	J	71	Total 71	O 71	0	0
8	K	160	Total 160	O 160	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	123	Total 123	O 123	0	0
8	M	7	Total 7	O 7	0	0
8	N	5	Total 5	O 5	0	0
8	O	5	Total 5	O 5	0	0
8	P	5	Total 5	O 5	0	0
8	Q	3	Total 3	O 3	0	0
8	R	3	Total 3	O 3	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.
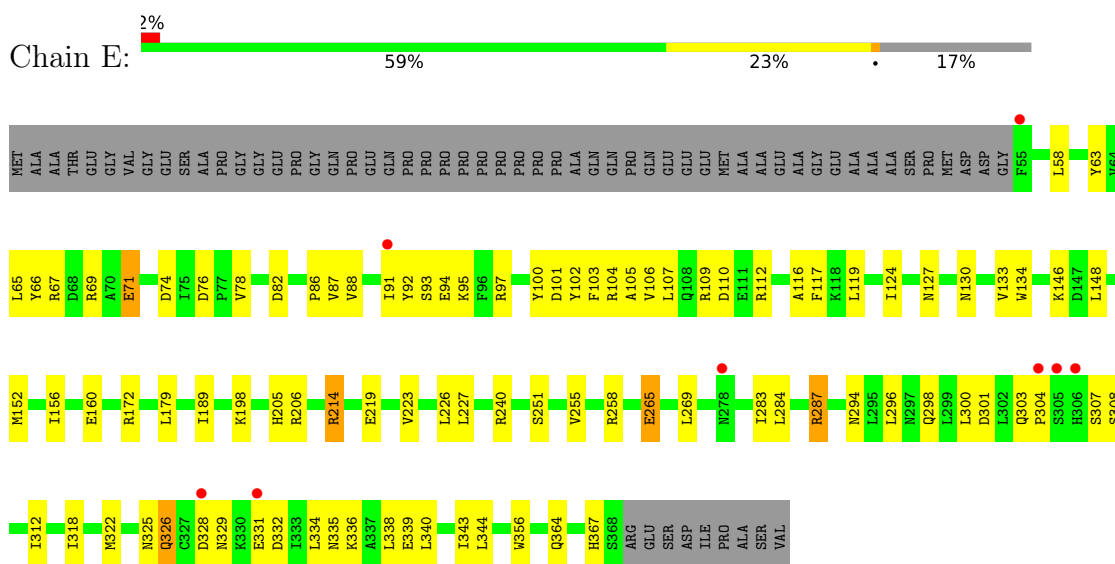
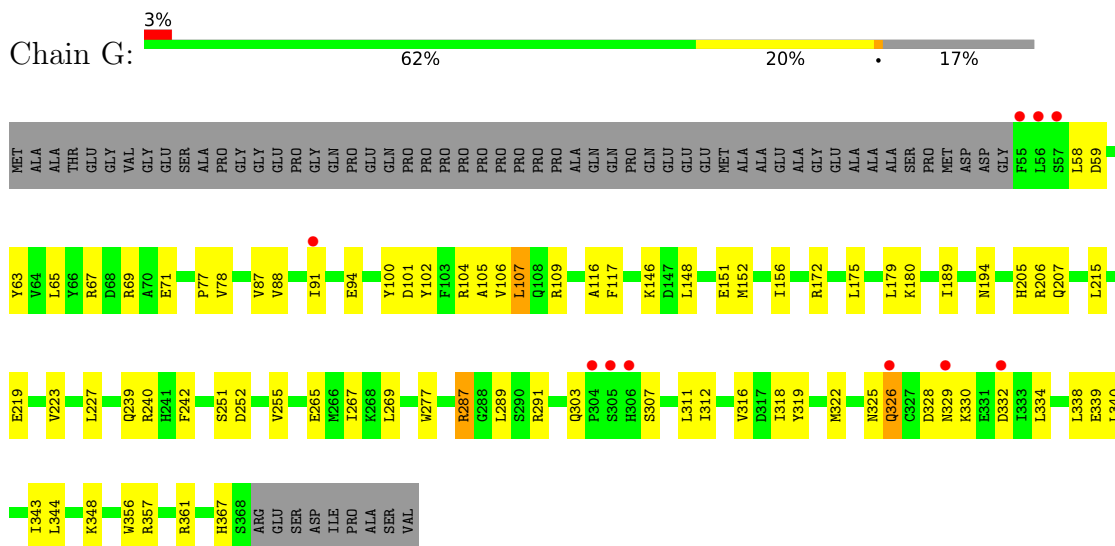• Molecule 1: geranylgeranyltransferase type I alpha subunit

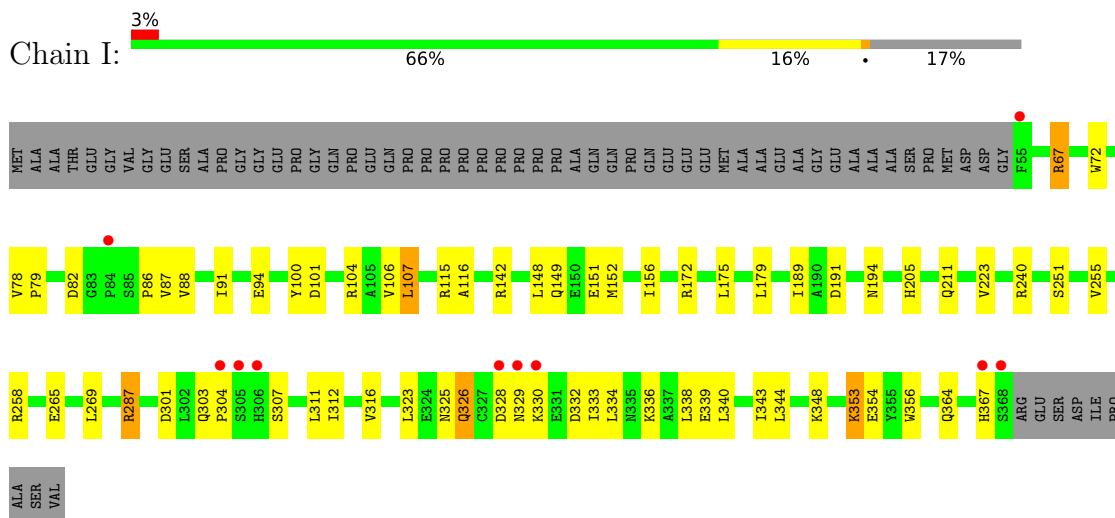• Molecule 1: geranylgeranyltransferase type I alpha subunit

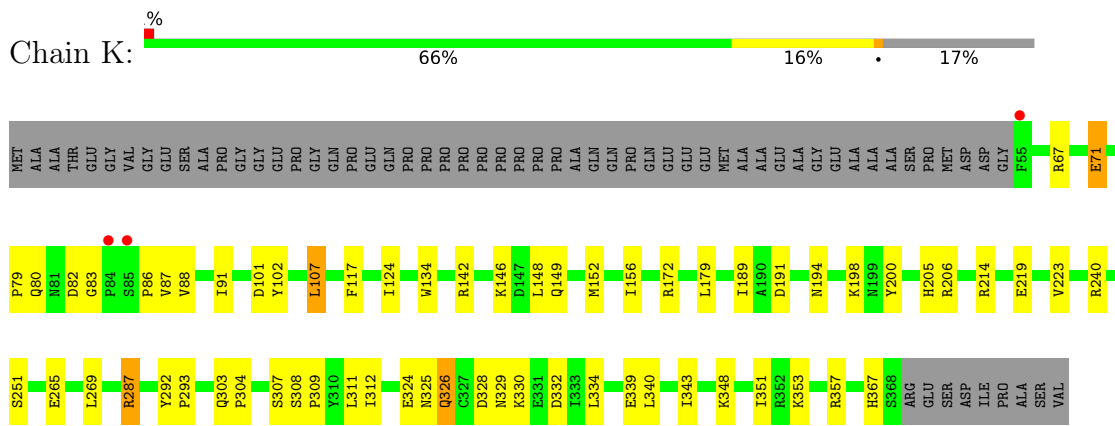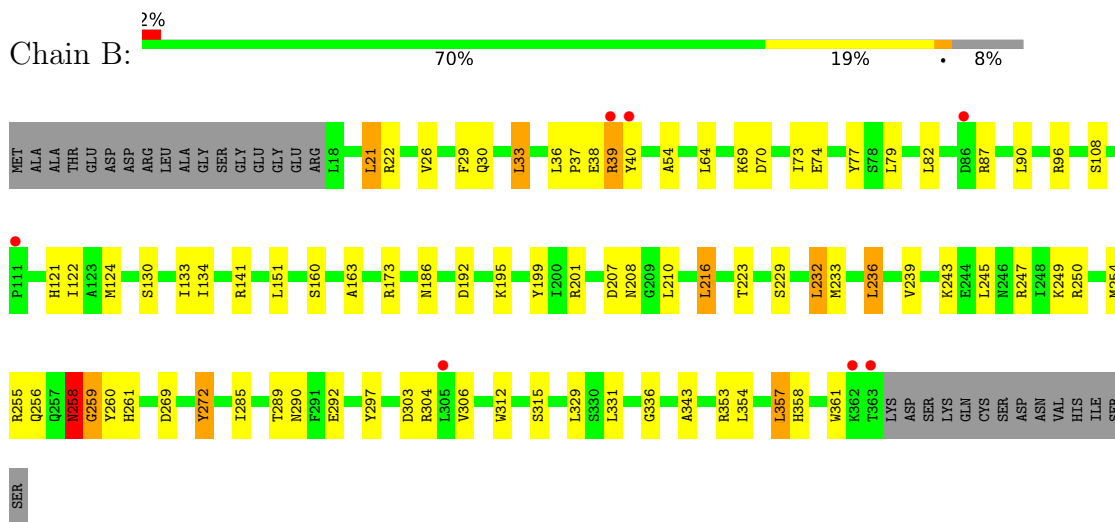• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain E:

• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain G:

• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain I:

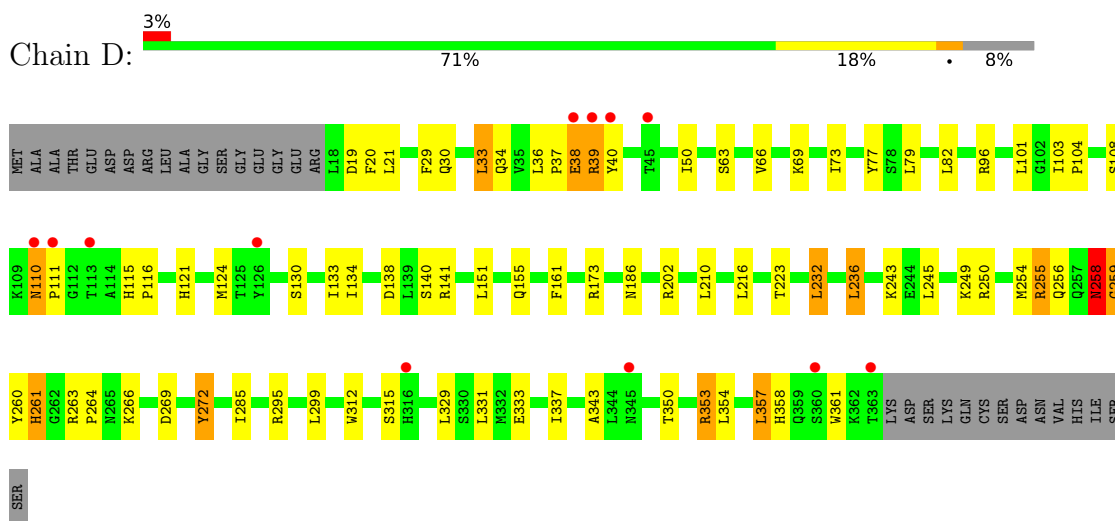• Molecule 1: geranylgeranyltransferase type I alpha subunit

Chain K:

• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain B:

• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain D:

• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain F:

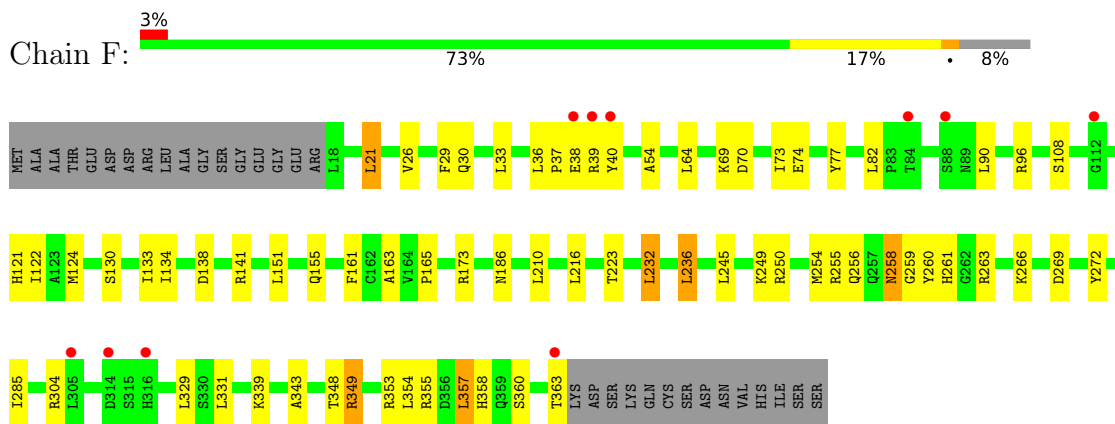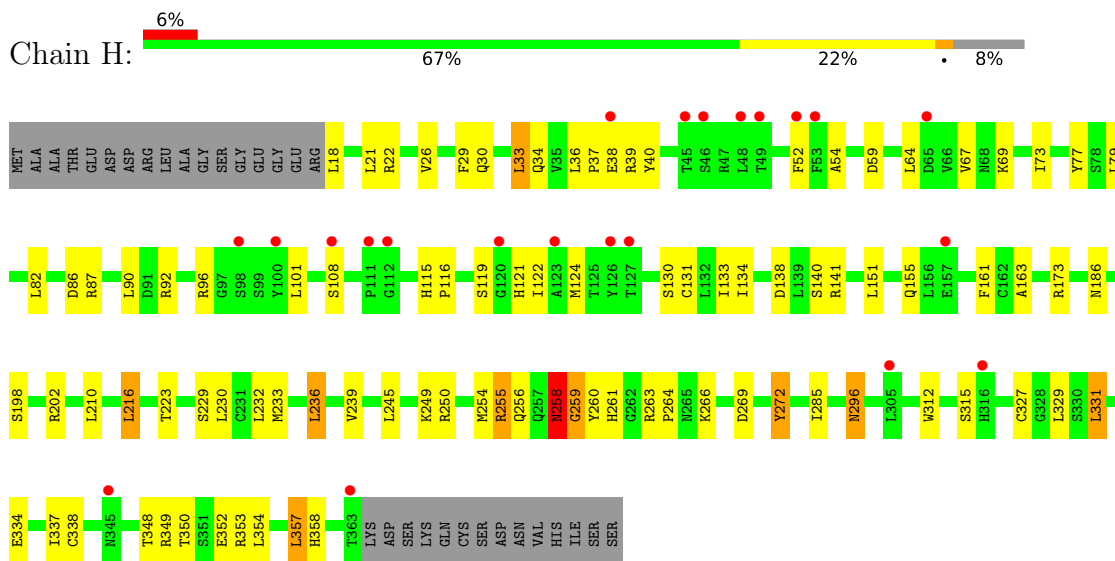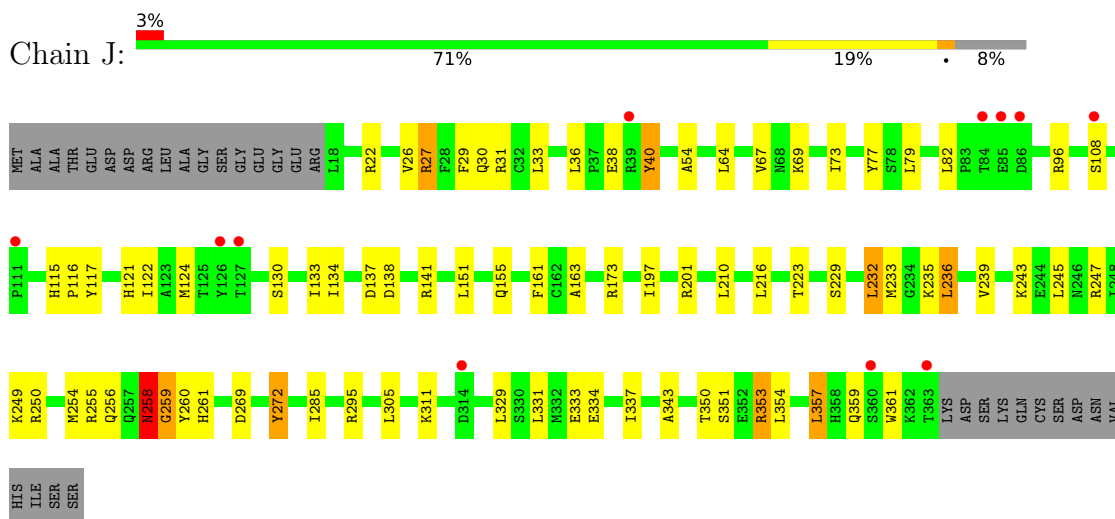• Molecule 2: Geranylgeranyl transferase type I beta subunit
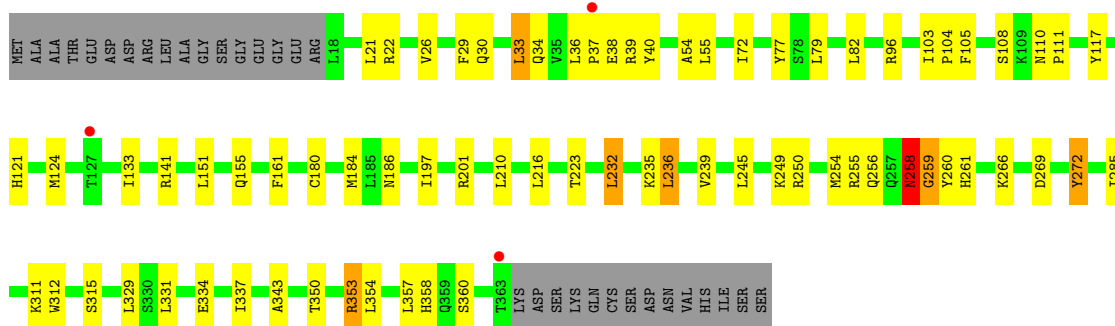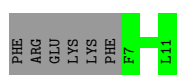
Chain H:

• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain J:

• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain L:

MET ALA ALA THR GLU ASP ASP ARG LEU ALA GLY SER GLU GLU GLY ARG L18 L21 R22 V26 F29 Q30 L33 Q34 V35 L36 P37 E38 R39 Y40 A54 L55 I72 Y77 S78 L79 L82 R96 I103 P104 F105 S108 K109 N110 P111 Y117

H121 M124 T127 I133 R141 L151 Q155 F161 C180 M184 L185 N186 I197 R201 L210 L216 T223 L232 K235 L236 V239 L245 K249 R250 M254 R255 Q256 Q257 N258 G259 Y260 H261 K266 D269 Y272 I285

K311 W312 S315 L329 S330 L331 E334 I337 A343 T350 R353 L354 L357 H358 Q359 S360 T363 LYS ASP SER LYS GLN CYS SER ASP ASN VAL HIS ILE SER SER

- Molecule 3: guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit

Chain M:

45%   55%

PHE ARG GLU LYS LYS PHE F7 L11

- Molecule 3: guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit

Chain N:

36%   9%   55%

PHE ARG GLU LYS LYS PHE F7 L11

- Molecule 3: guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit

Chain O:

45%   55%

PHE ARG GLU LYS LYS PHE F7 L11

- Molecule 3: guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit

9%

Chain P:

36%   9%   55%

PHE ARG GLU LYS LYS PHE F7 L11

- Molecule 3: guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit

Chain Q:

36%   9%   55%
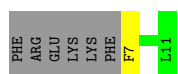
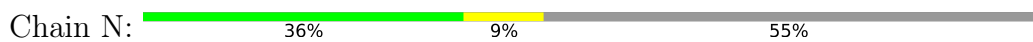PHE ARG GLU LYS LYS PHE F7 L11

- Molecule 3: guanine nucleotide-binding protein G(I)/G(S)/G(O) gamma-2 subunit

Chain R:

36%   9%   55%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	270.95Å 264.01Å 184.99Å 90.00° 131.72° 90.00°	Depositor
Resolution (Å)	29.91 – 2.70 29.91 – 2.49	Depositor EDS
% Data completeness (in resolution range)	91.8 (29.91-2.70) 82.7 (29.91-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	0.77 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.212 0.181 , 0.200	Depositor DCC
R_{free} test set	10710 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å²)	47.8	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.35 , 50.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.079 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33566	wwPDB-VP
Average B, all atoms (Å²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: MGM, MES, ZN, 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	0.37	0/2709	0.53	0/3684
1	E	0.36	0/2708	0.54	0/3684
1	G	0.38	0/2699	0.53	0/3672
1	I	0.37	0/2722	0.53	0/3700
1	K	0.39	0/2737	0.55	0/3717
2	B	0.37	0/2759	0.59	2/3733 (0.1%)
2	D	0.37	0/2775	0.59	2/3752 (0.1%)
2	F	0.39	0/2780	0.61	2/3758 (0.1%)
2	H	0.35	0/2756	0.58	2/3729 (0.1%)
2	J	0.37	0/2773	0.59	2/3750 (0.1%)
2	L	0.39	0/2785	0.61	2/3764 (0.1%)
3	M	0.74	0/38	0.53	0/48
3	N	0.63	0/39	0.53	0/50
3	O	0.77	0/39	0.61	0/50
3	P	0.65	0/39	0.61	0/50
3	Q	0.65	0/39	0.56	0/50
3	R	0.57	0/39	0.53	0/50
All	All	0.37	0/33131	0.57	12/44909 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
2	B	0	2
2	D	0	1
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	7

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	F	259	GLY	N-CA-C	-6.00	98.10	113.10
2	D	259	GLY	N-CA-C	-5.91	98.33	113.10
2	L	259	GLY	N-CA-C	-5.82	98.56	113.10
2	J	259	GLY	N-CA-C	-5.80	98.61	113.10
2	H	259	GLY	N-CA-C	-5.75	98.74	113.10

There are no chirality outliers.

5 of 7 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
1	E	102	TYR	Sidechain
2	H	272	TYR	Sidechain

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	2629	0	2520	66	0
1	C	2643	0	2540	61	0
1	E	2642	0	2534	72	0
1	G	2633	0	2524	64	0
1	I	2656	0	2560	54	0
1	K	2671	0	2588	50	0
2	B	2697	0	2600	66	0
2	D	2713	0	2628	63	0
2	F	2718	0	2635	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2694	0	2590	68	0
2	J	2711	0	2616	56	0
2	L	2723	0	2643	51	0
3	M	38	0	38	0	0
3	N	39	0	39	0	0
3	O	39	0	39	0	0
3	P	39	0	39	0	0
3	Q	39	0	39	1	0
3	R	39	0	39	1	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	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
6	B	29	0	34	2	0
6	D	29	0	34	3	0
6	F	29	0	34	1	0
6	H	29	0	34	3	0
6	J	29	0	34	3	0
6	L	29	0	34	2	0
7	F	12	0	13	1	0
8	A	66	0	0	1	0
8	B	54	0	0	2	0
8	C	69	0	0	1	0
8	D	79	0	0	4	0
8	E	63	0	0	0	0
8	F	84	0	0	2	0
8	G	70	0	0	2	0
8	H	58	0	0	2	0
8	I	80	0	0	0	0
8	J	71	0	0	0	0
8	K	160	0	0	3	0
8	L	123	0	0	0	0
8	M	7	0	0	0	0
8	N	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	5	0	0	0	0
8	P	5	0	0	0	0
8	Q	3	0	0	0	0
8	R	3	0	0	0	0
All	All	33566	0	31428	682	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 11.

The worst 5 of 682 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	1.00	1.15
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.06	1.10
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.14	1.08
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.17	1.05
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.18	1.03

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	312/377 (83%)	286 (92%)	25 (8%)	1 (0%)	41	66
1	C	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	41	66
1	E	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	41	66
1	G	312/377 (83%)	291 (93%)	20 (6%)	1 (0%)	41	66
1	I	312/377 (83%)	291 (93%)	20 (6%)	1 (0%)	41	66
1	K	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	41	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	41	66
2	D	344/377 (91%)	330 (96%)	11 (3%)	3 (1%)	17	40
2	F	344/377 (91%)	330 (96%)	13 (4%)	1 (0%)	41	66
2	H	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	41	66
2	J	344/377 (91%)	328 (95%)	14 (4%)	2 (1%)	25	50
2	L	344/377 (91%)	334 (97%)	9 (3%)	1 (0%)	41	66
3	M	3/11 (27%)	3 (100%)	0	0	100	100
3	N	3/11 (27%)	3 (100%)	0	0	100	100
3	O	3/11 (27%)	3 (100%)	0	0	100	100
3	P	3/11 (27%)	3 (100%)	0	0	100	100
3	Q	3/11 (27%)	2 (67%)	1 (33%)	0	100	100
3	R	3/11 (27%)	2 (67%)	1 (33%)	0	100	100
All	All	3954/4590 (86%)	3735 (94%)	204 (5%)	15 (0%)	34	60

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	38	GLU
1	G	326	GLN
2	B	258	ASN
1	C	326	GLN
1	E	326	GLN

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	280/338 (83%)	273 (98%)	7 (2%)	47	76
1	C	283/338 (84%)	276 (98%)	7 (2%)	47	76
1	E	284/338 (84%)	277 (98%)	7 (2%)	47	76
1	G	281/338 (83%)	277 (99%)	4 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	I	287/338 (85%)	281 (98%)	6 (2%)		53	80
1	K	291/338 (86%)	285 (98%)	6 (2%)		53	80
2	B	289/326 (89%)	276 (96%)	13 (4%)		27	55
2	D	293/326 (90%)	278 (95%)	15 (5%)		24	50
2	F	294/326 (90%)	282 (96%)	12 (4%)		30	59
2	H	288/326 (88%)	275 (96%)	13 (4%)		27	55
2	J	292/326 (90%)	278 (95%)	14 (5%)		25	53
2	L	296/326 (91%)	284 (96%)	12 (4%)		30	59
3	M	3/10 (30%)	3 (100%)	0		100	100
3	N	4/10 (40%)	3 (75%)	1 (25%)		0	1
3	O	4/10 (40%)	4 (100%)	0		100	100
3	P	4/10 (40%)	3 (75%)	1 (25%)		0	1
3	Q	4/10 (40%)	3 (75%)	1 (25%)		0	1
3	R	4/10 (40%)	3 (75%)	1 (25%)		0	1
All	All	3481/4044 (86%)	3361 (97%)	120 (3%)		37	66

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	331	LEU
2	L	255	ARG
2	H	255	ARG
2	L	236	LEU
3	Q	7	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	184	GLN
1	I	149	GLN
1	G	201	HIS
1	G	335	ASN
1	I	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	$\#|Z| > 2$
7	MES	F	380	-	12,12,12	8.99	8 (66%)	14,16,16	2.52	5 (35%)
6	MGM	F	381	-	26,28,28	0.92	1 (3%)	33,37,37	1.98	6 (18%)
6	MGM	D	380	-	26,28,28	0.85	0	33,37,37	1.89	5 (15%)
6	MGM	B	380	-	26,28,28	0.91	1 (3%)	33,37,37	1.98	6 (18%)
6	MGM	H	380	-	26,28,28	0.82	0	33,37,37	1.87	5 (15%)
6	MGM	L	380	-	26,28,28	0.93	1 (3%)	33,37,37	1.98	5 (15%)
6	MGM	J	380	-	26,28,28	0.87	1 (3%)	33,37,37	1.93	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
7	MES	F	380	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MGM	F	381	-	-	8/31/31/31	-
6	MGM	D	380	-	-	10/31/31/31	-
6	MGM	B	380	-	-	10/31/31/31	-
6	MGM	H	380	-	-	10/31/31/31	-
6	MGM	L	380	-	-	9/31/31/31	-
6	MGM	J	380	-	-	9/31/31/31	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	380	MES	C8-S	-23.21	1.44	1.77
7	F	380	MES	O2S-S	12.36	1.81	1.45
7	F	380	MES	O1S-S	12.14	1.80	1.45
7	F	380	MES	O3S-S	9.30	1.80	1.47
7	F	380	MES	C7-C8	-4.49	1.40	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	380	MGM	C1-C2-N3	7.16	130.77	113.31
6	F	381	MGM	C1-C2-N3	7.10	130.61	113.31
6	L	380	MGM	C1-C2-N3	6.86	130.03	113.31
6	J	380	MGM	C1-C2-N3	6.78	129.83	113.31
6	H	380	MGM	C1-C2-N3	6.70	129.64	113.31

There are no chirality outliers.

5 of 59 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	D	380	MGM	C1-C2-N3-C4
6	D	380	MGM	O1-C1-C2-N3

There are no ring outliers.

7 monomers are involved in 15 short contacts:

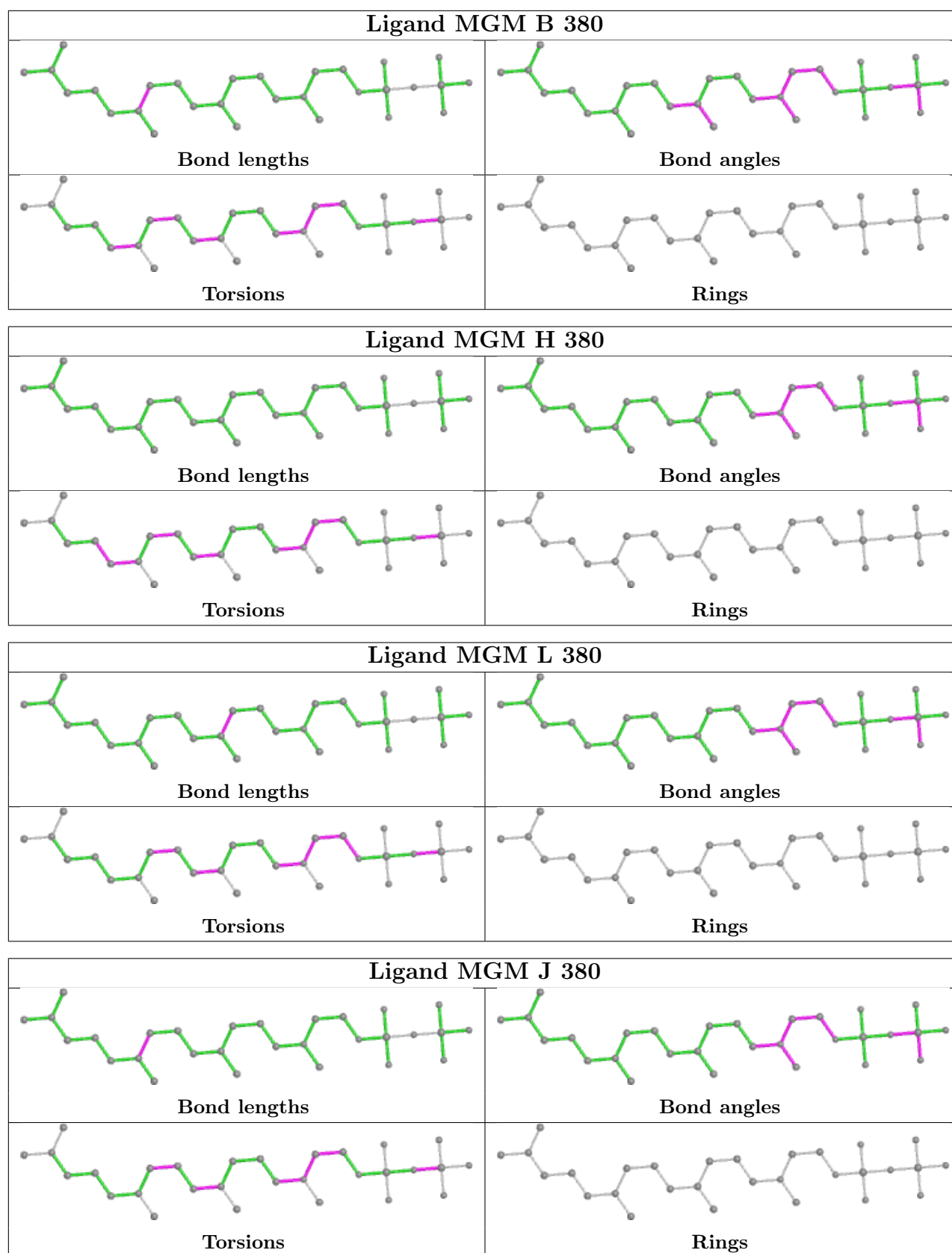| Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	380	MES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	381	MGM	1	0
6	D	380	MGM	3	0
6	B	380	MGM	2	0
6	H	380	MGM	3	0
6	L	380	MGM	2	0
6	J	380	MGM	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 MGM F 381

Bond lengths

Bond angles

Torsions

Rings

Ligand MGM D 380

Bond lengths

Bond angles

Torsions

Rings

Ligand MGM B 380

Bond lengths

Bond angles

Torsions

Rings

Ligand MGM H 380

Bond lengths

Bond angles

Torsions

Rings

Ligand MGM L 380

Bond lengths

Bond angles

Torsions

Rings

Ligand MGM J 380

Bond lengths

Bond angles

Torsions

Rings
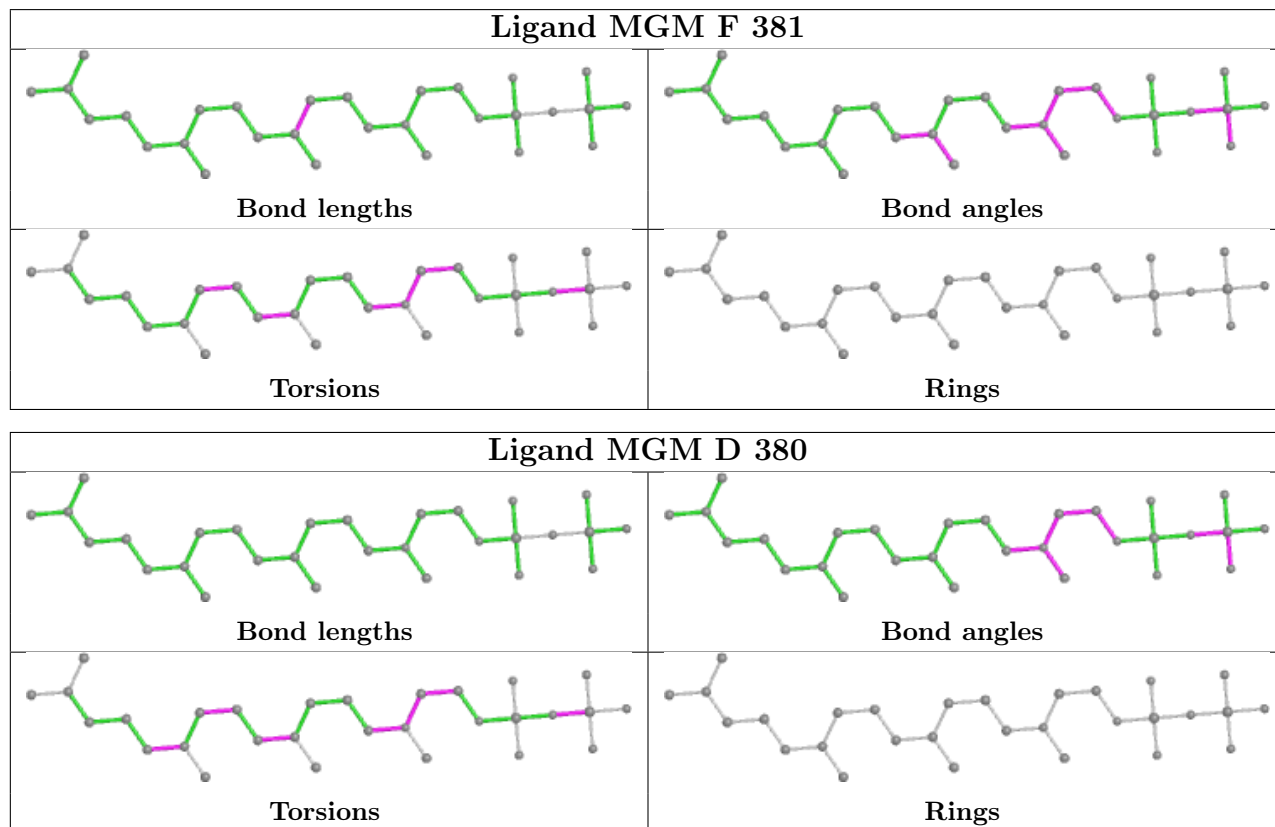
5.7 Other polymers ⓘ

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	314/377 (83%)	-0.08	11 (3%)	44	44	37, 59, 92, 108	0
1	C	314/377 (83%)	-0.18	10 (3%)	47	48	34, 56, 83, 100	0
1	E	314/377 (83%)	-0.13	8 (2%)	57	59	32, 57, 86, 102	0
1	G	314/377 (83%)	-0.18	10 (3%)	47	48	32, 54, 84, 98	0
1	I	314/377 (83%)	-0.06	10 (3%)	47	48	32, 57, 88, 98	0
1	K	314/377 (83%)	-0.36	3 (0%)	82	83	25, 44, 69, 83	0
2	B	346/377 (91%)	-0.11	7 (2%)	65	67	38, 53, 79, 102	0
2	D	346/377 (91%)	-0.12	12 (3%)	44	44	32, 48, 75, 93	0
2	F	346/377 (91%)	-0.17	10 (2%)	51	52	31, 46, 73, 97	0
2	H	346/377 (91%)	0.12	22 (6%)	19	18	33, 61, 91, 108	0
2	J	346/377 (91%)	-0.05	11 (3%)	47	48	34, 54, 82, 106	0
2	L	346/377 (91%)	-0.21	3 (0%)	84	85	28, 42, 66, 95	0
3	M	5/11 (45%)	-0.23	0	100	100	37, 40, 50, 74	0
3	N	5/11 (45%)	-0.12	0	100	100	40, 42, 53, 70	0
3	O	5/11 (45%)	0.20	0	100	100	41, 42, 55, 76	0
3	P	5/11 (45%)	0.01	1 (20%)	1	0	43, 46, 59, 77	0
3	Q	5/11 (45%)	0.17	0	100	100	36, 37, 48, 67	0
3	R	5/11 (45%)	-0.09	0	100	100	30, 31, 51, 68	0
All	All	3990/4590 (86%)	-0.12	118 (2%)	50	51	25, 52, 83, 108	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	6.9
1	C	55	PHE	5.5
1	I	329	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	40	TYR	4.2
1	A	304	PRO	4.2

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

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

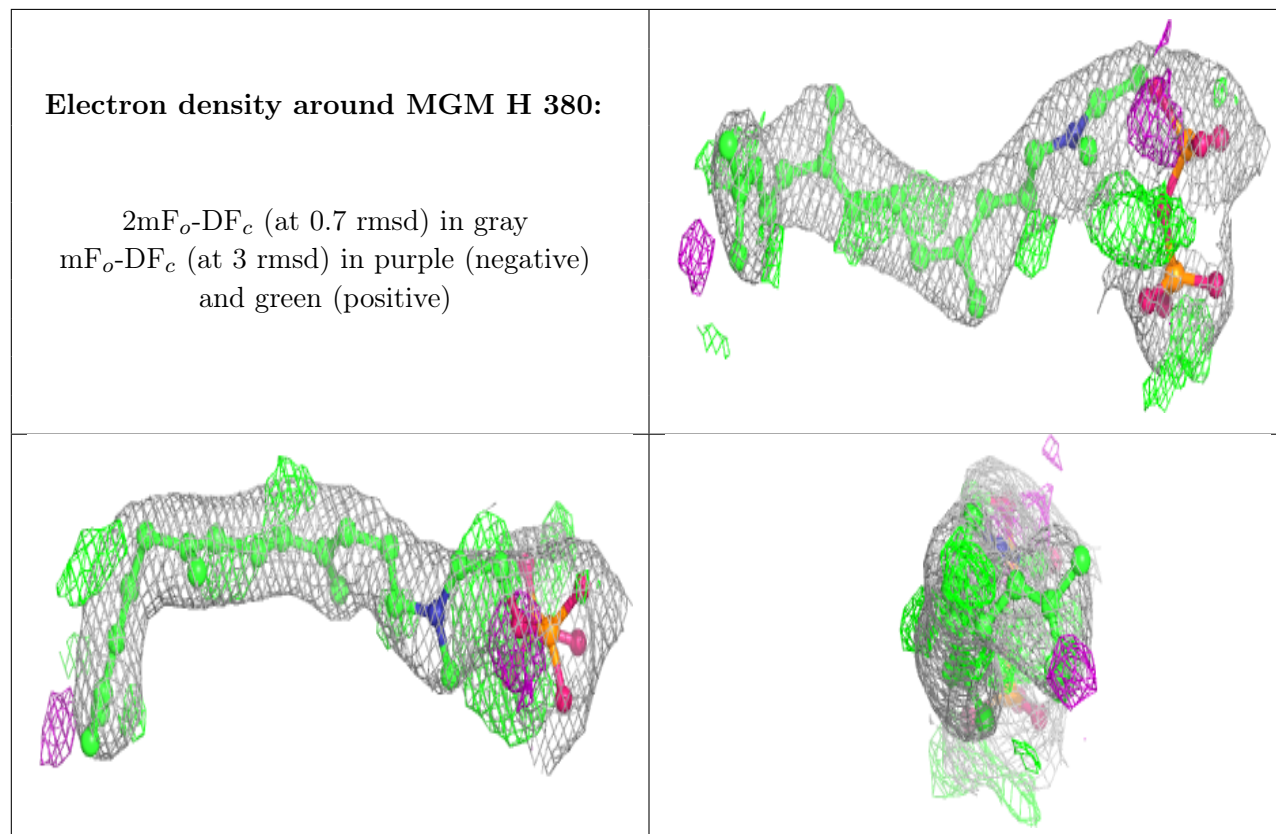## 6.3 Carbohydrates ⓘ

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MES	F	380	12/12	0.90	0.27	85,87,87,88	0
6	MGM	H	380	29/29	0.92	0.22	38,50,71,73	0
6	MGM	D	380	29/29	0.93	0.22	38,49,66,67	0
6	MGM	B	380	29/29	0.94	0.21	37,50,67,67	0
6	MGM	J	380	29/29	0.94	0.22	30,40,57,57	0
6	MGM	L	380	29/29	0.94	0.24	27,39,55,58	0
6	MGM	F	381	29/29	0.94	0.23	38,48,65,65	0
5	CL	J	379	1/1	0.96	0.05	68,68,68,68	0
5	CL	B	379	1/1	0.96	0.09	64,64,64,64	0
5	CL	H	379	1/1	0.97	0.07	54,54,54,54	0
4	ZN	H	378	1/1	0.98	0.06	51,51,51,51	0
4	ZN	L	378	1/1	0.99	0.06	38,38,38,38	0
4	ZN	F	378	1/1	0.99	0.05	44,44,44,44	0
5	CL	D	379	1/1	0.99	0.07	49,49,49,49	0
5	CL	F	379	1/1	0.99	0.04	49,49,49,49	0
4	ZN	B	378	1/1	0.99	0.05	46,46,46,46	0
4	ZN	J	378	1/1	0.99	0.06	43,43,43,43	0
5	CL	L	379	1/1	0.99	0.04	47,47,47,47	0
4	ZN	D	378	1/1	1.00	0.06	44,44,44,44	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.
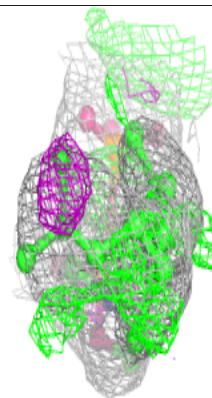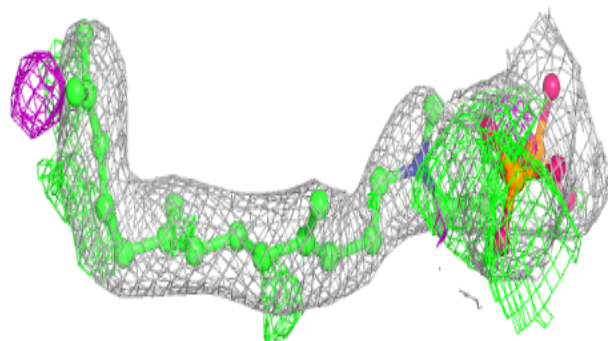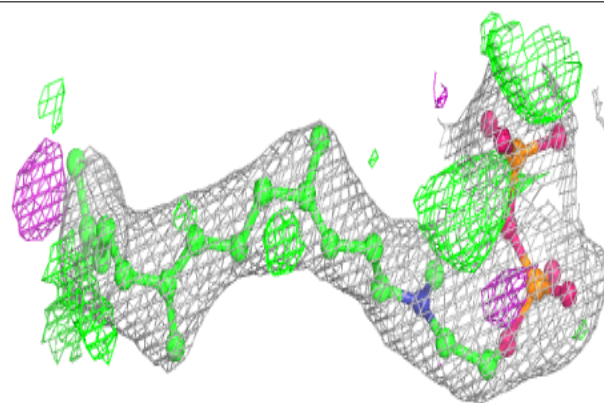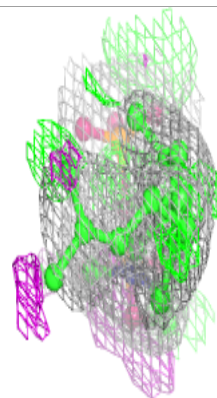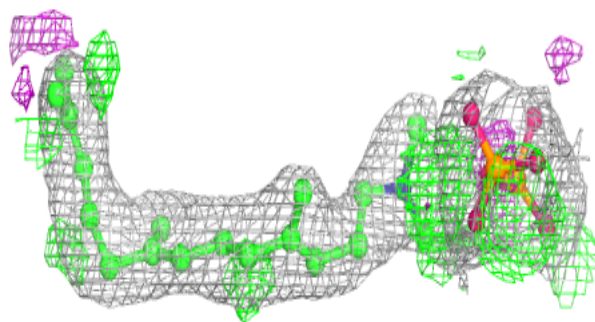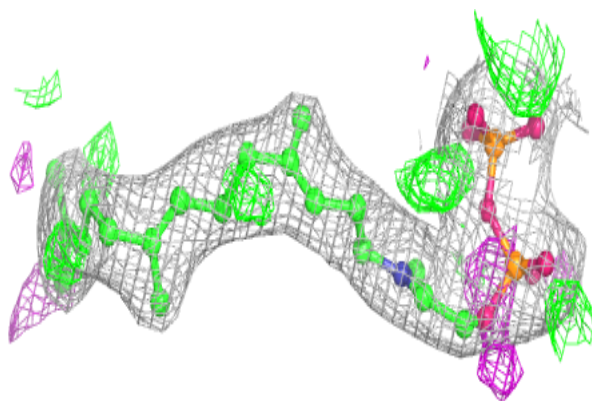
Electron density around MGM H 380:

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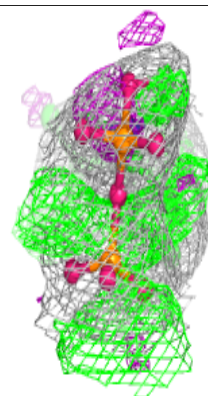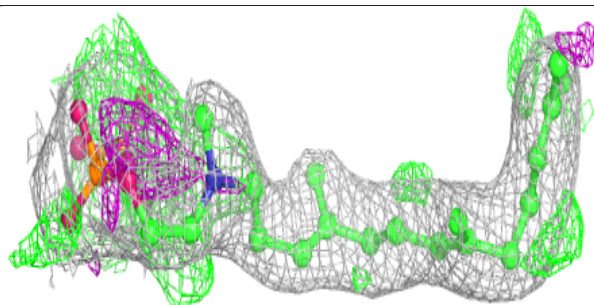mF_o-DF_c (at 3 rmsd) in purple (negative)
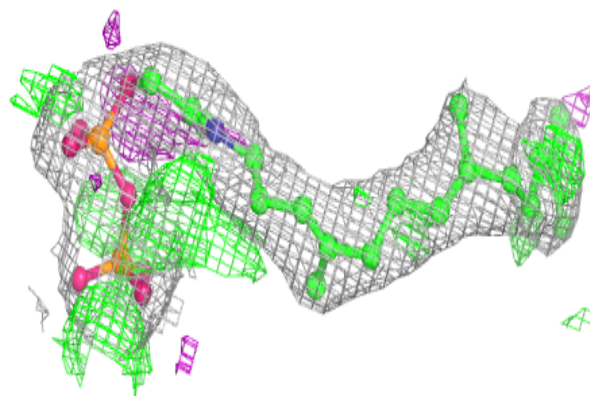and green (positive)

Electron density around MGM D 380:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
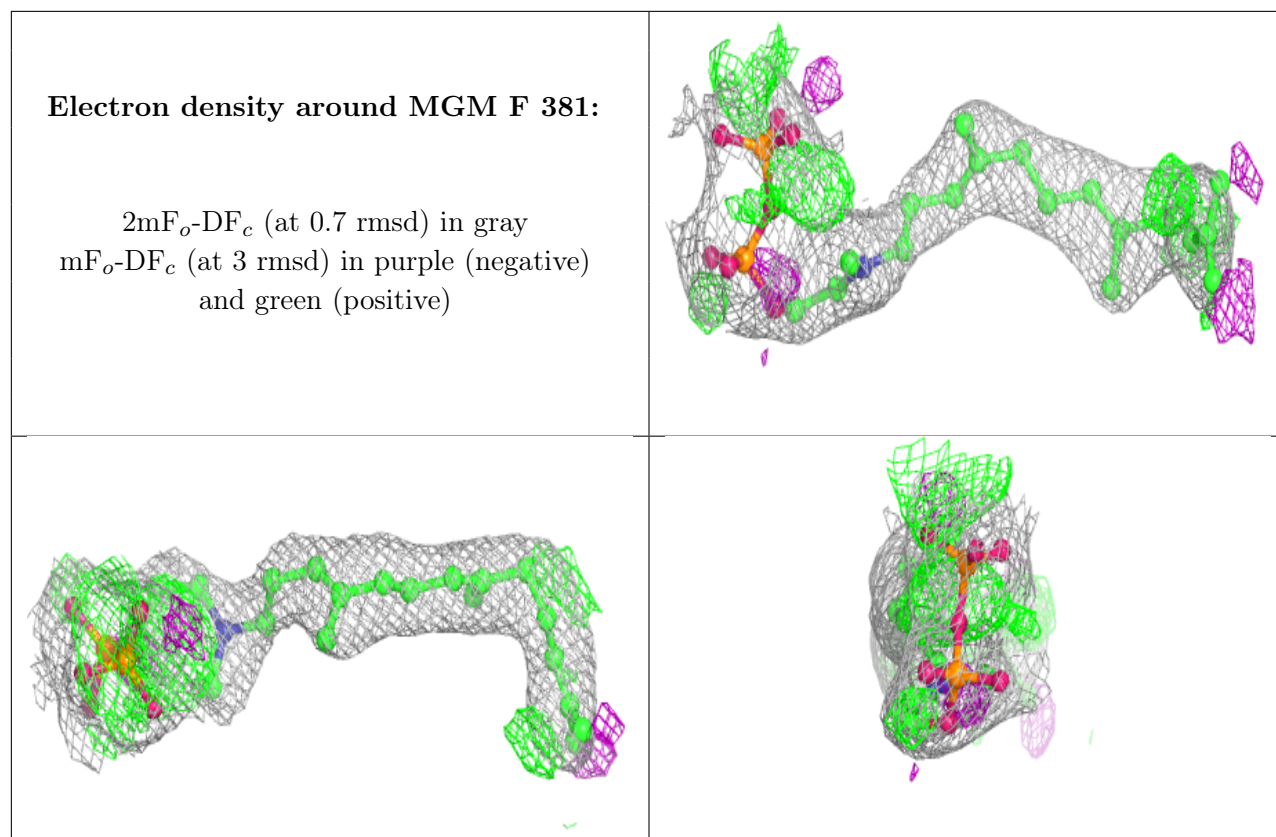mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
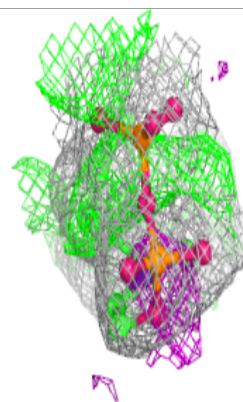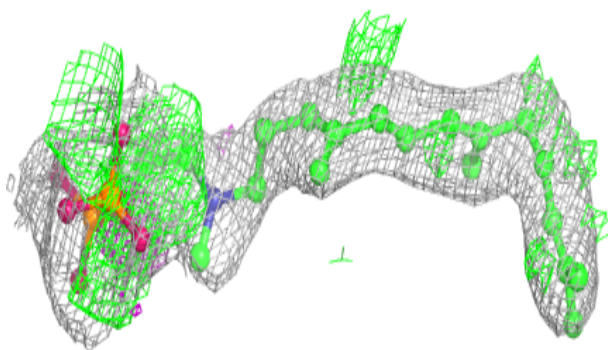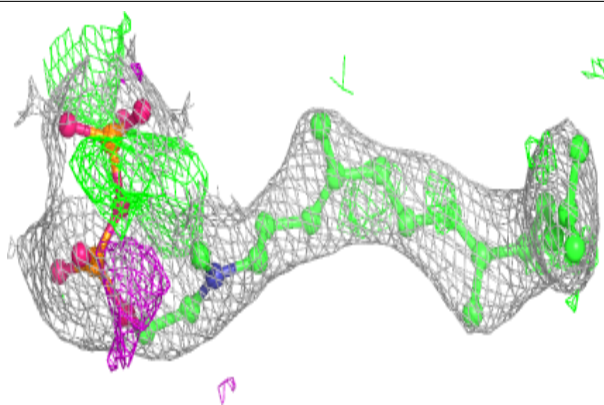
Electron density around MGM B 380:

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

Electron density around MGM J 380:

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

Electron density around MGM L 380:

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

Electron density around MGM 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.