



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2024 – 07:26 PM EDT

PDB ID : 1N4Q
Title : Protein Geranylgeranyltransferase type-I Complexed with a GGPP Analog and a KKKSCTKCVIL Peptide
Authors : Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on : 2002-11-01
Resolution : 2.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

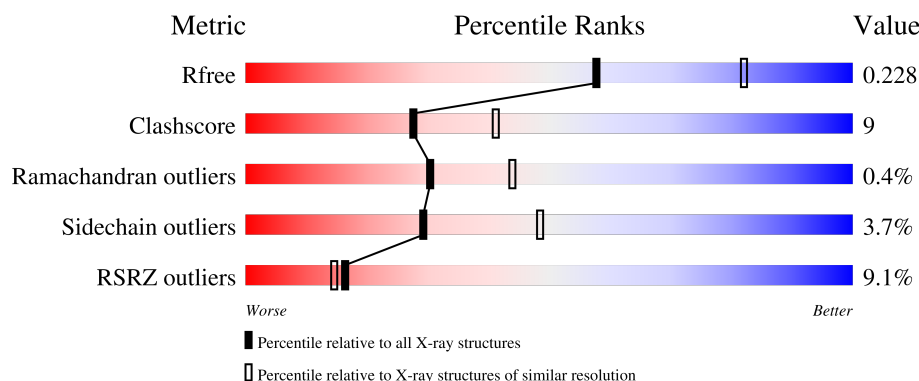
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 $\leq 5\%$. 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	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	377	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	377	<div> <div>9%</div> <div> <div></div> <div>64%</div> <div>18%</div> <div>•</div> <div>17%</div> </div> </div>
1	G	377	<div> <div>10%</div> <div> <div></div> <div>65%</div> <div>18%</div> <div>•</div> <div>17%</div> </div> </div>
1	I	377	<div> <div>9%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>

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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	
3	M	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33546 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-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2611	1672	458	476	5			
1	C	314	Total	C	N	O	S	0	0	0
			2630	1683	457	485	5			
1	E	314	Total	C	N	O	S	0	0	0
			2639	1685	461	488	5			
1	G	314	Total	C	N	O	S	0	0	0
			2621	1677	455	484	5			
1	I	314	Total	C	N	O	S	0	0	0
			2645	1690	460	490	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-1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2689	1702	467	496	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
			2700	1708	468	500	24			
2	H	346	Total	C	N	O	S	0	0	0
			2680	1698	460	498	24			
2	J	346	Total	C	N	O	S	0	0	0
			2706	1710	471	501	24			
2	L	346	Total	C	N	O	S	0	0	0
			2710	1713	471	502	24			

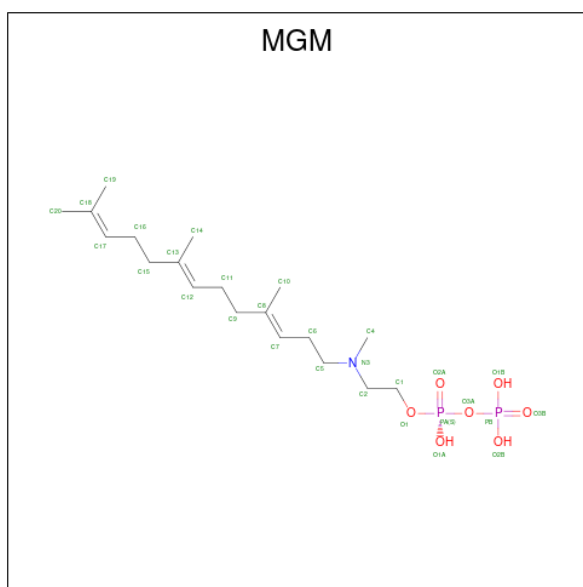
- Molecule 3 is a protein called Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	N	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	O	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	P	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	Q	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			
3	R	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			

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

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

- Molecule 5 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (three-letter code: MGM) (formula: C₁₉H₃₇NO₇P₂).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

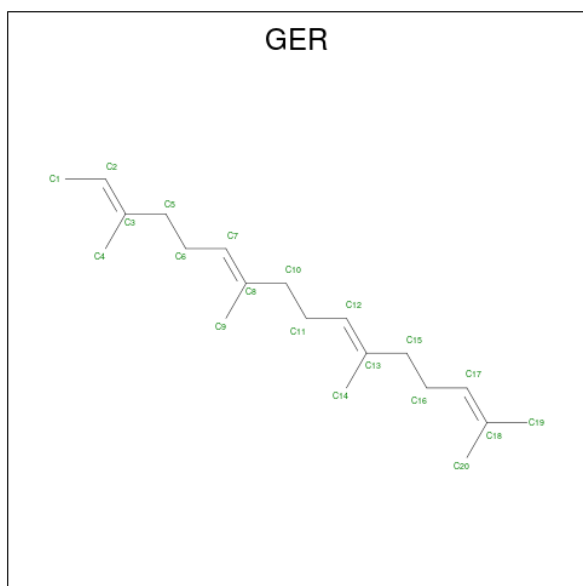
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Cl	0	0
			1	1		
6	D	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		
6	G	1	Total	Cl	0	0
			1	1		
6	H	1	Total	Cl	0	0
			1	1		
6	J	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GERAN-8-YL GERAN (three-letter code: GER) (formula: $C_{20}H_{34}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	R	1	Total	C	0	0
			20	20		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	78	Total	O	0	0
			78	78		
8	B	64	Total	O	0	0
			64	64		
8	C	82	Total	O	0	0
			82	82		
8	D	89	Total	O	0	0
			89	89		
8	E	81	Total	O	0	0
			81	81		
8	F	91	Total	O	0	0
			91	91		
8	G	75	Total	O	0	0
			75	75		

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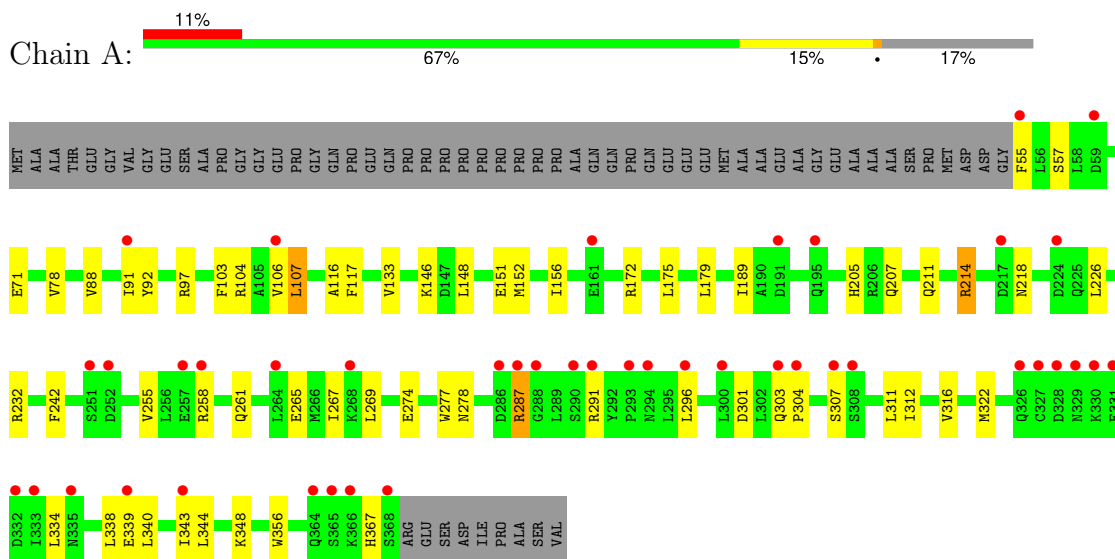
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	56	Total 56	O 56	0	0
8	I	104	Total 104	O 104	0	0
8	J	82	Total 82	O 82	0	0
8	K	169	Total 169	O 169	0	0
8	L	121	Total 121	O 121	0	0
8	M	7	Total 7	O 7	0	0
8	N	4	Total 4	O 4	0	0
8	O	4	Total 4	O 4	0	0
8	P	1	Total 1	O 1	0	0
8	Q	6	Total 6	O 6	0	0
8	R	3	Total 3	O 3	0	0

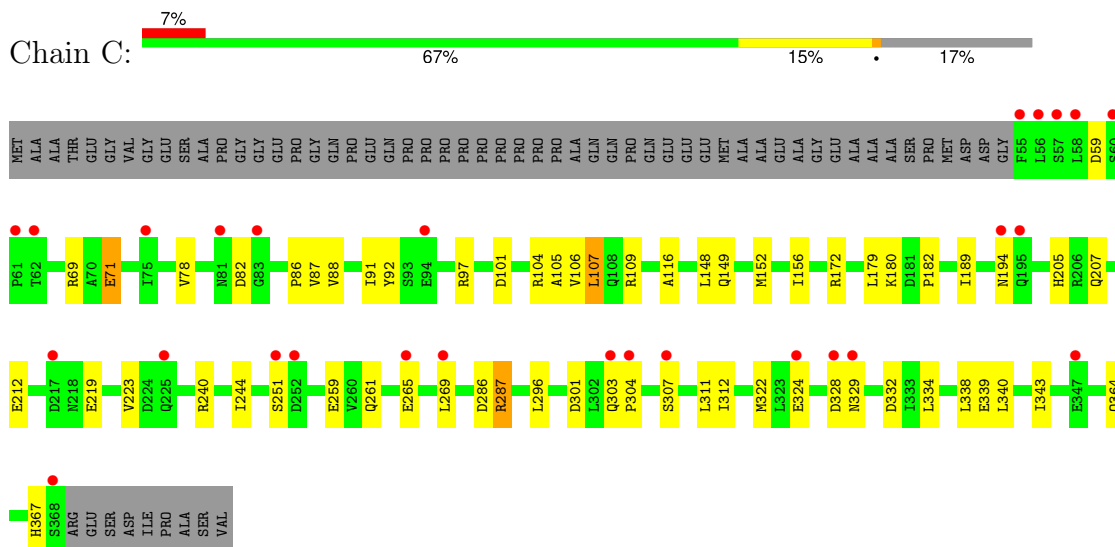
3 Residue-property plots [i](#)

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-1 subunit alpha



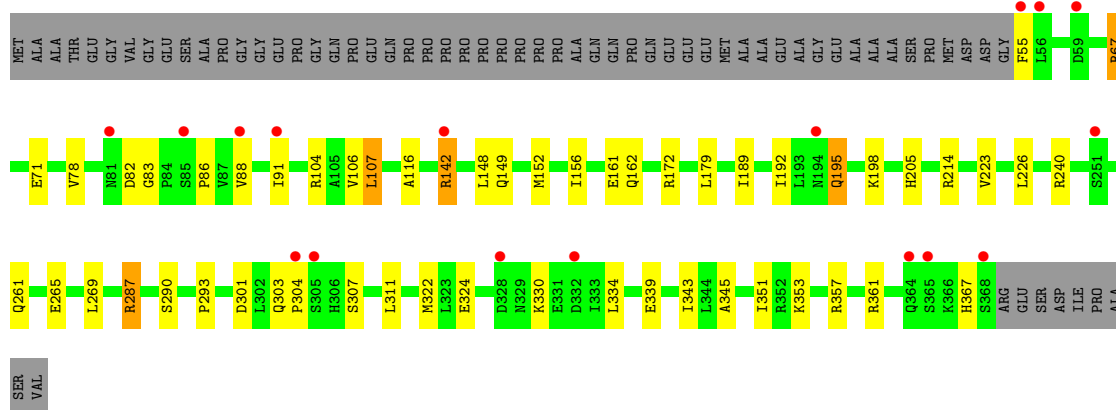
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



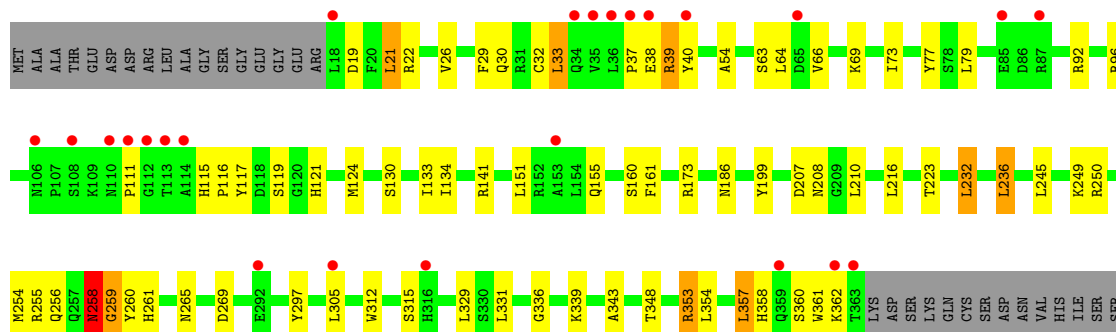
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



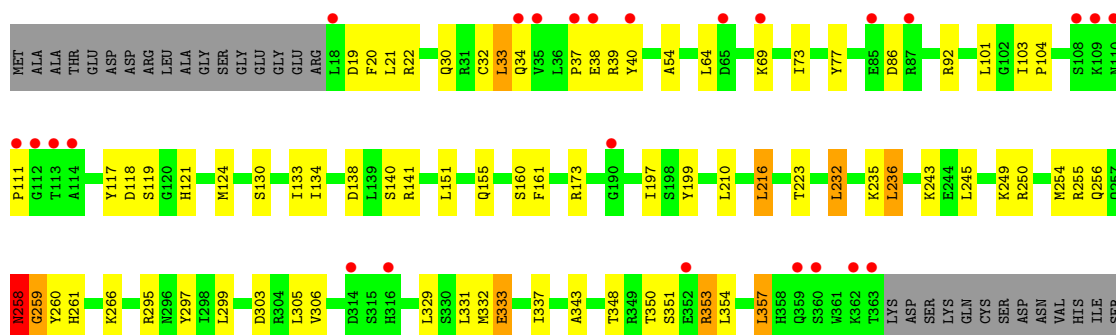
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

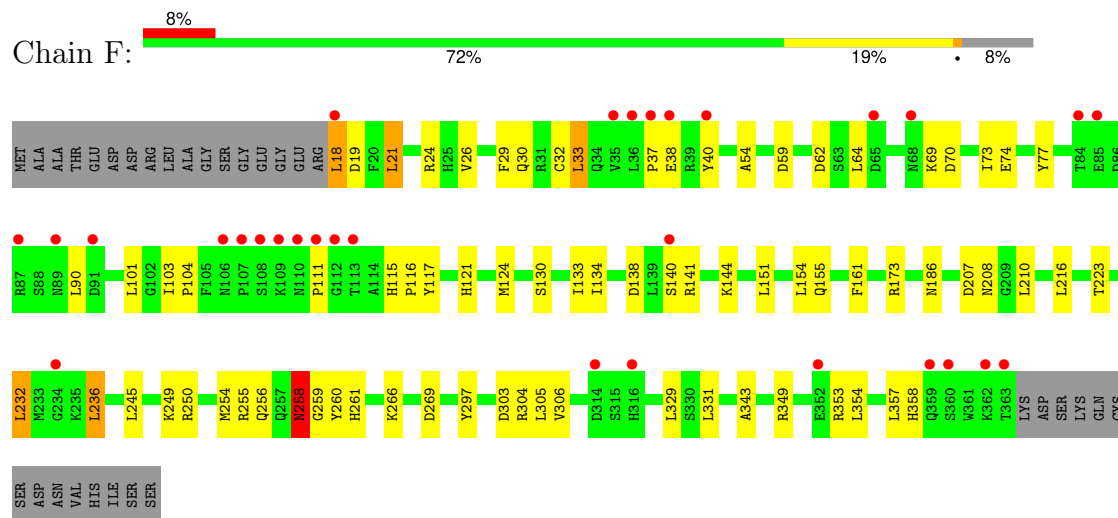


- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

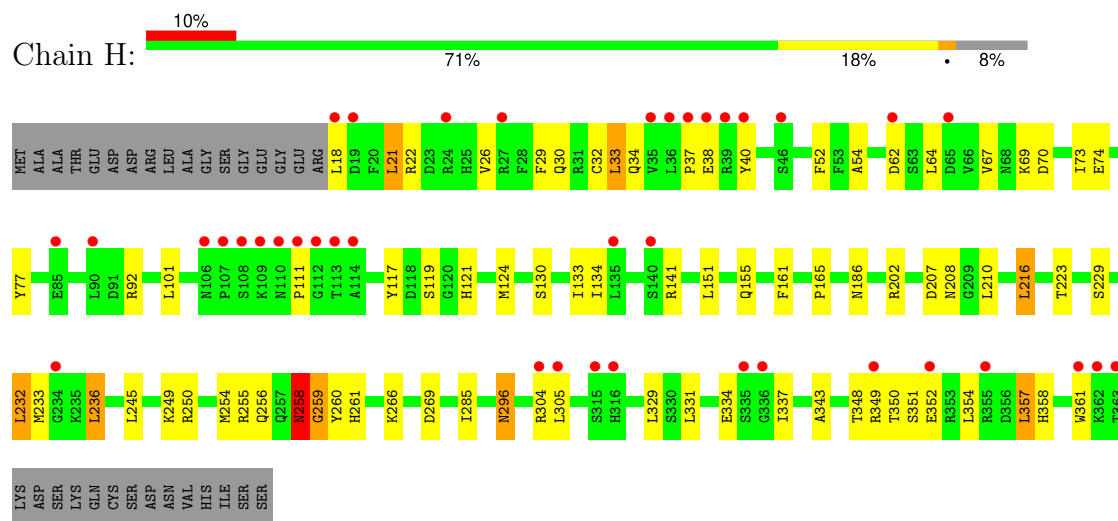


SER

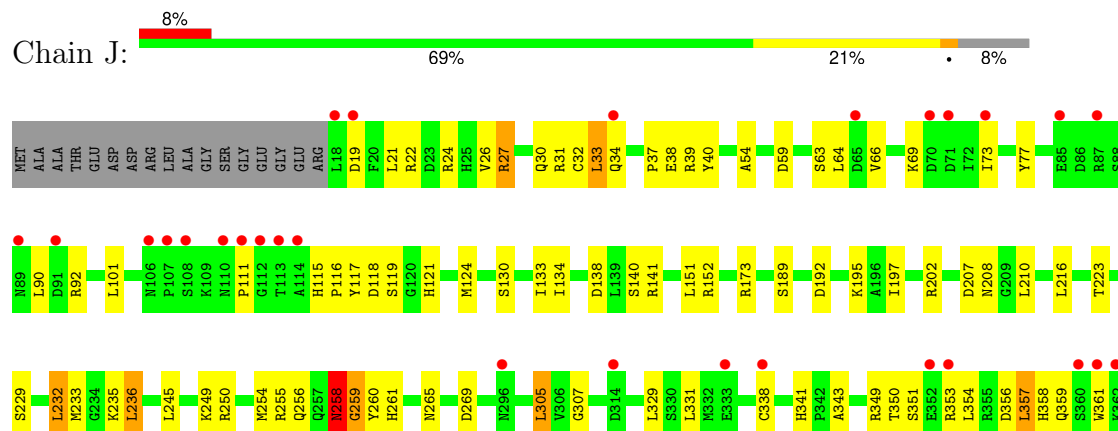
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

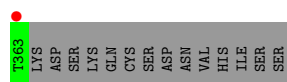


- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



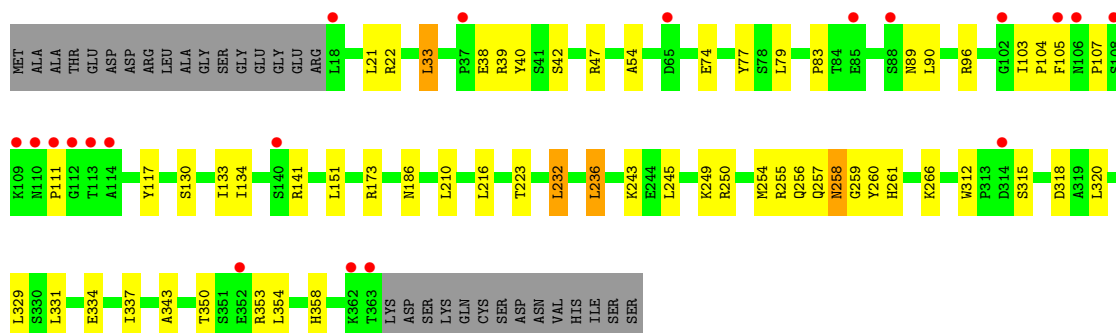
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta





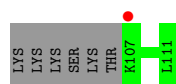
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain L: 5% 76% 15% 8%



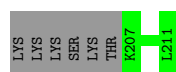
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain M: 9% 45% 55%



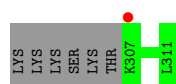
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain N: 45% 55%



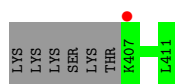
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain O: 9% 45% 55%

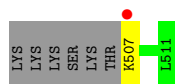
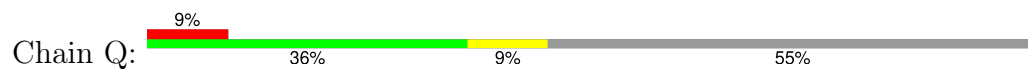


- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain P: 9% 45% 55%



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.06Å 268.03Å 184.97Å 90.00° 131.73° 90.00°	Depositor
Resolution (Å)	29.99 – 2.40 29.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.8 (29.99-2.40) 92.9 (29.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.234 0.207 , 0.228	Depositor DCC
R_{free} test set	17766 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33546	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 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.32	0/2677	0.52	0/3645
1	C	0.35	0/2696	0.53	0/3668
1	E	0.33	0/2705	0.53	0/3680
1	G	0.34	0/2687	0.52	0/3658
1	I	0.35	0/2711	0.53	0/3686
1	K	0.39	0/2733	0.55	0/3713
2	B	0.35	0/2750	0.60	2/3720 (0.1%)
2	D	0.36	0/2751	0.60	2/3720 (0.1%)
2	F	0.37	0/2761	0.60	2/3733 (0.1%)
2	H	0.35	0/2741	0.59	2/3710 (0.1%)
2	J	0.36	0/2767	0.60	2/3741 (0.1%)
2	L	0.39	0/2771	0.62	2/3745 (0.1%)
3	M	0.56	0/38	0.52	0/48
3	N	0.53	0/38	0.54	0/48
3	O	0.57	0/38	0.54	0/48
3	P	0.53	0/38	0.51	0/48
3	Q	0.55	0/38	0.52	0/48
3	R	0.67	0/38	1.08	0/48
All	All	0.36	0/32978	0.57	12/44707 (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	D	0	1
2	F	0	1
All	All	0	3

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	-6.07	97.93	113.10
2	L	259	GLY	N-CA-C	-5.91	98.32	113.10
2	H	259	GLY	N-CA-C	-5.90	98.34	113.10
2	D	259	GLY	N-CA-C	-5.87	98.43	113.10
2	F	259	GLY	N-CA-C	-5.82	98.54	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	D	297	TYR	Sidechain
2	F	297	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	2611	0	2497	46	0
1	C	2630	0	2521	41	0
1	E	2639	0	2532	56	0
1	G	2621	0	2502	58	0
1	I	2645	0	2543	40	0
1	K	2667	0	2577	45	0
2	B	2689	0	2585	50	0
2	D	2690	0	2588	50	0
2	F	2700	0	2602	48	0
2	H	2680	0	2562	60	0
2	J	2706	0	2608	54	0
2	L	2710	0	2617	38	0
3	M	39	0	47	0	0
3	N	39	0	47	0	0
3	O	39	0	47	0	0
3	P	39	0	47	0	0
3	Q	39	0	47	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	39	0	47	6	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	29	0	34	3	0
5	D	29	0	34	3	0
5	F	29	0	34	2	0
5	H	29	0	34	2	0
5	J	29	0	34	3	0
5	L	29	0	34	4	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	1	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	1	0
7	R	20	0	33	7	0
8	A	78	0	0	3	0
8	B	64	0	0	1	0
8	C	82	0	0	2	0
8	D	89	0	0	1	0
8	E	81	0	0	0	0
8	F	91	0	0	3	0
8	G	75	0	0	5	0
8	H	56	0	0	1	0
8	I	104	0	0	1	0
8	J	82	0	0	3	0
8	K	169	0	0	7	0
8	L	121	0	0	3	0
8	M	7	0	0	0	0
8	N	4	0	0	0	0
8	O	4	0	0	0	0
8	P	1	0	0	0	0
8	Q	6	0	0	1	0
8	R	3	0	0	0	0
All	All	33546	0	31253	569	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 9.

The worst 5 of 569 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	1.03	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.08	1.13
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.13	1.12
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.14	1.07
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.14	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%)	23 (7%)	0	100	100
1	C	312/377 (83%)	292 (94%)	20 (6%)	0	100	100
1	E	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	I	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
1	K	312/377 (83%)	294 (94%)	18 (6%)	0	100	100
2	B	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	14	22
2	D	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	14	22
2	F	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	22	33
2	H	344/377 (91%)	330 (96%)	12 (4%)	2 (1%)	22	33
2	J	344/377 (91%)	327 (95%)	14 (4%)	3 (1%)	14	22
2	L	344/377 (91%)	331 (96%)	11 (3%)	2 (1%)	22	33
3	M	3/11 (27%)	3 (100%)	0	0	100	100
3	N	3/11 (27%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	3 (100%)	0	0	100	100
3	R	3/11 (27%)	3 (100%)	0	0	100	100
All	All	3954/4590 (86%)	3742 (95%)	197 (5%)	15 (0%)	30	44

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
2	H	258	ASN
2	B	362	LYS
2	D	258	ASN
2	F	258	ASN

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	275/338 (81%)	269 (98%)	6 (2%)	47	67
1	C	280/338 (83%)	272 (97%)	8 (3%)	37	58
1	E	283/338 (84%)	274 (97%)	9 (3%)	34	54
1	G	278/338 (82%)	273 (98%)	5 (2%)	54	73
1	I	284/338 (84%)	278 (98%)	6 (2%)	48	69
1	K	290/338 (86%)	281 (97%)	9 (3%)	35	56
2	B	286/326 (88%)	271 (95%)	15 (5%)	19	34
2	D	286/326 (88%)	272 (95%)	14 (5%)	21	36
2	F	289/326 (89%)	274 (95%)	15 (5%)	19	34
2	H	284/326 (87%)	270 (95%)	14 (5%)	21	36
2	J	290/326 (89%)	274 (94%)	16 (6%)	18	31
2	L	291/326 (89%)	279 (96%)	12 (4%)	26	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	5/11 (46%)	5 (100%)	0	100	100
3	N	5/11 (46%)	5 (100%)	0	100	100
3	O	5/11 (46%)	5 (100%)	0	100	100
3	P	5/11 (46%)	5 (100%)	0	100	100
3	Q	5/11 (46%)	5 (100%)	0	100	100
3	R	5/11 (46%)	5 (100%)	0	100	100
All	All	3446/4050 (85%)	3317 (96%)	129 (4%)	29	48

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	324	GLU
2	L	151	LEU
1	E	107	LEU
1	E	94	GLU
2	L	232	LEU

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

Mol	Chain	Res	Type
1	G	297	ASN
1	I	285	GLN
1	G	325	ASN
1	I	89	GLN
2	J	208	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 13 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	GER	R	1300	3	19,19,19	0.97	0	21,22,22	0.62	0
5	MGM	D	1402	-	27,28,28	1.18	1 (3%)	34,37,37	1.86	6 (17%)
5	MGM	F	1403	-	27,28,28	1.04	1 (3%)	34,37,37	1.87	6 (17%)
5	MGM	H	1404	-	27,28,28	0.97	1 (3%)	34,37,37	1.83	6 (17%)
5	MGM	J	1405	-	27,28,28	0.96	1 (3%)	34,37,37	1.82	6 (17%)
5	MGM	B	1401	-	27,28,28	0.97	1 (3%)	34,37,37	1.85	6 (17%)
5	MGM	L	1406	-	27,28,28	1.02	2 (7%)	34,37,37	1.76	7 (20%)

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	GER	R	1300	3	-	9/20/20/20	-
5	MGM	D	1402	-	-	9/31/31/31	-
5	MGM	F	1403	-	-	9/31/31/31	-
5	MGM	H	1404	-	-	9/31/31/31	-
5	MGM	J	1405	-	-	9/31/31/31	-
5	MGM	B	1401	-	-	9/31/31/31	-
5	MGM	L	1406	-	-	9/31/31/31	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1402	MGM	PA-O3A	4.07	1.63	1.59
5	L	1406	MGM	PA-O3A	3.13	1.62	1.59
5	F	1403	MGM	PA-O3A	3.12	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1404	MGM	PA-O3A	2.72	1.62	1.59
5	J	1405	MGM	PA-O3A	2.52	1.62	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1403	MGM	C1-C2-N3	6.83	129.69	113.30
5	B	1401	MGM	C1-C2-N3	6.77	129.54	113.30
5	D	1402	MGM	C1-C2-N3	6.69	129.35	113.30
5	H	1404	MGM	C1-C2-N3	6.65	129.27	113.30
5	J	1405	MGM	C1-C2-N3	6.51	128.94	113.30

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1401	MGM	C1-C2-N3-C4
5	B	1401	MGM	O1-C1-C2-N3
5	B	1401	MGM	PA-O3A-PB-O1B
5	D	1402	MGM	C1-C2-N3-C4
5	D	1402	MGM	O1-C1-C2-N3

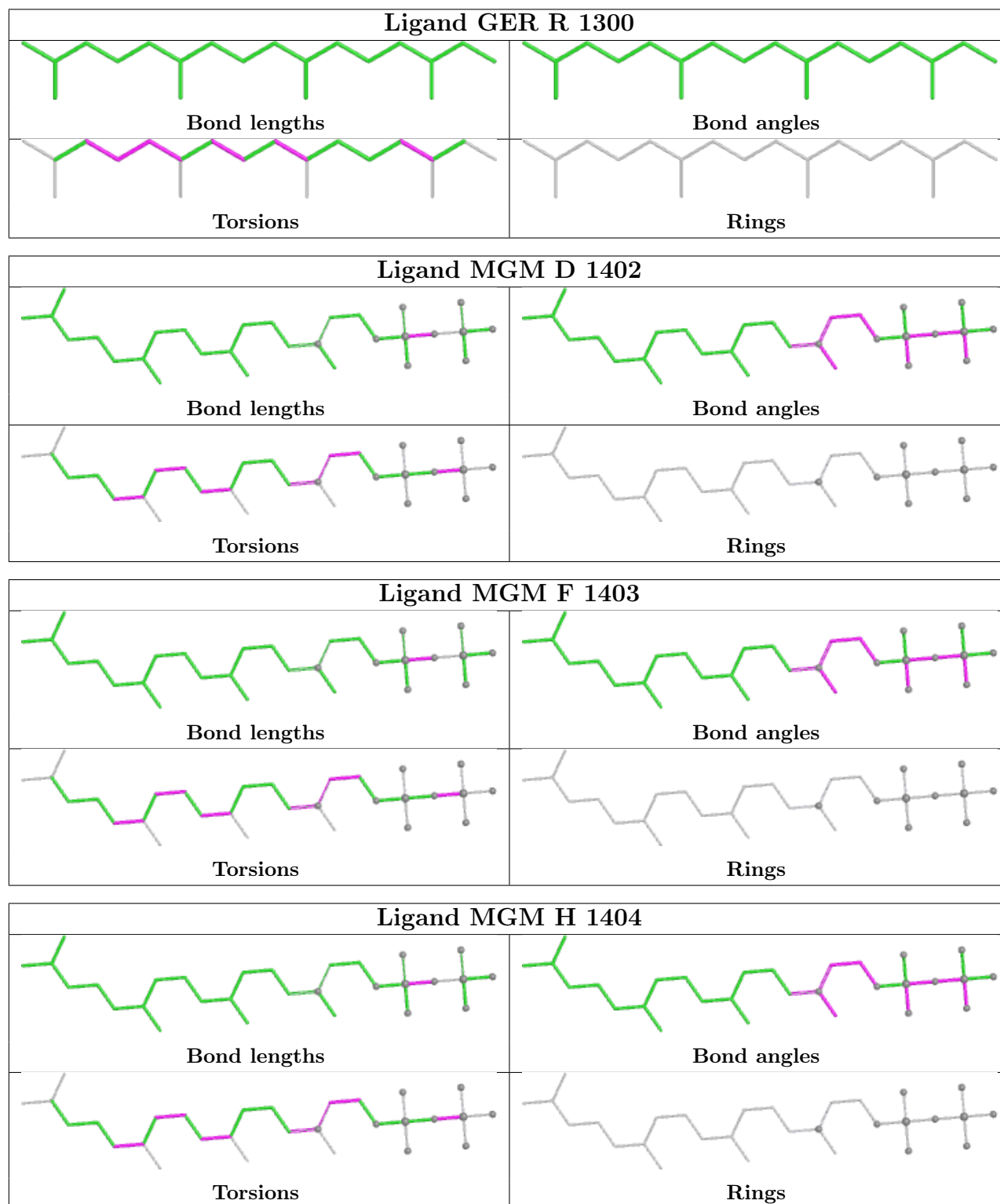
There are no ring outliers.

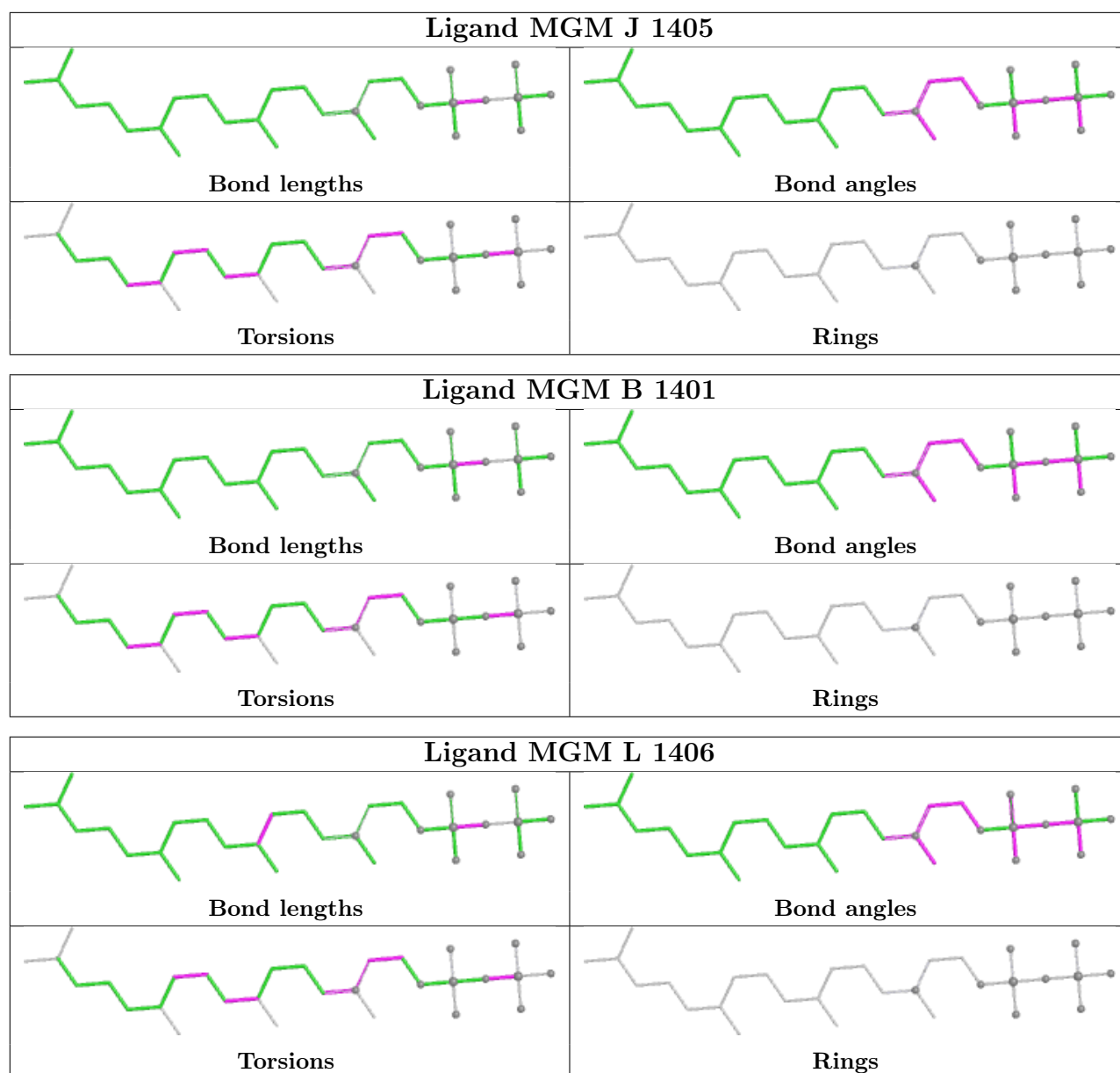
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1300	GER	7	0
5	D	1402	MGM	3	0
5	F	1403	MGM	2	0
5	H	1404	MGM	2	0
5	J	1405	MGM	3	0
5	B	1401	MGM	3	0
5	L	1406	MGM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

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%)	0.76	43 (13%) 8 7	42, 63, 91, 106	0
1	C	314/377 (83%)	0.65	27 (8%) 18 16	41, 59, 87, 138	0
1	E	314/377 (83%)	0.76	35 (11%) 12 10	40, 63, 86, 105	0
1	G	314/377 (83%)	0.80	36 (11%) 11 9	42, 62, 89, 140	0
1	I	314/377 (83%)	0.68	33 (10%) 13 11	35, 60, 88, 100	0
1	K	314/377 (83%)	0.09	17 (5%) 32 30	30, 48, 71, 87	0
2	B	346/377 (91%)	0.40	24 (6%) 24 22	41, 57, 81, 103	0
2	D	346/377 (91%)	0.20	25 (7%) 23 21	37, 51, 84, 101	0
2	F	346/377 (91%)	0.22	30 (8%) 17 16	36, 51, 83, 105	0
2	H	346/377 (91%)	0.82	39 (11%) 11 10	43, 64, 90, 112	0
2	J	346/377 (91%)	0.36	29 (8%) 18 17	36, 55, 83, 103	0
2	L	346/377 (91%)	-0.04	20 (5%) 30 27	32, 46, 72, 95	0
3	M	5/11 (45%)	0.80	1 (20%) 3 3	52, 53, 60, 71	0
3	N	5/11 (45%)	0.25	0 100 100	51, 55, 60, 73	0
3	O	5/11 (45%)	0.52	1 (20%) 3 3	53, 56, 60, 74	0
3	P	5/11 (45%)	1.11	1 (20%) 3 3	62, 62, 73, 83	0
3	Q	5/11 (45%)	1.00	1 (20%) 3 3	51, 51, 67, 78	0
3	R	5/11 (45%)	1.98	3 (60%) 0 0	50, 52, 78, 79	0
All	All	3990/4590 (86%)	0.47	365 (9%) 16 14	30, 57, 86, 140	0

The worst 5 of 365 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	PHE	8.0
1	G	55	PHE	7.8
2	B	110	ASN	6.9

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Mol	Chain	Res	Type	RSRZ
2	H	18	LEU	6.4
2	H	362	LYS	6.3

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

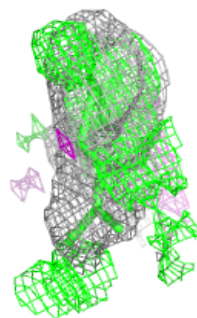
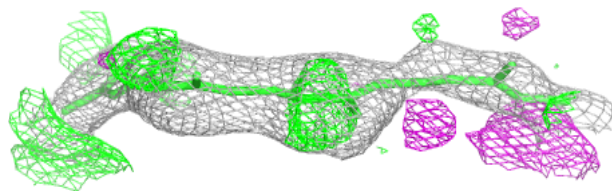
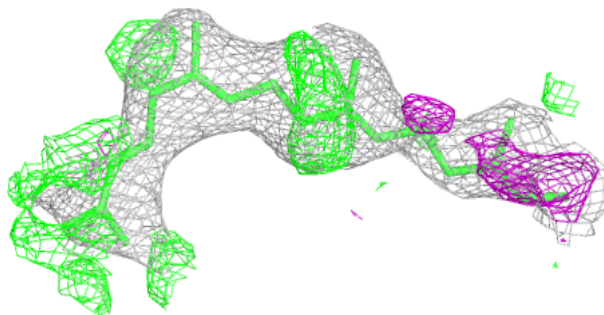
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GER	R	1300	20/20	0.84	0.26	66,71,80,81	0
5	MGM	L	1406	29/29	0.86	0.19	39,54,79,80	0
5	MGM	J	1405	29/29	0.88	0.17	41,58,81,82	0
5	MGM	F	1403	29/29	0.89	0.16	46,58,81,83	0
5	MGM	H	1404	29/29	0.90	0.17	59,69,91,94	0
5	MGM	D	1402	29/29	0.90	0.17	43,59,80,80	0
5	MGM	B	1401	29/29	0.91	0.15	46,66,88,88	0
6	CL	J	1315	1/1	0.92	0.12	60,60,60,60	0
6	CL	C	1301	1/1	0.95	0.26	65,65,65,65	0
6	CL	K	1317	1/1	0.97	0.16	61,61,61,61	0
6	CL	F	1309	1/1	0.98	0.07	51,51,51,51	0
6	CL	G	1311	1/1	0.98	0.21	59,59,59,59	0
6	CL	H	1312	1/1	0.98	0.05	59,59,59,59	0
4	ZN	H	378	1/1	0.99	0.03	60,60,60,60	0
6	CL	D	1306	1/1	0.99	0.04	45,45,45,45	0
4	ZN	L	378	1/1	1.00	0.02	36,36,36,36	0
4	ZN	D	378	1/1	1.00	0.02	39,39,39,39	0
4	ZN	F	378	1/1	1.00	0.01	45,45,45,45	0
4	ZN	B	378	1/1	1.00	0.02	47,47,47,47	0
4	ZN	J	378	1/1	1.00	0.03	42,42,42,42	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.

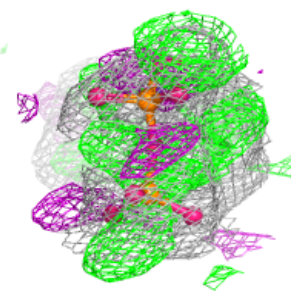
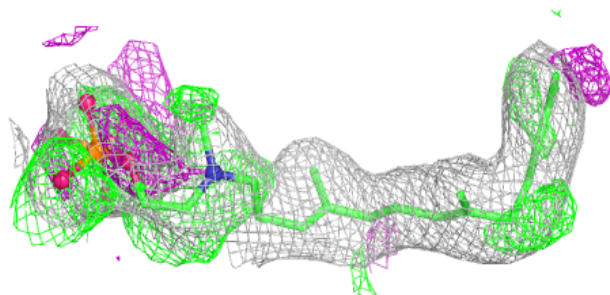
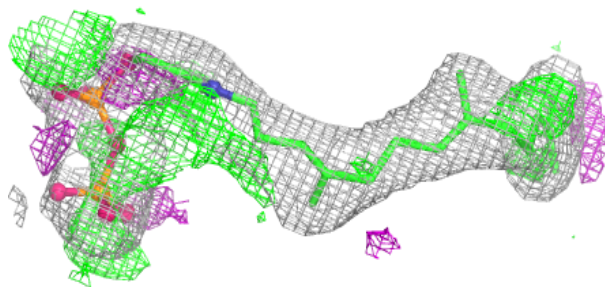
Electron density around GER R 1300:

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

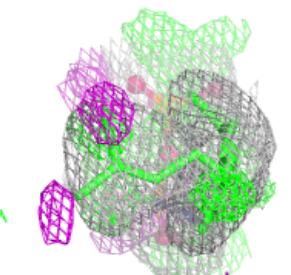
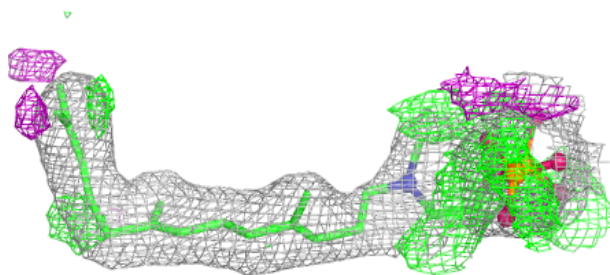
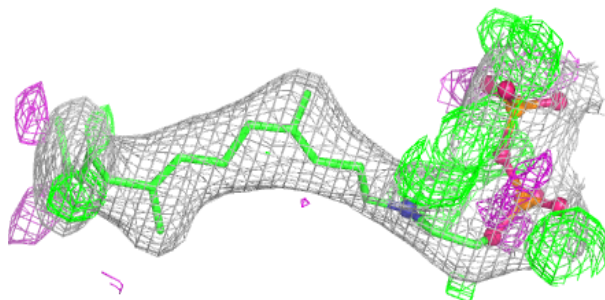


Electron density around MGM L 1406:

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

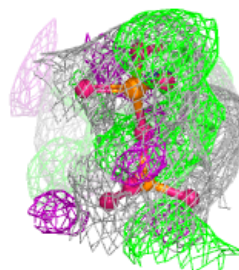
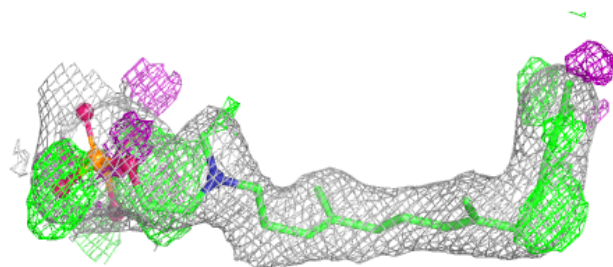
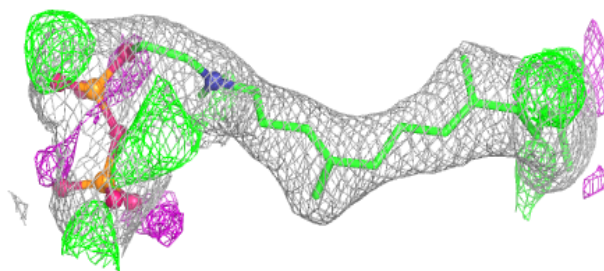
**Electron density around MGM J 1405:**

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and green (positive)

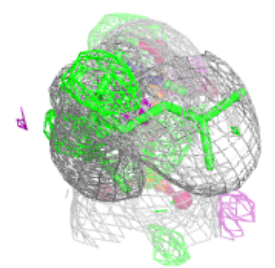
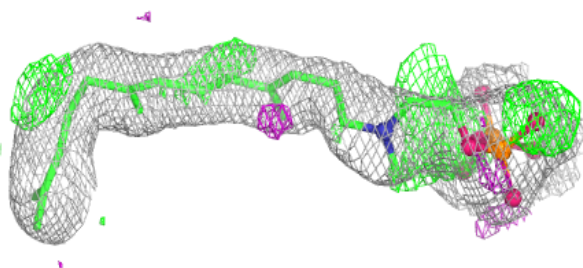
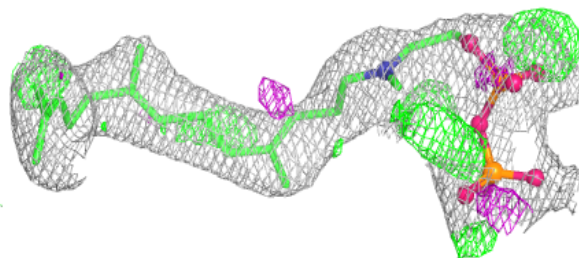


Electron density around MGM F 1403:

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

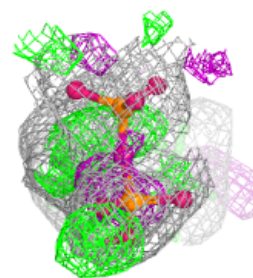
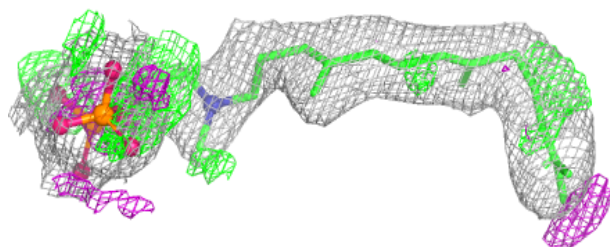
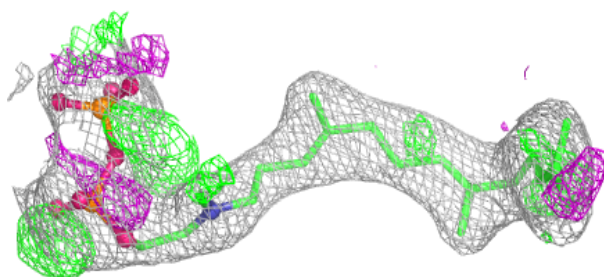
**Electron density around MGM H 1404:**

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and green (positive)

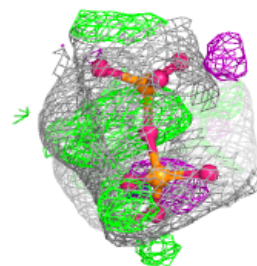
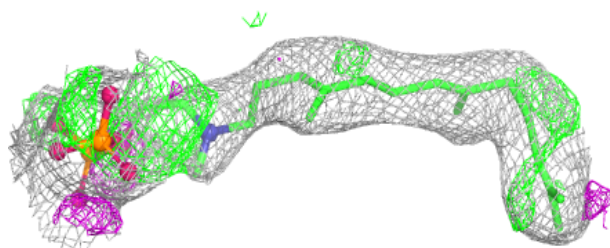
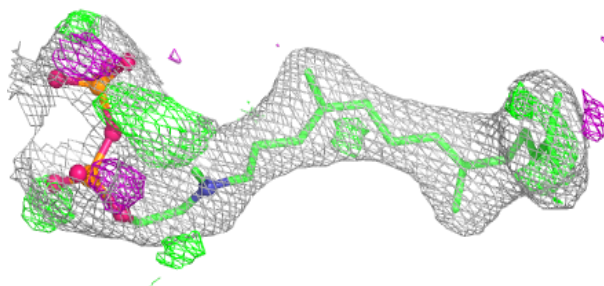


Electron density around MGM D 1402:

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

**Electron density around MGM B 1401:**

$2mF_o-DF_c$ (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.