wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2024 – 09:22 PM EDT

PDB ID	:	1N4R
Title	:	Protein Geranylgeranyltransferase type-I Complexed with a Geranylgeranylated KKKSKTKCVIL Peptide Product
Authors	:	Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on	:	2002-11-01
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

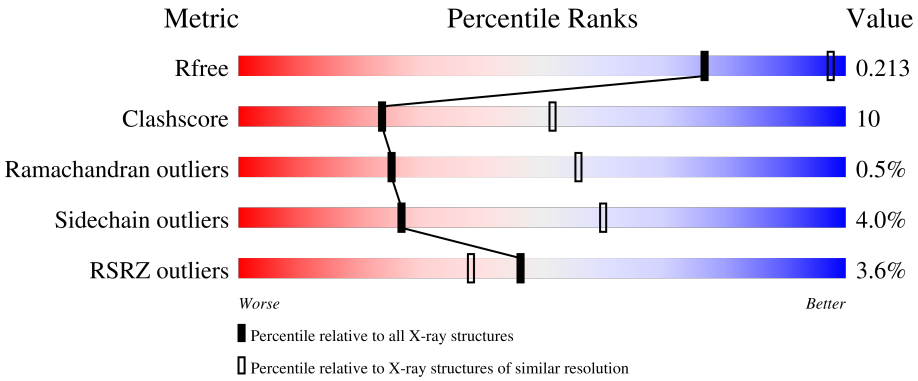
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	2% 64% 19% • 17%
1	C	377	2% 65% 17% • 17%
1	E	377	2% 62% 20% • 17%
1	G	377	5% 65% 17% • 17%
1	I	377	2% 62% 20% • 17%

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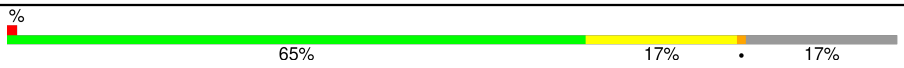
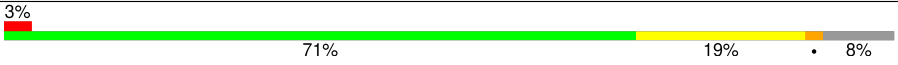
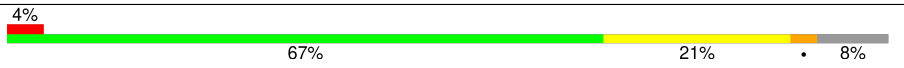
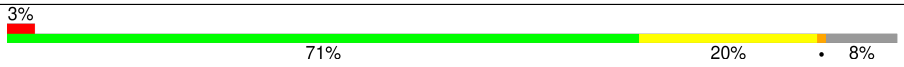
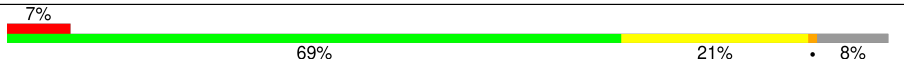
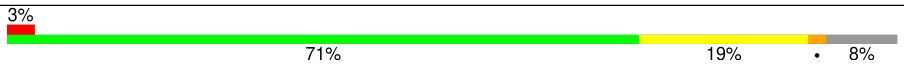
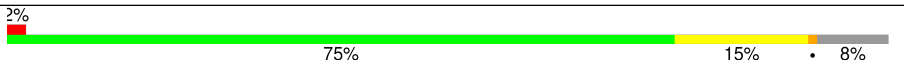
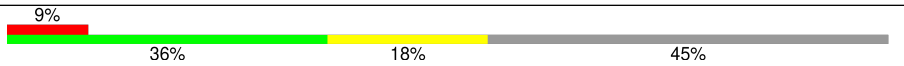
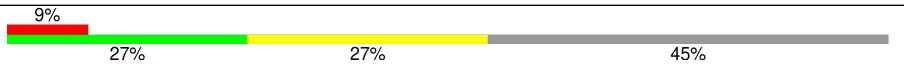
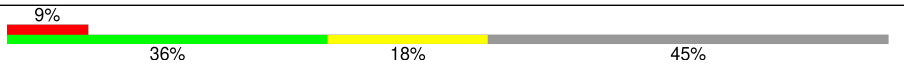
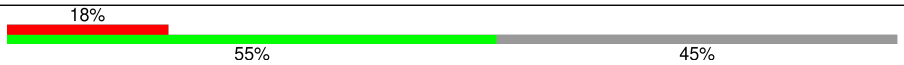
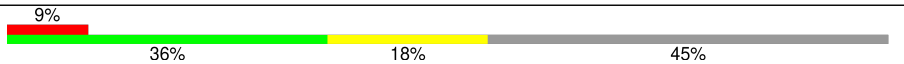
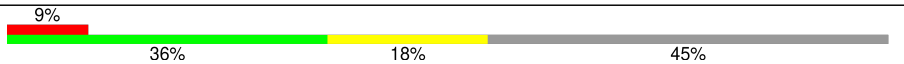
Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MES	I	905	-	X	-	-
7	CL	G	804	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 33129 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
			2614	1673	458	478	5			
1	C	314	Total	C	N	O	S	0	0	0
			2648	1691	462	490	5			
1	E	314	Total	C	N	O	S	0	0	0
			2630	1682	460	483	5			
1	G	314	Total	C	N	O	S	0	0	0
			2632	1683	459	485	5			
1	I	314	Total	C	N	O	S	0	0	0
			2654	1693	461	495	5			
1	K	314	Total	C	N	O	S	0	0	0
			2667	1700	466	496	5			

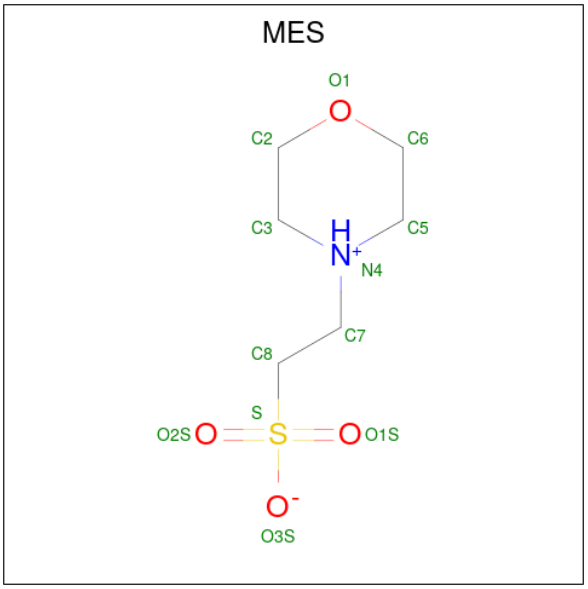
- Molecule 2 is a protein called Geranylgeranyl transferase type-1 subunit beta.

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
			2693	1704	467	498	24			
2	F	346	Total	C	N	O	S	0	0	0
			2708	1711	471	502	24			
2	H	346	Total	C	N	O	S	0	0	0
			2670	1692	458	496	24			
2	J	346	Total	C	N	O	S	0	0	0
			2709	1711	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2714	1715	471	504	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	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	N	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	O	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	P	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	Q	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			
3	R	6	Total	C	N	O	S	0	0	0
			46	30	7	8	1			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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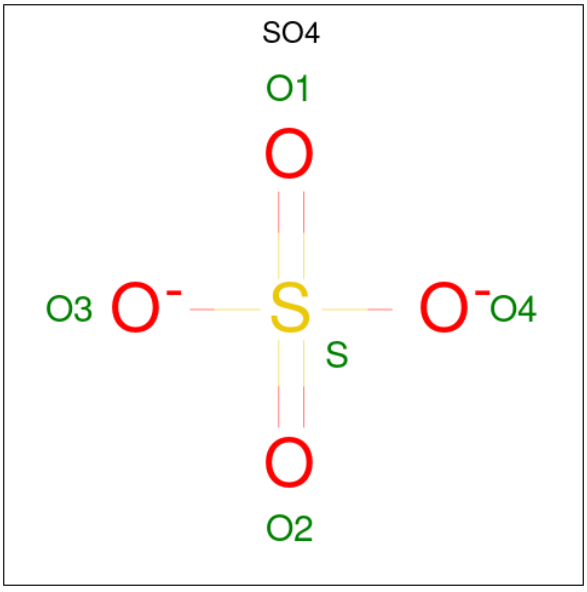
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

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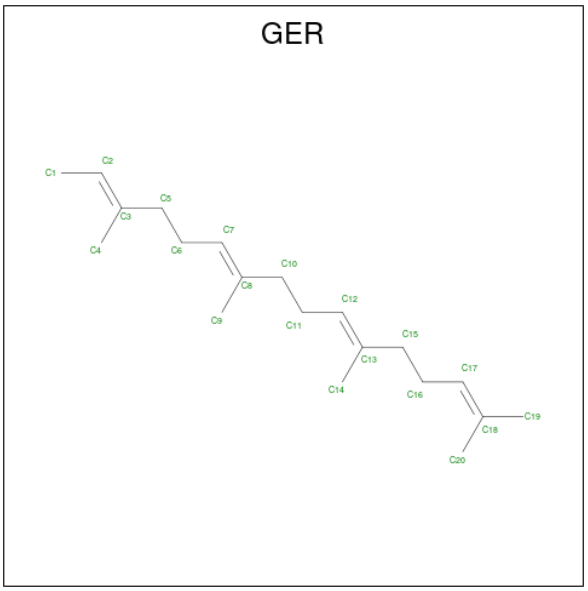
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	J	1	Total O S 5 4 1	0	0
6	L	1	Total O S 5 4 1	0	0

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

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C 20 20	0	0
8	N	1	Total C 20 20	0	0
8	O	1	Total C 20 20	0	0
8	P	1	Total C 20 20	0	0
8	Q	1	Total C 20 20	0	0
8	R	1	Total C 20 20	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	45	Total O 45 45	0	0
9	B	35	Total O 35 35	0	0
9	C	49	Total O 49 49	0	0
9	D	45	Total O 45 45	0	0
9	E	40	Total O 40 40	0	0
9	F	51	Total O 51 51	0	0

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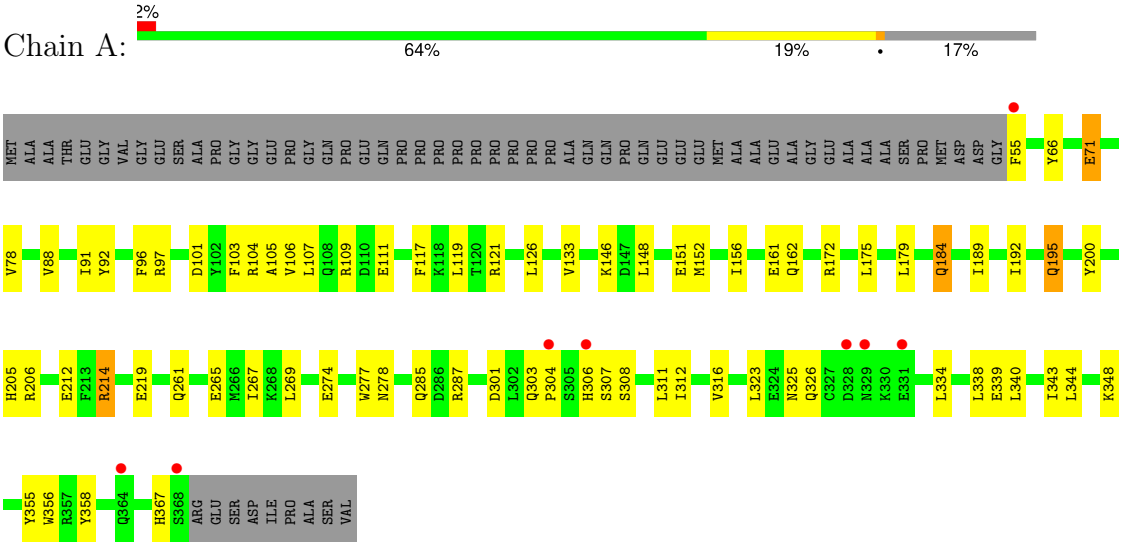
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	40	Total O 40 40	0	0
9	H	23	Total O 23 23	0	0
9	I	52	Total O 52 52	0	0
9	J	36	Total O 36 36	0	0
9	K	101	Total O 101 101	0	0
9	L	60	Total O 60 60	0	0
9	M	1	Total O 1 1	0	0
9	N	3	Total O 3 3	0	0
9	O	1	Total O 1 1	0	0
9	Q	3	Total O 3 3	0	0
9	R	5	Total O 5 5	0	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.

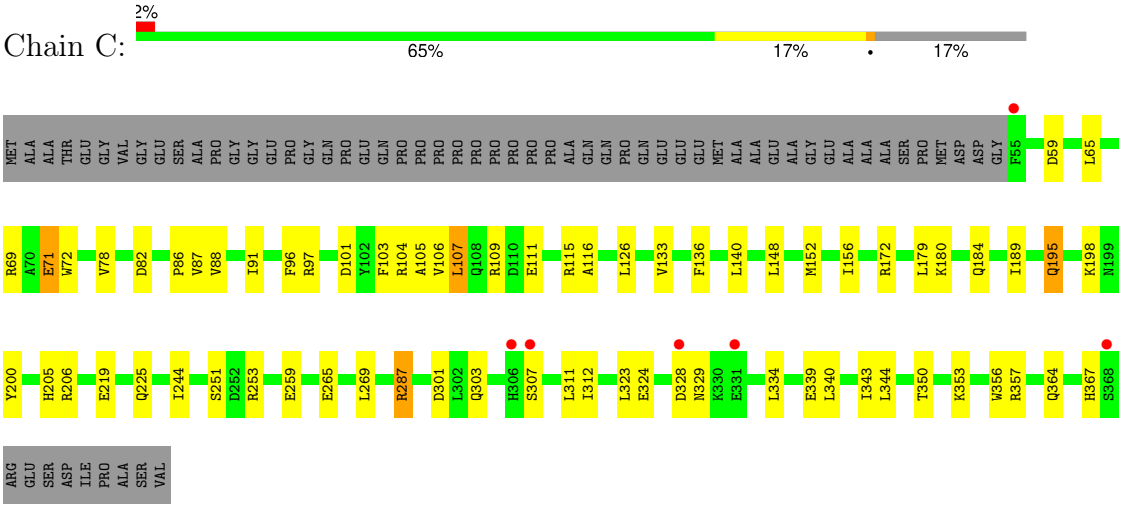
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain A:



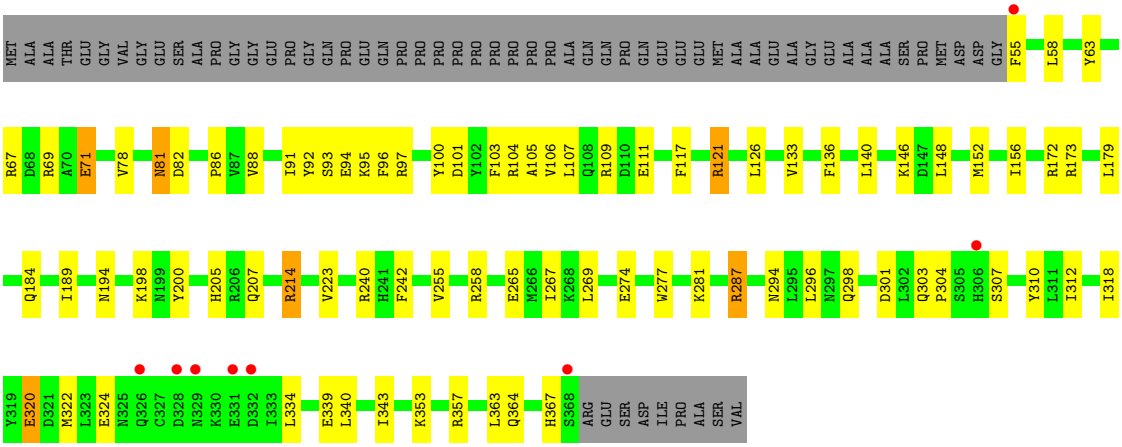
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain C:



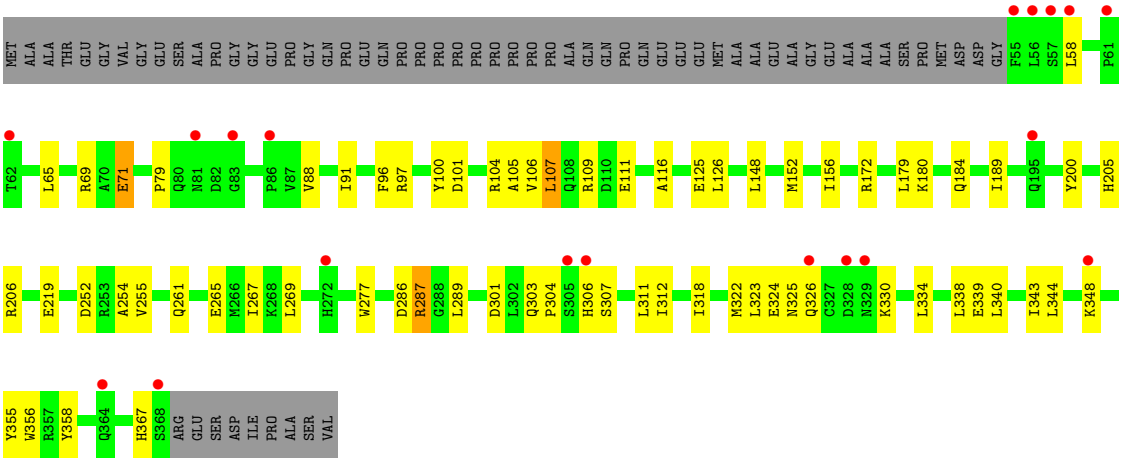
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain E:



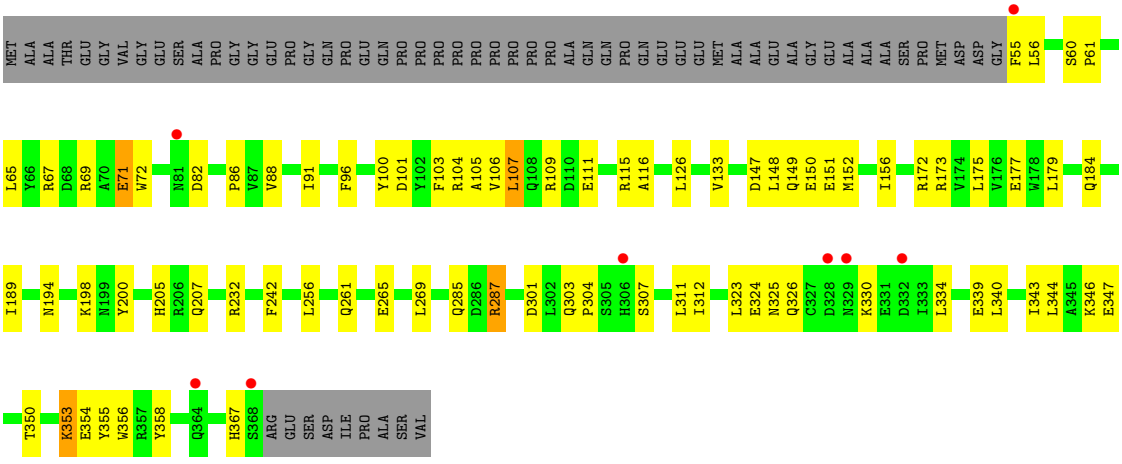
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain G:



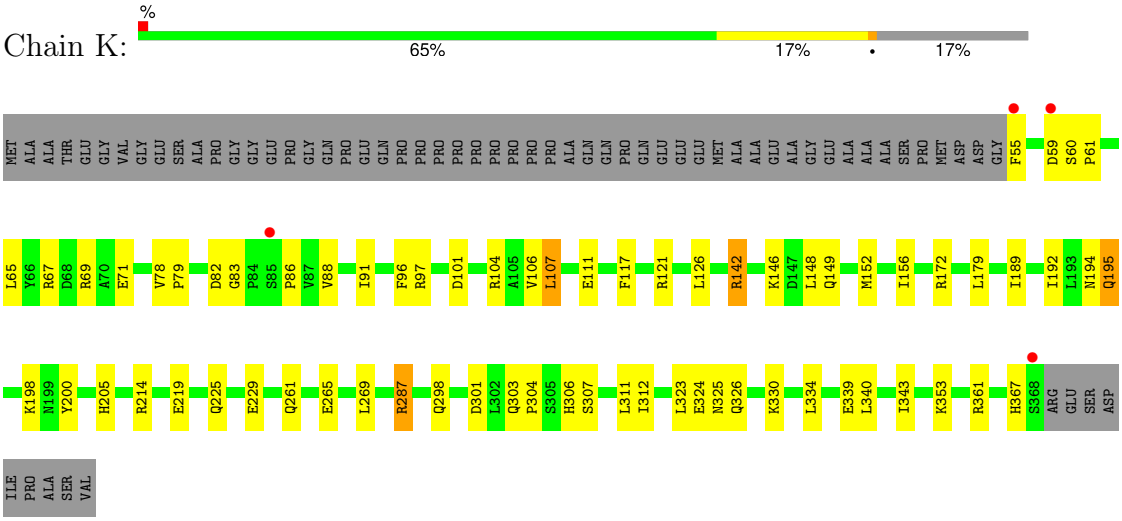
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain I:



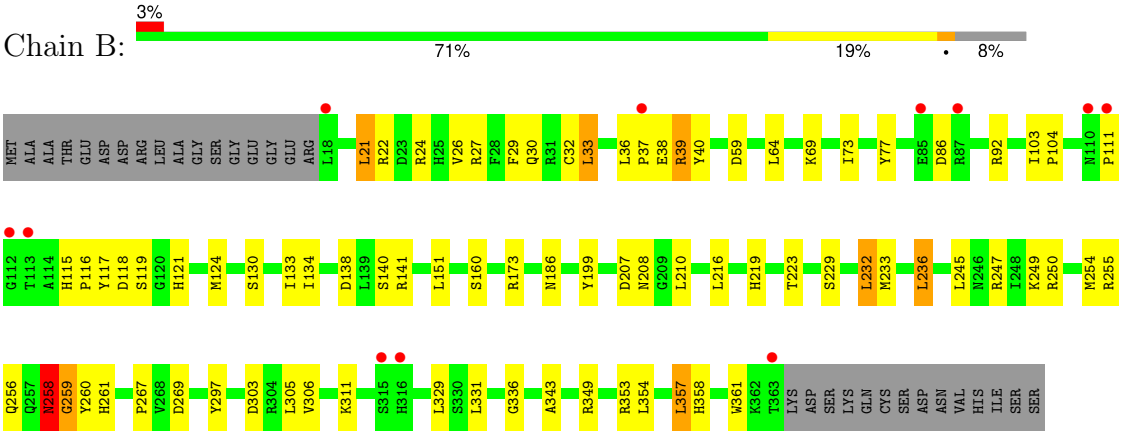
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain K:



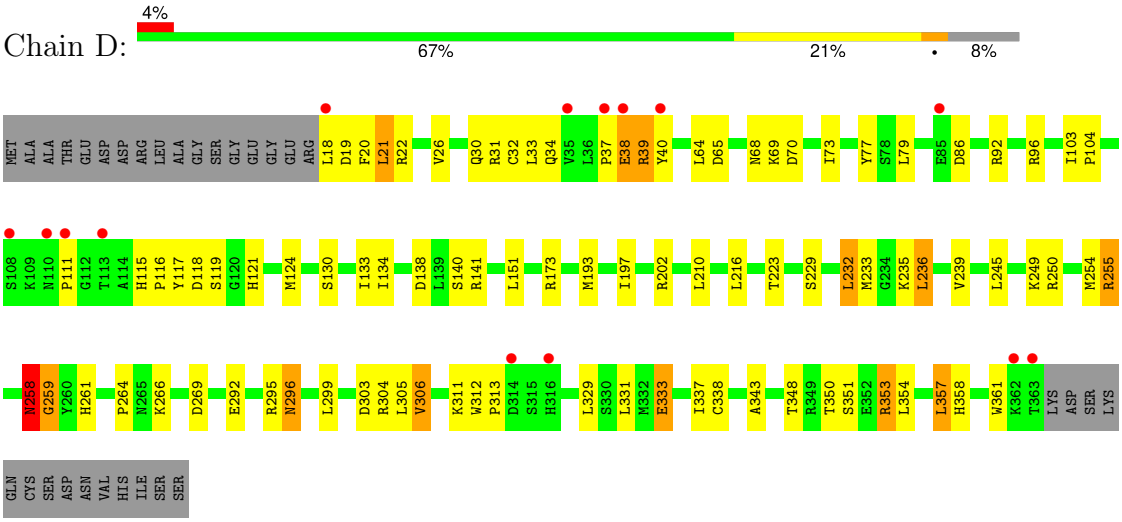
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain B:



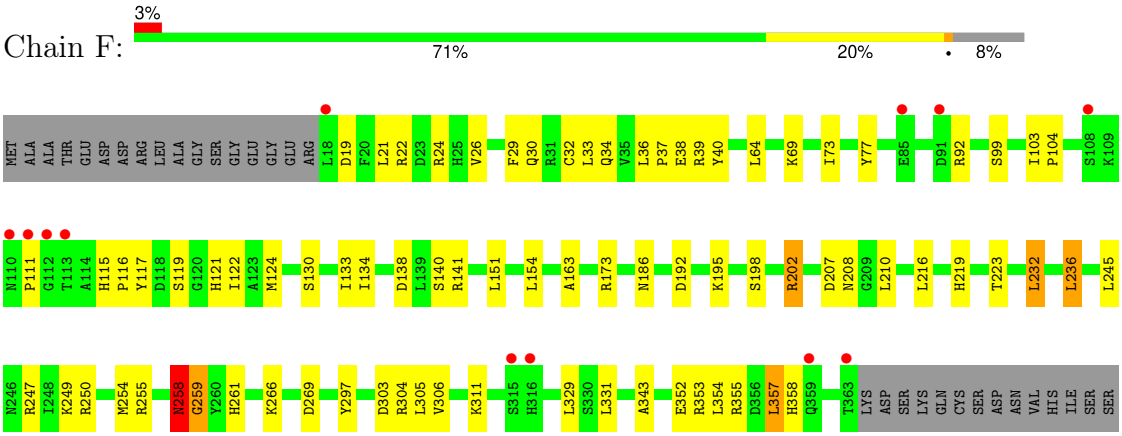
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain D:



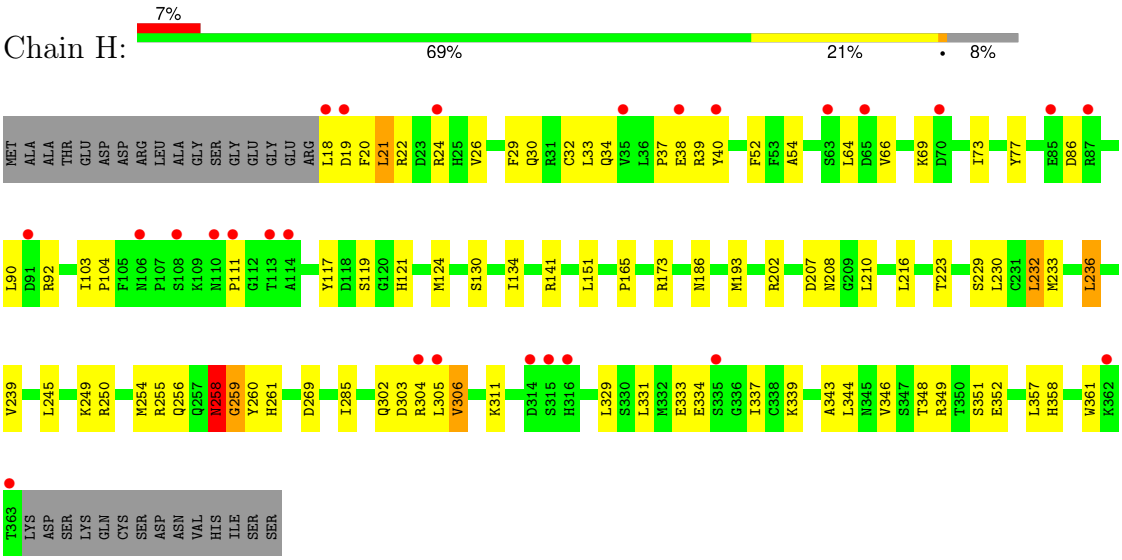
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain F:



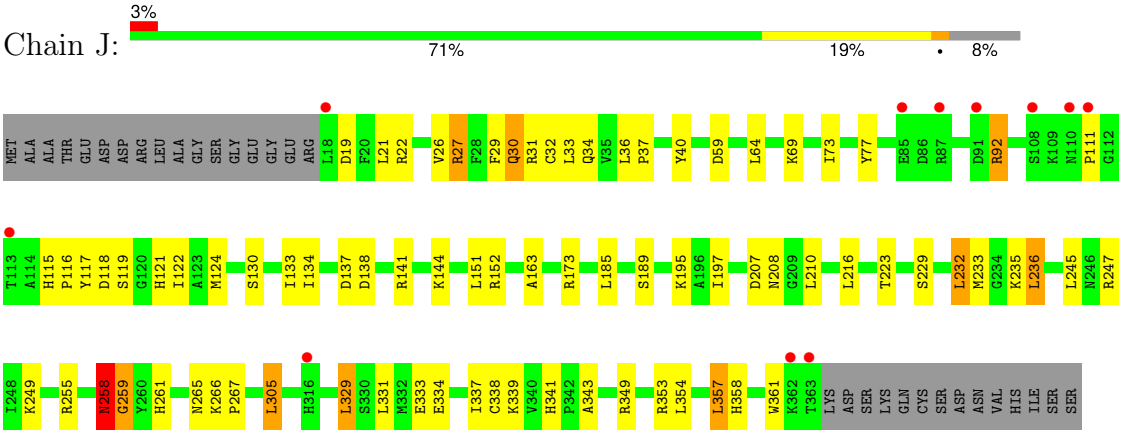
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain H:



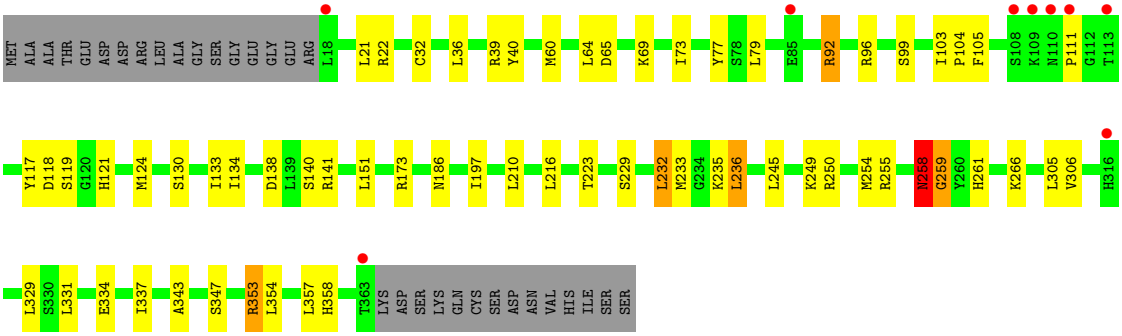
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain J:



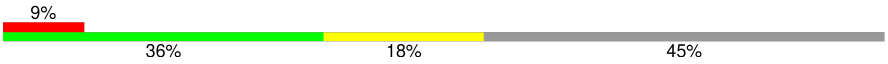
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain L:



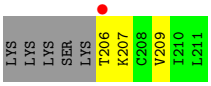
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain M:



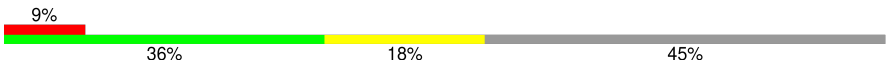
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

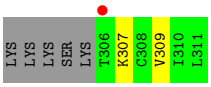
Chain N:



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

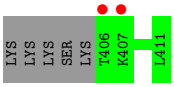
Chain O:





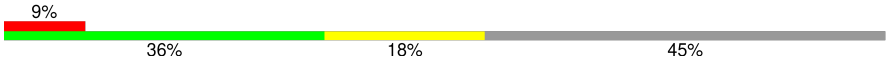
• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

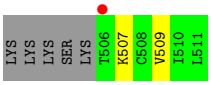
Chain P:



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

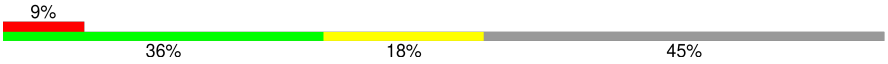
Chain Q:

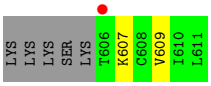




• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	272.07Å 268.80Å 185.31Å 90.00° 131.55° 90.00°	Depositor
Resolution (Å)	29.86 – 2.80 29.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.86-2.80) 99.2 (29.86-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.218 0.195 , 0.213	Depositor DCC
R_{free} test set	12102 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.085 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	33129	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.33	0/2680	0.52	0/3649
1	C	0.36	0/2714	0.53	0/3690
1	E	0.35	0/2696	0.53	0/3668
1	G	0.36	0/2698	0.53	0/3670
1	I	0.36	0/2720	0.54	0/3698
1	K	0.39	0/2733	0.56	0/3713
2	B	0.36	0/2750	0.60	2/3720 (0.1%)
2	D	0.37	0/2754	0.59	2/3725 (0.1%)
2	F	0.38	0/2769	0.60	2/3743 (0.1%)
2	H	0.35	0/2730	0.58	2/3696 (0.1%)
2	J	0.36	0/2770	0.59	2/3745 (0.1%)
2	L	0.39	0/2775	0.61	2/3750 (0.1%)
3	M	0.54	0/45	0.50	0/58
3	N	0.52	0/45	0.51	0/58
3	O	0.54	0/45	0.53	0/58
3	P	0.50	0/45	0.51	0/58
3	Q	0.55	0/45	0.52	0/58
3	R	0.56	0/45	0.53	0/58
All	All	0.37	0/33059	0.57	12/44815 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	259	GLY	N-CA-C	-5.88	98.40	113.10
2	F	259	GLY	N-CA-C	-5.80	98.61	113.10
2	L	259	GLY	N-CA-C	-5.79	98.62	113.10
2	H	259	GLY	N-CA-C	-5.75	98.73	113.10
2	D	259	GLY	N-CA-C	-5.65	98.97	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2614	0	2499	58	0
1	C	2648	0	2549	50	0
1	E	2630	0	2524	69	0
1	G	2632	0	2527	57	0
1	I	2654	0	2551	54	0
1	K	2667	0	2577	54	0
2	B	2689	0	2585	55	0
2	D	2693	0	2589	64	0
2	F	2708	0	2613	48	0
2	H	2670	0	2551	66	0
2	J	2709	0	2610	46	0
2	L	2714	0	2621	39	0
3	M	46	0	54	1	0
3	N	46	0	54	2	0
3	O	46	0	54	1	0
3	P	46	0	54	0	0
3	Q	46	0	54	1	0
3	R	46	0	54	1	0
4	A	12	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	12	0	13	1	0
4	E	12	0	13	2	0
4	G	12	0	13	2	0
4	I	12	0	13	2	0
4	K	12	0	13	1	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	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	H	5	0	0	0	0
6	J	5	0	0	0	0
6	L	5	0	0	0	0
7	C	1	0	0	1	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	2	0
7	H	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	1	0
8	M	20	0	32	1	0
8	N	20	0	32	1	0
8	O	20	0	32	1	0
8	P	20	0	32	1	0
8	Q	20	0	32	1	0
8	R	20	0	32	2	0
9	A	45	0	0	3	0
9	B	35	0	0	1	0
9	C	49	0	0	2	0
9	D	45	0	0	2	0
9	E	40	0	0	2	0
9	F	51	0	0	2	0
9	G	40	0	0	4	0
9	H	23	0	0	0	0
9	I	52	0	0	0	0
9	J	36	0	0	2	0
9	K	101	0	0	4	0
9	L	60	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	1	0	0	0	0
9	N	3	0	0	0	0
9	O	1	0	0	0	0
9	Q	3	0	0	0	0
9	R	5	0	0	0	0
All	All	33129	0	31390	639	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 10.

The worst 5 of 639 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.12	1.14
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.14
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.12	1.12
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.15	1.11
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.16	1.09

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%)	288 (92%)	23 (7%)	1 (0%)	37 67
1	C	312/377 (83%)	292 (94%)	20 (6%)	0	100 100
1	E	312/377 (83%)	291 (93%)	21 (7%)	0	100 100
1	G	312/377 (83%)	287 (92%)	24 (8%)	1 (0%)	37 67
1	I	312/377 (83%)	290 (93%)	22 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	37	67
2	B	344/377 (91%)	324 (94%)	18 (5%)	2 (1%)	22	51
2	D	344/377 (91%)	326 (95%)	14 (4%)	4 (1%)	11	34
2	F	344/377 (91%)	323 (94%)	19 (6%)	2 (1%)	22	51
2	H	344/377 (91%)	318 (92%)	22 (6%)	4 (1%)	11	34
2	J	344/377 (91%)	324 (94%)	17 (5%)	3 (1%)	14	42
2	L	344/377 (91%)	325 (94%)	17 (5%)	2 (1%)	22	51
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%)	3704 (94%)	236 (6%)	20 (0%)	25	56

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	111	PRO
2	B	258	ASN
2	D	111	PRO
2	D	258	ASN
2	F	111	PRO

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	276/338 (82%)	270 (98%)	6 (2%)	47	79
1	C	285/338 (84%)	275 (96%)	10 (4%)	31	65
1	E	280/338 (83%)	269 (96%)	11 (4%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	281/338 (83%)	276 (98%)	5 (2%)	54 83
1	I	287/338 (85%)	278 (97%)	9 (3%)	35 69
1	K	290/338 (86%)	279 (96%)	11 (4%)	28 62
2	B	286/326 (88%)	273 (96%)	13 (4%)	23 55
2	D	287/326 (88%)	270 (94%)	17 (6%)	16 44
2	F	291/326 (89%)	276 (95%)	15 (5%)	19 50
2	H	282/326 (86%)	271 (96%)	11 (4%)	27 61
2	J	291/326 (89%)	274 (94%)	17 (6%)	17 45
2	L	292/326 (90%)	279 (96%)	13 (4%)	23 55
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%)	6 (100%)	0	100 100
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	3464/4050 (86%)	3326 (96%)	138 (4%)	27 60

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	59	ASP
1	K	142	ARG
2	L	232	LEU
1	E	81	ASN
1	E	71	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	89	GLN
1	I	81	ASN
1	K	297	ASN
1	G	162	GLN
2	H	246	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 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	L	815	-	4,4,4	0.28	0	6,6,6	0.25	0
8	GER	M	1108	3	19,19,19	0.70	0	21,22,22	0.66	0
4	MES	A	901	-	12,12,12	9.12	8 (66%)	15,16,16	2.37	5 (33%)
8	GER	P	1408	3	19,19,19	0.59	0	21,22,22	0.67	0
4	MES	G	904	-	12,12,12	8.99	8 (66%)	15,16,16	2.39	6 (40%)
4	MES	E	903	-	12,12,12	9.01	8 (66%)	15,16,16	2.39	6 (40%)
6	SO4	J	814	-	4,4,4	0.33	0	6,6,6	0.22	0
8	GER	O	1308	3	19,19,19	0.67	0	21,22,22	0.69	0
6	SO4	B	810	-	4,4,4	0.34	0	6,6,6	0.16	0
4	MES	I	905	-	12,12,12	8.91	8 (66%)	15,16,16	2.49	8 (53%)
8	GER	N	1208	3	19,19,19	0.65	0	21,22,22	0.66	0
6	SO4	D	811	-	4,4,4	0.34	0	6,6,6	0.19	0
6	SO4	F	812	-	4,4,4	0.37	0	6,6,6	0.19	0
8	GER	R	1608	3	19,19,19	0.65	0	21,22,22	0.68	0
4	MES	K	906	-	12,12,12	9.03	8 (66%)	15,16,16	2.45	6 (40%)
4	MES	C	902	-	12,12,12	8.98	8 (66%)	15,16,16	2.36	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	H	813	-	4,4,4	0.32	0	6,6,6	0.18	0
8	GER	Q	1508	3	19,19,19	0.66	0	21,22,22	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GER	M	1108	3	-	3/20/20/20	-
4	MES	A	901	-	-	3/6/14/14	0/1/1/1
8	GER	P	1408	3	-	3/20/20/20	-
4	MES	G	904	-	-	3/6/14/14	0/1/1/1
4	MES	E	903	-	-	3/6/14/14	0/1/1/1
8	GER	O	1308	3	-	2/20/20/20	-
4	MES	I	905	-	-	3/6/14/14	0/1/1/1
8	GER	N	1208	3	-	3/20/20/20	-
8	GER	R	1608	3	-	2/20/20/20	-
4	MES	K	906	-	-	3/6/14/14	0/1/1/1
4	MES	C	902	-	-	3/6/14/14	0/1/1/1
8	GER	Q	1508	3	-	2/20/20/20	-

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	906	MES	C8-S	-23.87	1.44	1.77
4	A	901	MES	C8-S	-23.85	1.44	1.77
4	G	904	MES	C8-S	-23.37	1.44	1.77
4	E	903	MES	C8-S	-23.33	1.44	1.77
4	C	902	MES	C8-S	-23.28	1.44	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	904	MES	O3S-S-C8	4.71	115.23	106.00
4	I	905	MES	O3S-S-C8	4.64	115.08	106.00
4	E	903	MES	O3S-S-C8	4.61	115.02	106.00
4	A	901	MES	O3S-S-C8	4.57	114.94	106.00
4	K	906	MES	O3S-S-C8	4.54	114.89	106.00

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	MES	C7-C8-S-O1S
4	A	901	MES	C7-C8-S-O2S
4	A	901	MES	C7-C8-S-O3S
4	C	902	MES	C7-C8-S-O1S
4	C	902	MES	C7-C8-S-O3S

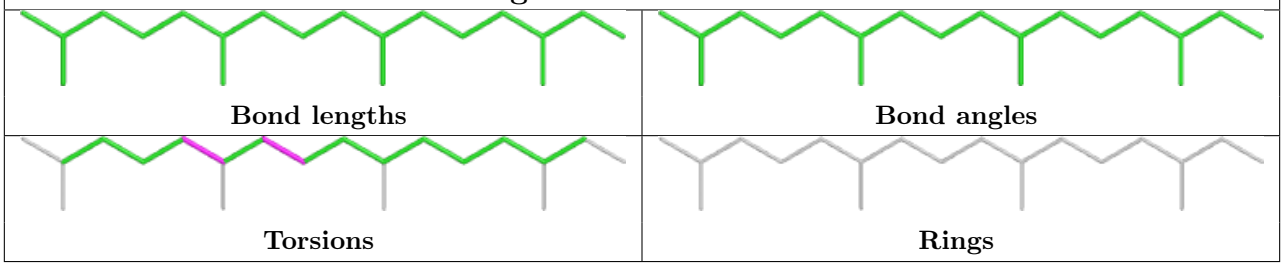
There are no ring outliers.

12 monomers are involved in 18 short contacts:

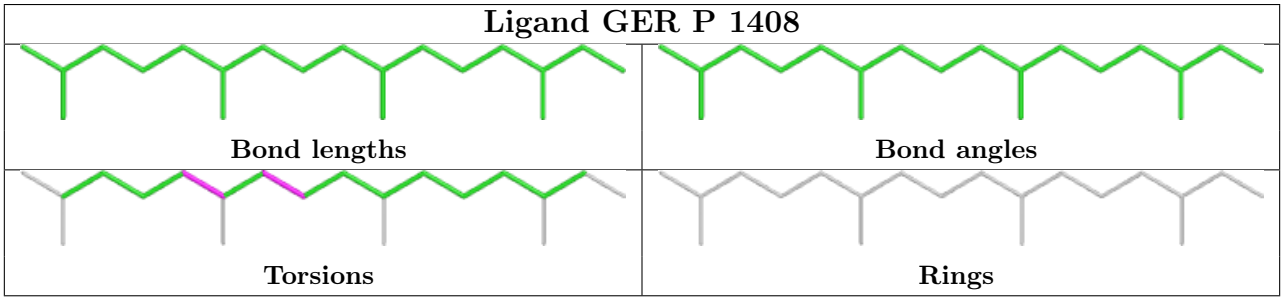
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1108	GER	1	0
4	A	901	MES	3	0
8	P	1408	GER	1	0
4	G	904	MES	2	0
4	E	903	MES	2	0
8	O	1308	GER	1	0
4	I	905	MES	2	0
8	N	1208	GER	1	0
8	R	1608	GER	2	0
4	K	906	MES	1	0
4	C	902	MES	1	0
8	Q	1508	GER	1	0

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 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.

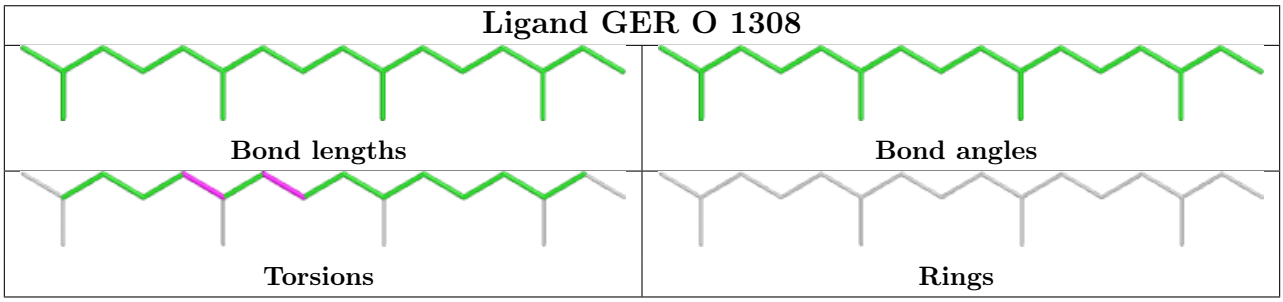
Ligand GER M 1108



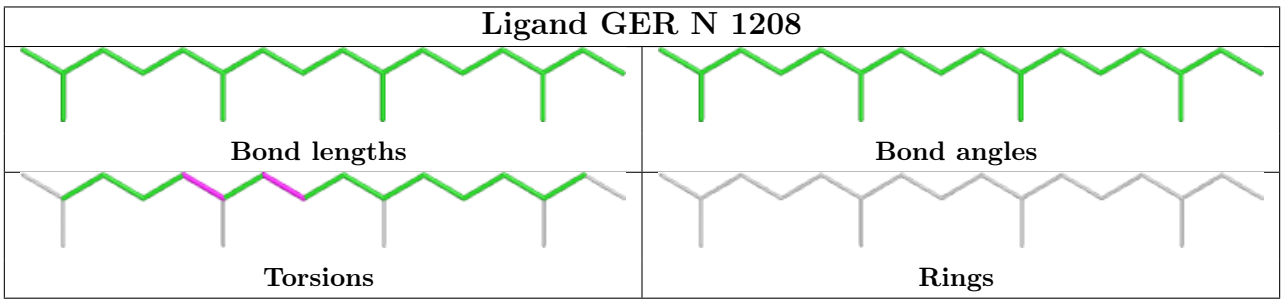
Ligand GER P 1408



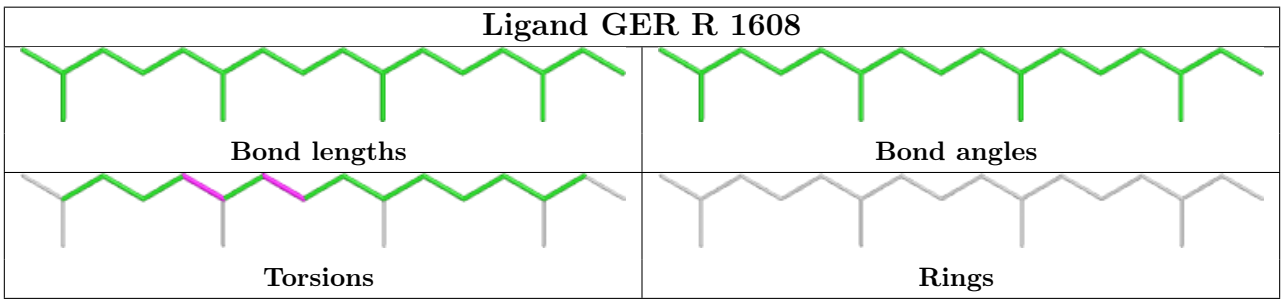
Ligand GER O 1308

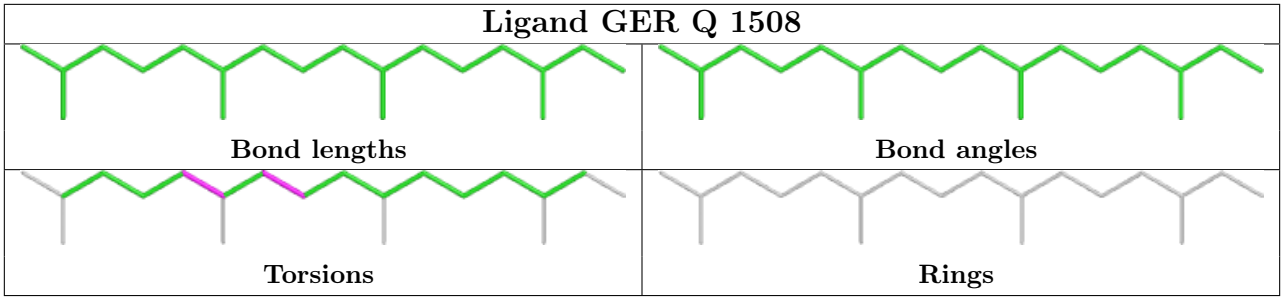


Ligand GER N 1208



Ligand GER R 1608





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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	314/377 (83%)	-0.04	8 (2%)	58	49	36, 57, 91, 105	0
1	C	314/377 (83%)	-0.02	6 (1%)	66	58	35, 55, 81, 99	0
1	E	314/377 (83%)	0.01	8 (2%)	58	49	34, 57, 83, 103	0
1	G	314/377 (83%)	0.10	19 (6%)	28	21	38, 58, 85, 104	0
1	I	314/377 (83%)	-0.12	8 (2%)	58	49	32, 52, 80, 91	0
1	K	314/377 (83%)	-0.45	4 (1%)	74	67	25, 43, 67, 82	0
2	B	346/377 (91%)	-0.21	11 (3%)	50	42	36, 52, 78, 100	0
2	D	346/377 (91%)	-0.28	14 (4%)	43	35	34, 48, 78, 92	0
2	F	346/377 (91%)	-0.27	12 (3%)	47	39	32, 48, 77, 103	0
2	H	346/377 (91%)	0.41	26 (7%)	22	16	37, 64, 92, 111	0
2	J	346/377 (91%)	-0.22	11 (3%)	50	42	31, 50, 79, 102	0
2	L	346/377 (91%)	-0.49	9 (2%)	57	49	27, 42, 66, 88	0
3	M	6/11 (54%)	0.68	1 (16%)	5	5	52, 58, 82, 89	0
3	N	6/11 (54%)	0.79	1 (16%)	5	5	56, 61, 79, 85	0
3	O	6/11 (54%)	0.55	1 (16%)	5	5	52, 59, 78, 84	0
3	P	6/11 (54%)	1.53	2 (33%)	1	1	64, 68, 89, 92	0
3	Q	6/11 (54%)	0.60	1 (16%)	5	5	51, 56, 72, 79	0
3	R	6/11 (54%)	0.77	1 (16%)	5	5	51, 57, 71, 76	0
All	All	3996/4590 (87%)	-0.13	143 (3%)	46	38	25, 52, 83, 111	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	18	LEU	7.3
1	G	55	PHE	6.9
1	C	55	PHE	6.6

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Mol	Chain	Res	Type	RSRZ
2	B	113	THR	5.9
1	E	55	PHE	5.5

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MES	A	901	12/12	0.89	0.22	96,103,106,106	0
4	MES	G	904	12/12	0.90	0.22	97,101,104,104	0
4	MES	I	905	12/12	0.90	0.22	78,84,88,89	0
4	MES	C	902	12/12	0.91	0.22	86,93,95,96	0
4	MES	K	906	12/12	0.91	0.19	65,77,83,84	0
4	MES	E	903	12/12	0.92	0.19	84,90,94,94	0
6	SO4	D	811	5/5	0.94	0.12	66,66,67,67	0
8	GER	N	1208	20/20	0.94	0.15	49,53,58,59	0
8	GER	O	1308	20/20	0.94	0.15	48,51,58,60	0
8	GER	P	1408	20/20	0.94	0.18	61,66,73,73	0
8	GER	R	1608	20/20	0.94	0.15	47,50,54,54	0
6	SO4	F	812	5/5	0.95	0.10	67,67,68,69	0
8	GER	Q	1508	20/20	0.95	0.14	47,50,55,56	0
8	GER	M	1108	20/20	0.95	0.14	48,52,61,61	0
6	SO4	B	810	5/5	0.96	0.09	67,68,68,69	0
6	SO4	J	814	5/5	0.97	0.07	52,52,54,55	0
6	SO4	L	815	5/5	0.97	0.08	54,54,56,56	0
7	CL	C	801	1/1	0.97	0.16	53,53,53,53	0
7	CL	H	805	1/1	0.97	0.06	60,60,60,60	0
7	CL	J	806	1/1	0.97	0.08	58,58,58,58	0
7	CL	K	807	1/1	0.97	0.10	44,44,44,44	0

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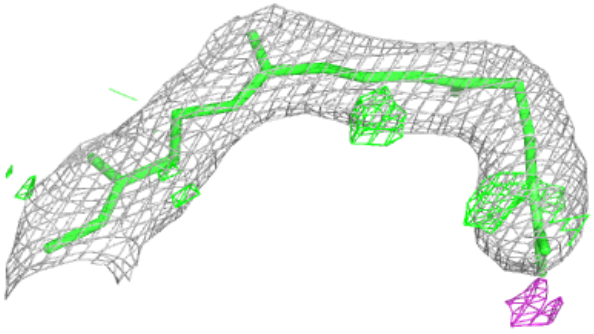
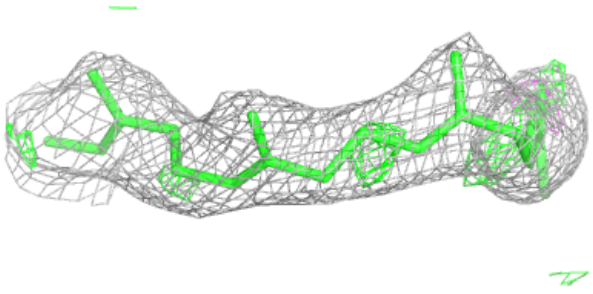
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CL	G	804	1/1	0.98	0.12	52,52,52,52	0
5	ZN	H	378	1/1	0.98	0.07	87,87,87,87	0
5	ZN	F	378	1/1	0.98	0.08	78,78,78,78	0
6	SO4	H	813	5/5	0.98	0.07	68,69,69,70	0
7	CL	D	802	1/1	0.98	0.04	45,45,45,45	0
5	ZN	B	378	1/1	0.99	0.06	77,77,77,77	0
5	ZN	D	378	1/1	0.99	0.04	66,66,66,66	0
5	ZN	J	378	1/1	0.99	0.05	68,68,68,68	0
5	ZN	L	378	1/1	0.99	0.04	58,58,58,58	0
7	CL	F	803	1/1	0.99	0.07	51,51,51,51	0

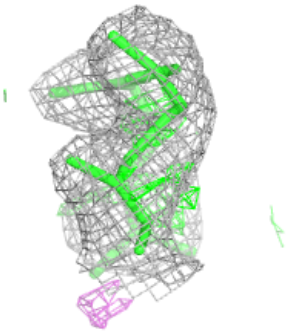
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GER N 1208:

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

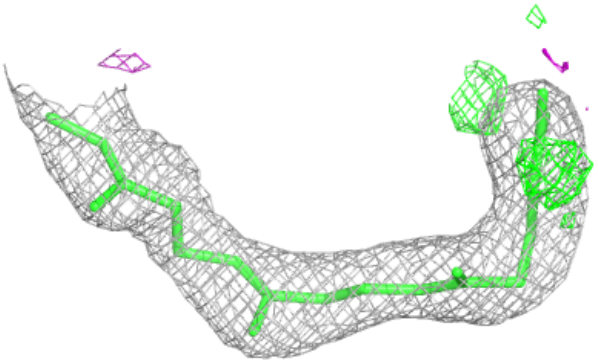


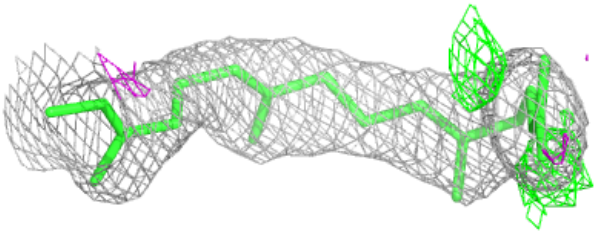


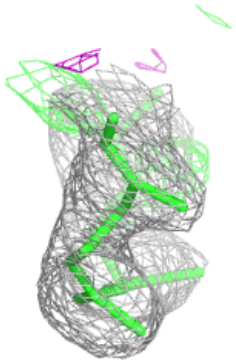


Electron density around GER O 1308:

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

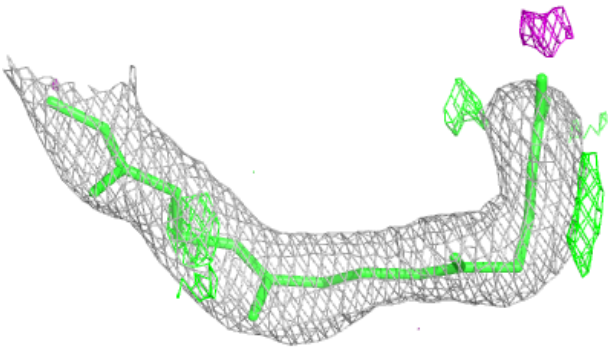


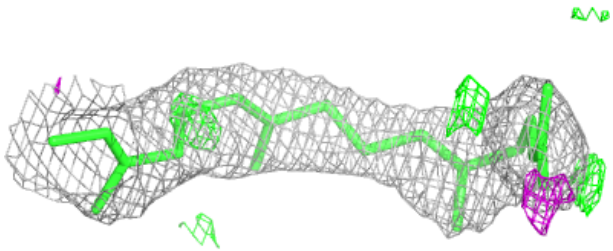


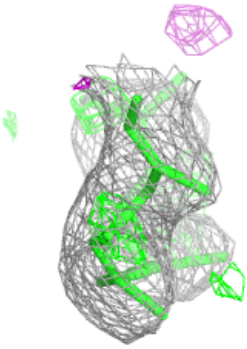


Electron density around GER P 1408:

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

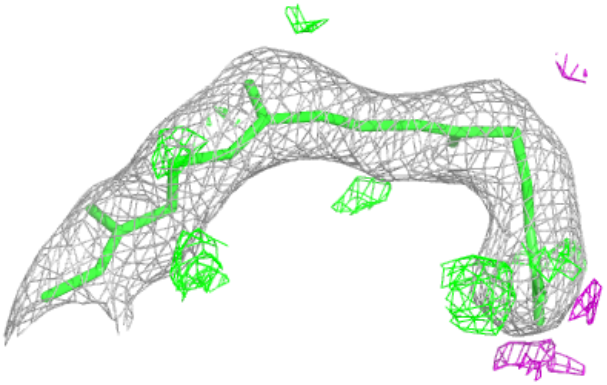


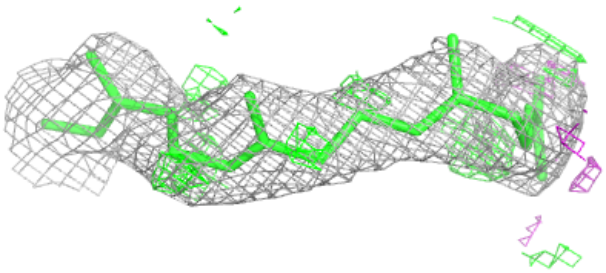


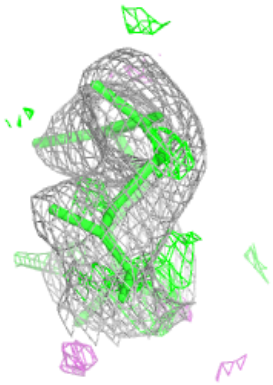


Electron density around GER R 1608:

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

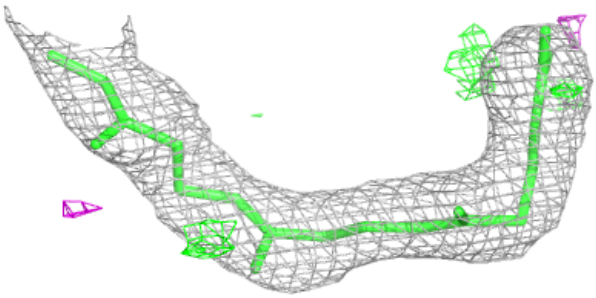


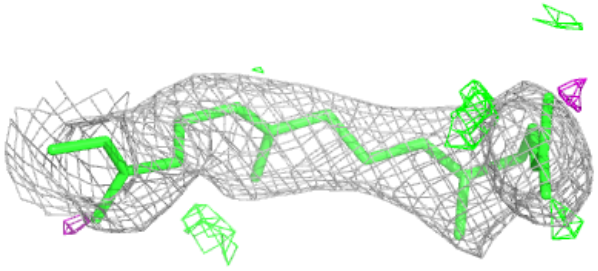


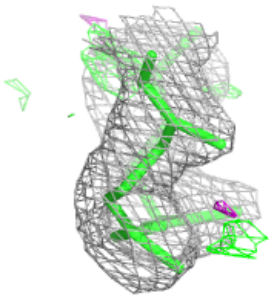


Electron density around GER Q 1508:

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

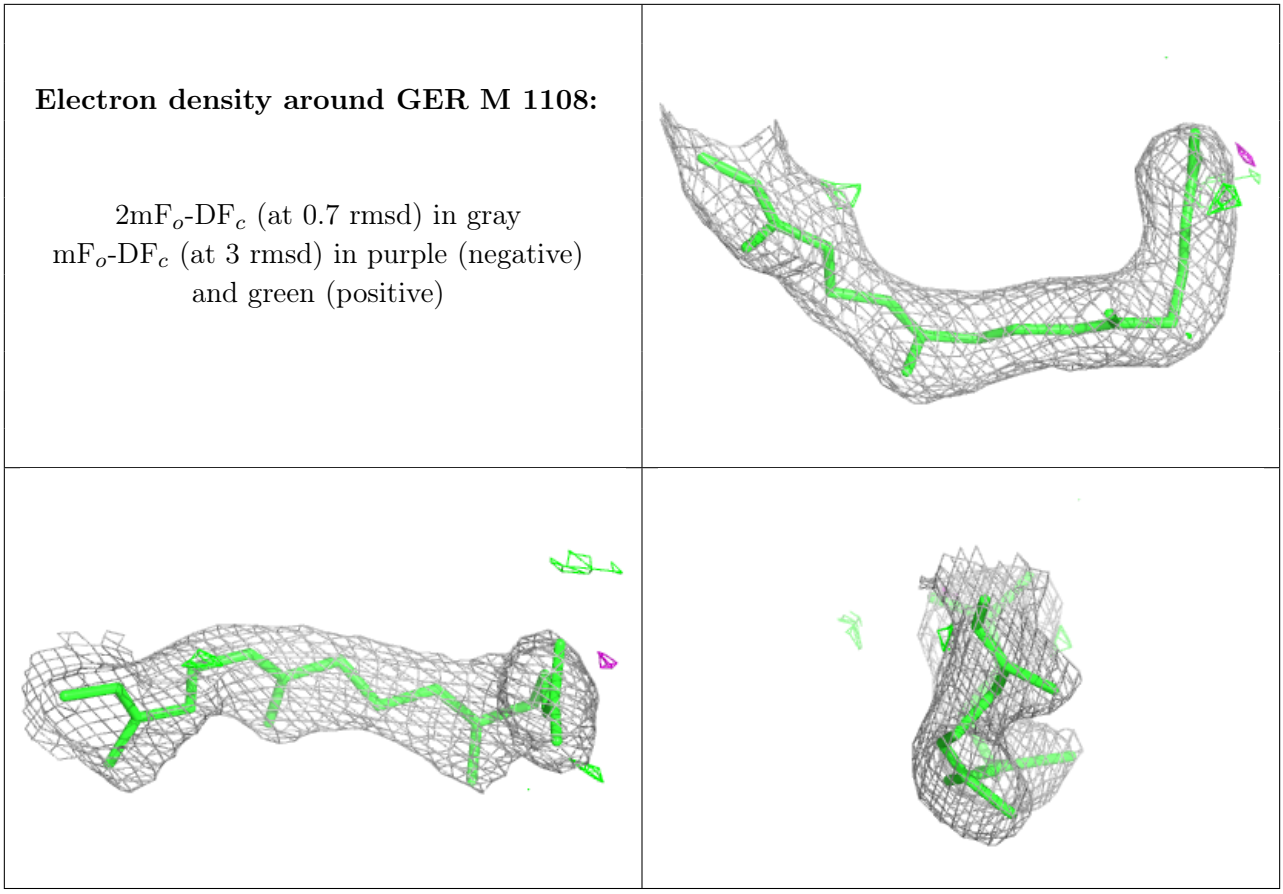






Electron density around GER M 1108:

$2mF_o$-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.