wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2024 – 01:20 AM EDT

PDB ID	:	1N4S
Title	:	Protein Geranylgeranyltransferase type-I Complexed with GGPP and a Geranylgeranylated KKKSKTKCVIL Peptide Product
Authors	:	Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on	:	2002-11-01
Resolution	:	2.60 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:

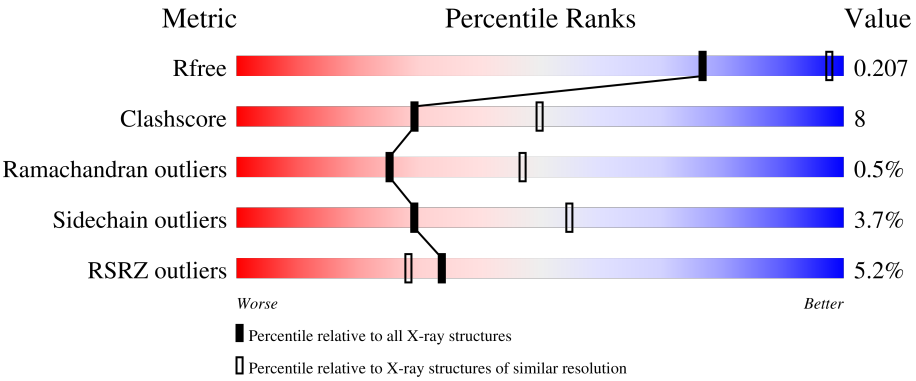
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & 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 2.60 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	4% 68% 14% • 17%
1	C	377	4% 67% 16% • 17%
1	E	377	3% 63% 19% • 17%
1	G	377	7% 66% 16% • 17%
1	I	377	3% 68% 15% • 17%

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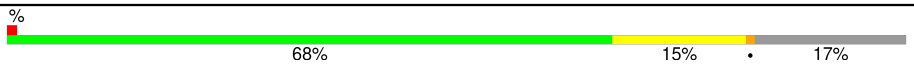
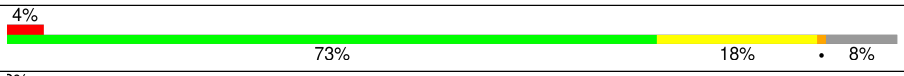
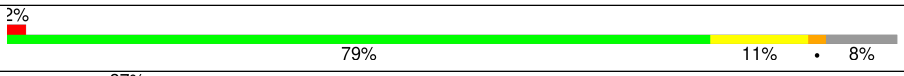
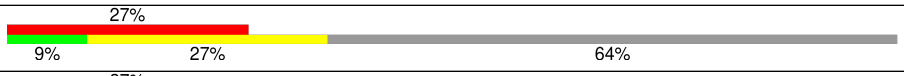
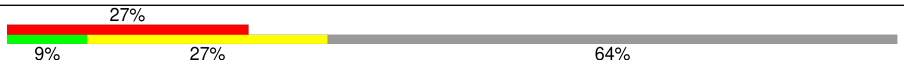
Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

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
7	GER	M	1108	-	-	-	X
7	GER	N	1208	-	-	-	X
7	GER	O	1308	-	-	-	X
7	GER	P	1408	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 33924 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
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2643	1689	461	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2656	1694	465	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2671	1703	467	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
			2697	1707	467	499	24			
2	D	346	Total	C	N	O	S	0	0	0
			2713	1715	472	502	24			
2	F	346	Total	C	N	O	S	0	0	0
			2718	1717	474	503	24			
2	H	346	Total	C	N	O	S	0	0	0
			2694	1706	464	500	24			
2	J	346	Total	C	N	O	S	0	0	0
			2711	1713	471	503	24			
2	L	346	Total	C	N	O	S	0	0	0
			2723	1720	473	506	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	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	N	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	O	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	P	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	Q	4	Total	C	N	O	S	0	0	0
			30	20	4	5	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		

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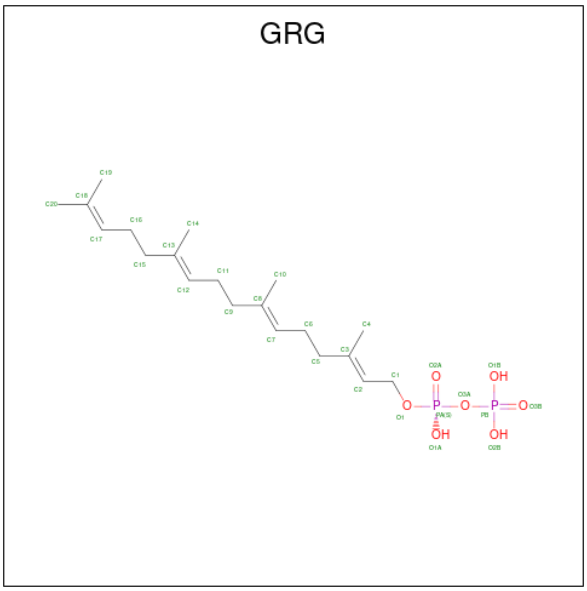
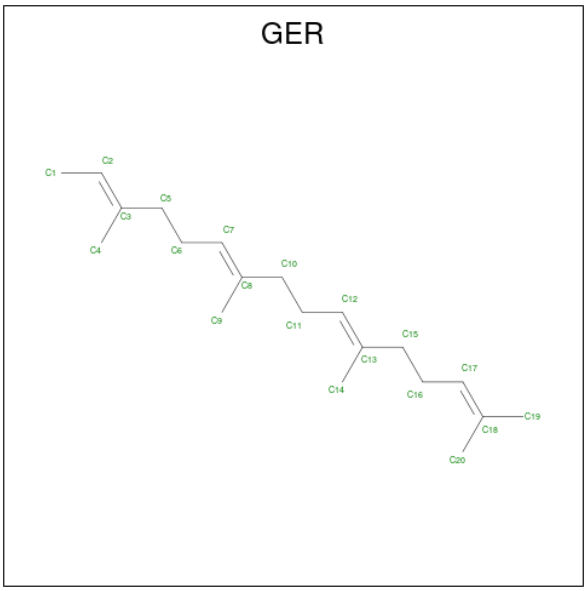
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total Cl 1 1	0	0
5	K	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0

- Molecule 6 is GERANYLGERANYL DIPHOSPHATE (three-letter code: GRG) (formula: $C_{20}H_{36}O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O P 29 20 7 2	0	0
6	D	1	Total C O P 29 20 7 2	0	0
6	F	1	Total C O P 29 20 7 2	0	0
6	H	1	Total C O P 29 20 7 2	0	0
6	J	1	Total C O P 29 20 7 2	0	0
6	L	1	Total C O P 29 20 7 2	0	0

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



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	89	Total O 89 89	0	0
8	B	79	Total O 79 79	0	0
8	C	93	Total O 93 93	0	0
8	D	121	Total O 121 121	0	0
8	E	85	Total O 85 85	0	0
8	F	100	Total O 100 100	0	0

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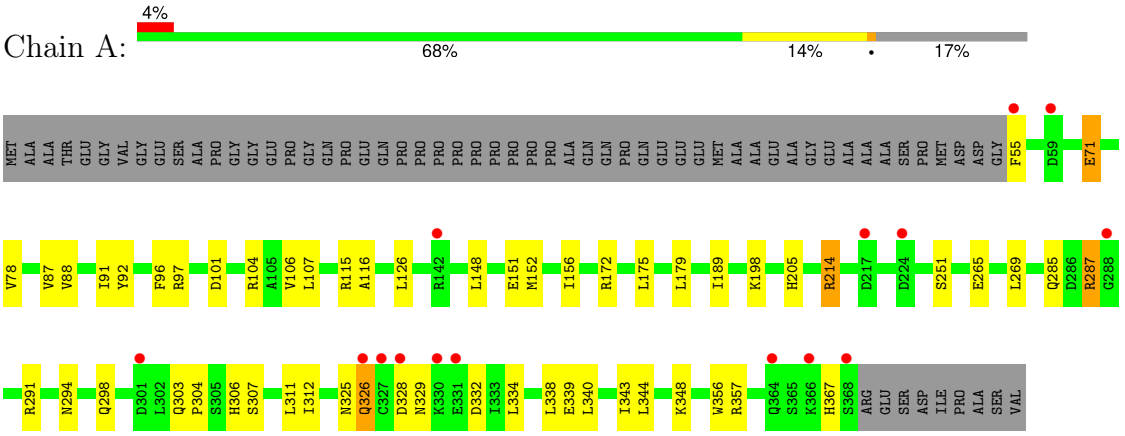
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	86	Total O 86 86	0	0
8	H	56	Total O 56 56	0	0
8	I	121	Total O 121 121	0	0
8	J	88	Total O 88 88	0	0
8	K	211	Total O 211 211	0	0
8	L	157	Total O 157 157	0	0
8	M	2	Total O 2 2	0	0
8	N	2	Total O 2 2	0	0
8	O	1	Total O 1 1	0	0
8	P	1	Total O 1 1	0	0
8	Q	1	Total O 1 1	0	0
8	R	3	Total O 3 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.

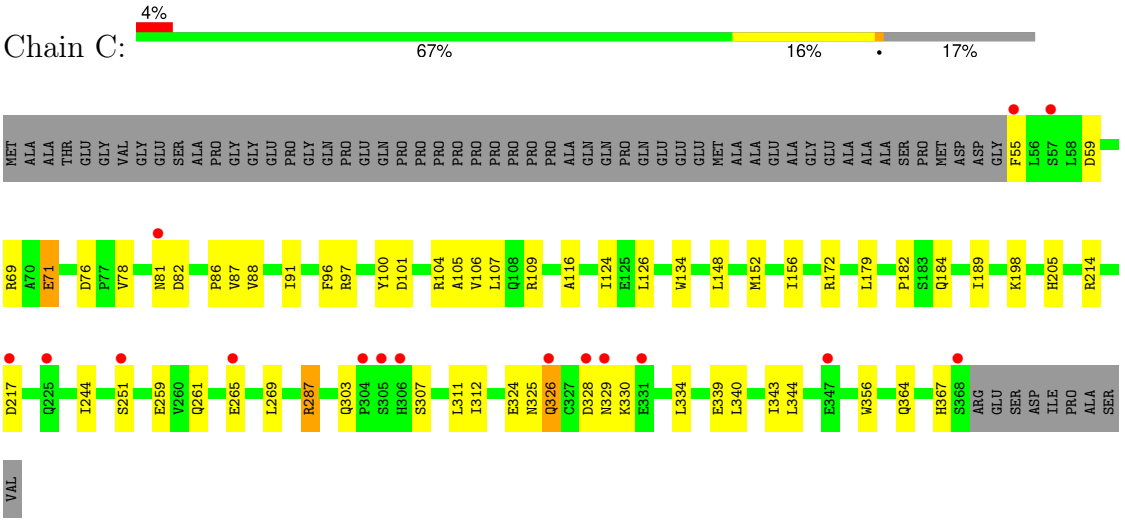
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain A:



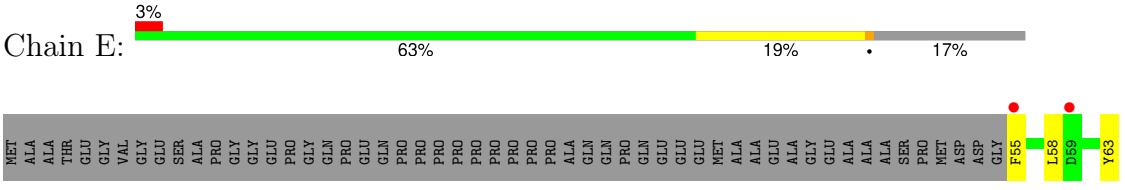
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

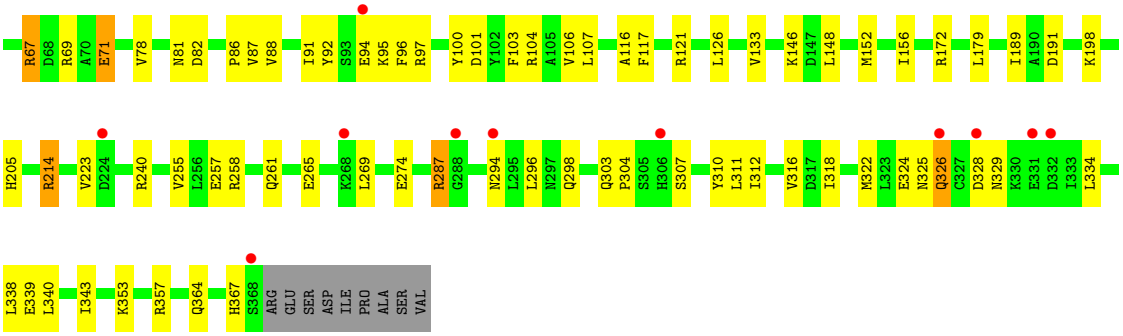
Chain C:



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

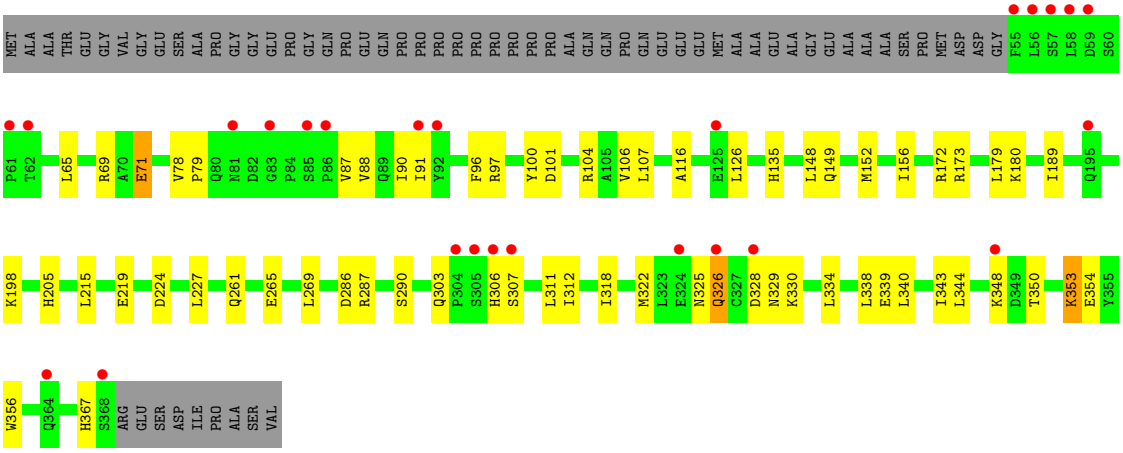
Chain E:





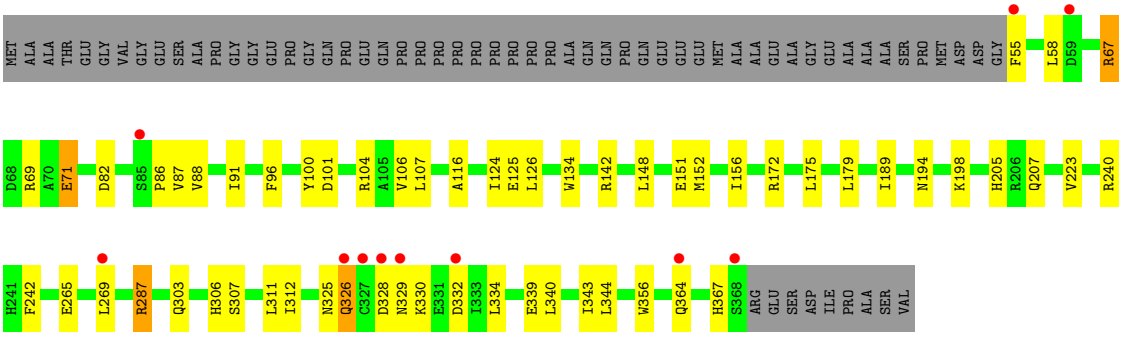
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

Chain G:



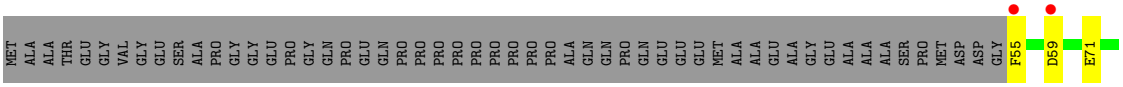
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

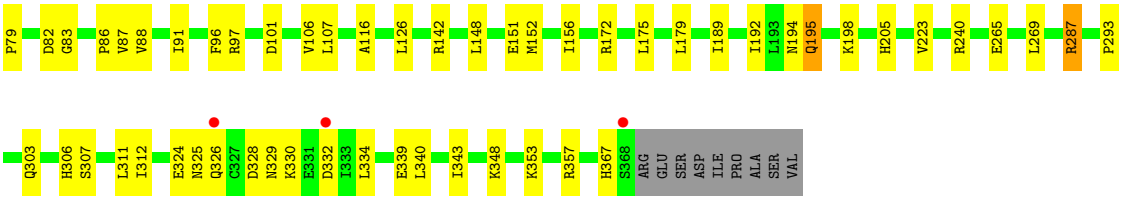
Chain I:



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

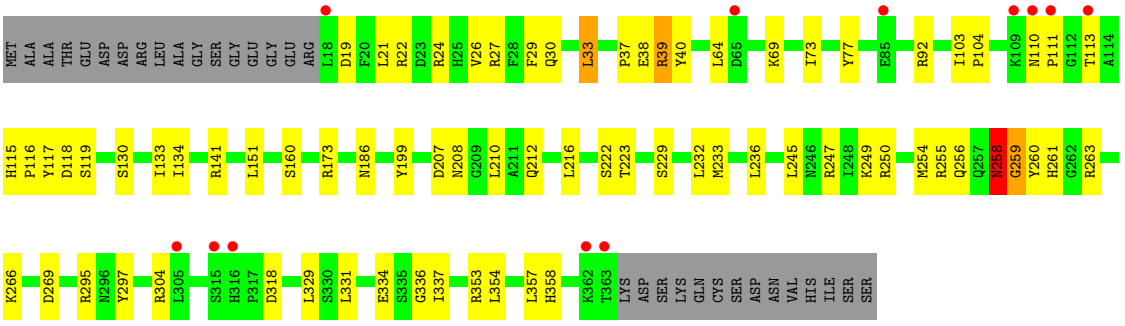
Chain K:





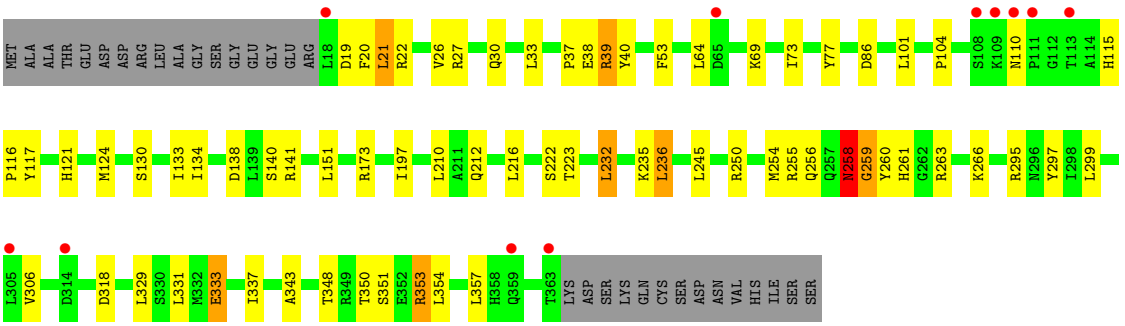
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain B:



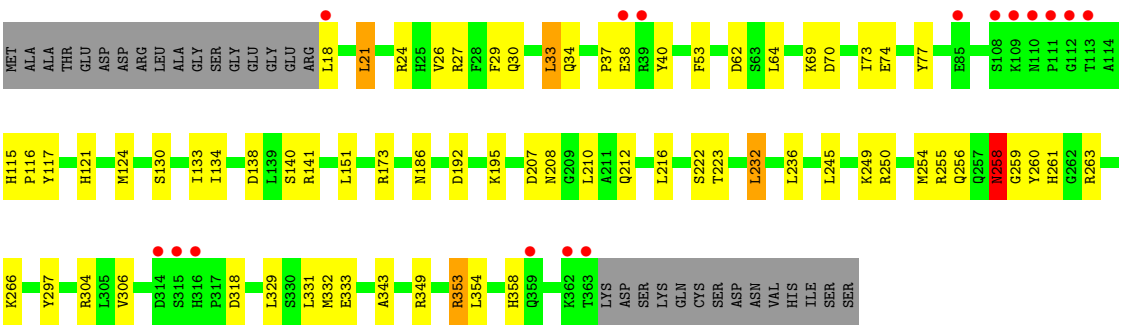
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain D:



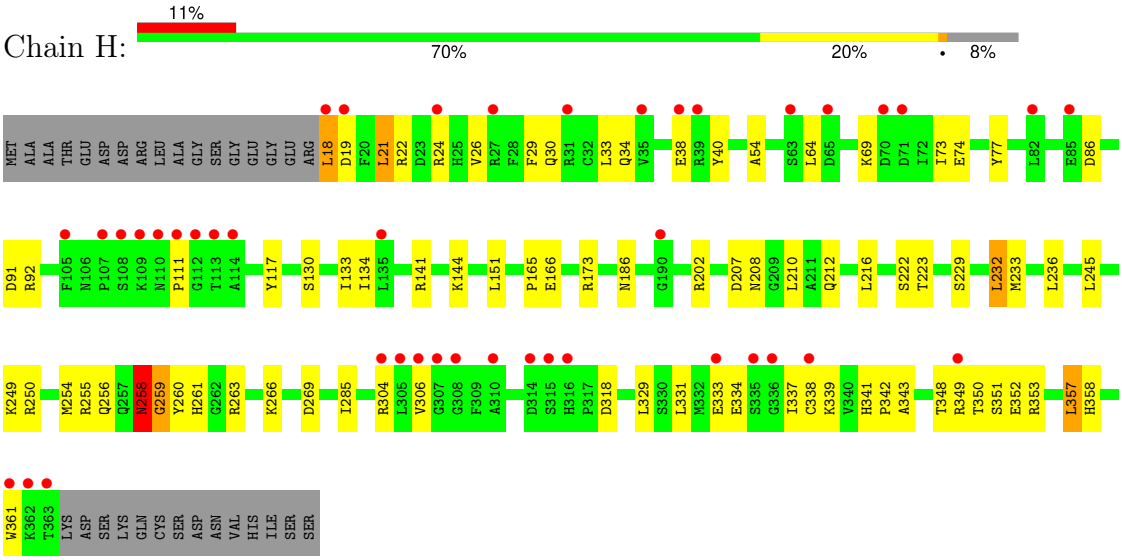
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain F:



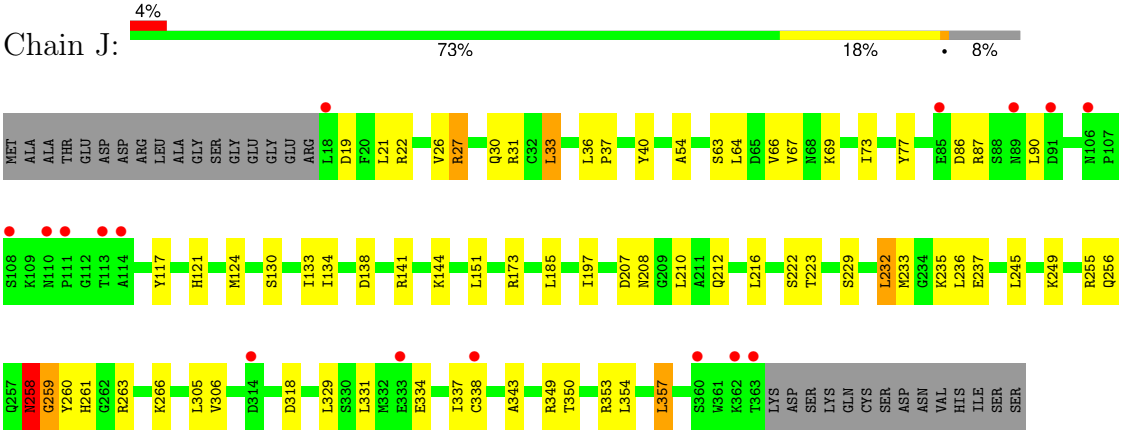
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain H:



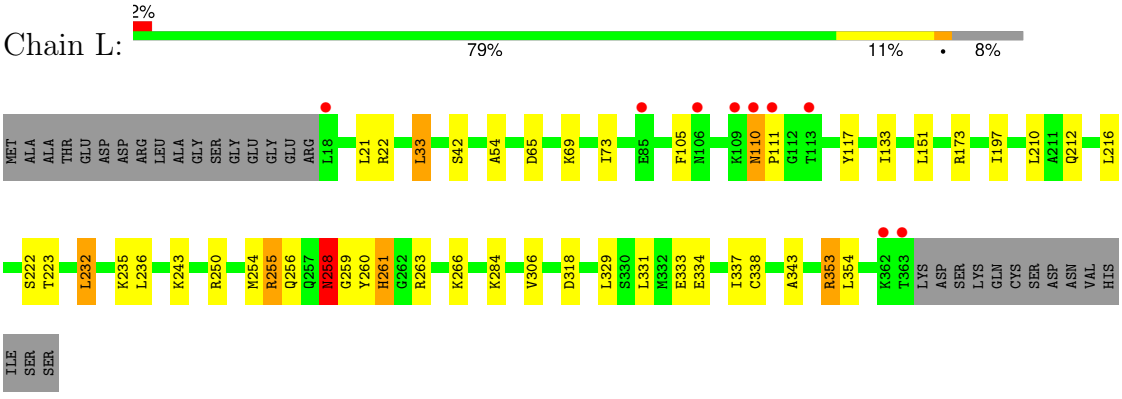
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain J:



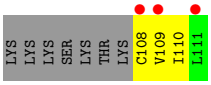
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

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

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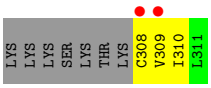
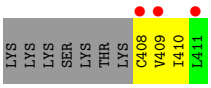
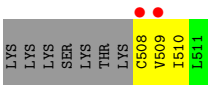


• Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



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



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.12Å 268.43Å 184.82Å 90.00° 131.58° 90.00°	Depositor
Resolution (Å)	29.98 – 2.60 29.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.98-2.60) 99.7 (29.98-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.214 0.189 , 0.207	Depositor DCC
R_{free} test set	14968 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	49.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.078 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	33924	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 2.25% 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, GER, ZN, GRG

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	0/2695	0.51	0/3668
1	C	0.35	0/2709	0.52	0/3684
1	E	0.34	0/2708	0.53	0/3684
1	G	0.35	0/2699	0.52	0/3672
1	I	0.35	0/2722	0.52	0/3700
1	K	0.39	0/2737	0.55	0/3717
2	B	0.35	0/2759	0.59	2/3733 (0.1%)
2	D	0.37	0/2775	0.59	2/3752 (0.1%)
2	F	0.37	0/2780	0.59	2/3758 (0.1%)
2	H	0.34	0/2756	0.58	2/3729 (0.1%)
2	J	0.36	0/2773	0.59	2/3750 (0.1%)
2	L	0.40	0/2785	0.61	2/3764 (0.1%)
3	M	0.62	0/29	0.88	0/37
3	N	0.57	0/29	0.91	0/37
3	O	0.60	0/29	0.91	0/37
3	P	0.56	0/29	0.89	0/37
3	Q	0.60	0/29	0.93	0/37
3	R	0.52	0/38	0.84	0/48
All	All	0.36	0/33081	0.56	12/44844 (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(^{o})	Ideal(^{o})
2	F	259	GLY	N-CA-C	-5.86	98.46	113.10
2	H	259	GLY	N-CA-C	-5.83	98.53	113.10
2	D	259	GLY	N-CA-C	-5.83	98.53	113.10
2	J	259	GLY	N-CA-C	-5.81	98.57	113.10
2	L	259	GLY	N-CA-C	-5.71	98.83	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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2520	43	0
1	C	2643	0	2540	39	0
1	E	2642	0	2534	52	0
1	G	2633	0	2524	52	0
1	I	2656	0	2560	35	0
1	K	2671	0	2588	38	0
2	B	2697	0	2600	51	0
2	D	2713	0	2628	51	0
2	F	2718	0	2635	38	0
2	H	2694	0	2590	63	0
2	J	2711	0	2616	47	0
2	L	2723	0	2643	27	0
3	M	30	0	34	4	0
3	N	30	0	34	3	0
3	O	30	0	34	4	0
3	P	30	0	34	5	0
3	Q	30	0	34	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	39	0	47	8	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	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	1	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	1	0
5	L	1	0	0	0	0
6	B	29	0	33	1	0
6	D	29	0	33	2	0
6	F	29	0	33	2	0
6	H	29	0	33	1	0
6	J	29	0	33	1	0
6	L	29	0	33	2	0
7	M	20	0	33	5	0
7	N	20	0	33	6	0
7	O	20	0	33	7	0
7	P	20	0	33	6	0
7	Q	20	0	33	4	0
7	R	20	0	33	6	0
8	A	89	0	0	1	0
8	B	79	0	0	2	0
8	C	93	0	0	1	0
8	D	121	0	0	2	0
8	E	85	0	0	0	0
8	F	100	0	0	3	0
8	G	86	0	0	5	0
8	H	56	0	0	4	0
8	I	121	0	0	1	0
8	J	88	0	0	2	0
8	K	211	0	0	4	0
8	L	157	0	0	2	0
8	M	2	0	0	0	0
8	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	1	0	0	0	0
8	P	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	3	0	0	2	0
All	All	33924	0	31591	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 545 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	1.01	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.12	1.10
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.11	1.07
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.06	1.06
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.18	1.04

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/377 (83%)	290 (93%)	20 (6%)	2 (1%)	22	43
1	C	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	37	59
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	37	59
1	G	312/377 (83%)	294 (94%)	16 (5%)	2 (1%)	22	43
1	I	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	22	43
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	37	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	344/377 (91%)	334 (97%)	9 (3%)	1 (0%)	37 59
2	D	344/377 (91%)	333 (97%)	9 (3%)	2 (1%)	22 43
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	37 59
2	H	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	14 31
2	J	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	37 59
2	L	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	37 59
3	M	2/11 (18%)	2 (100%)	0	0	100 100
3	N	2/11 (18%)	2 (100%)	0	0	100 100
3	O	2/11 (18%)	2 (100%)	0	0	100 100
3	P	2/11 (18%)	2 (100%)	0	0	100 100
3	Q	2/11 (18%)	2 (100%)	0	0	100 100
3	R	3/11 (27%)	3 (100%)	0	0	100 100
All	All	3949/4590 (86%)	3756 (95%)	175 (4%)	18 (0%)	25 47

5 of 18 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	280/338 (83%)	276 (99%)	4 (1%)	62 82
1	C	283/338 (84%)	273 (96%)	10 (4%)	31 57
1	E	284/338 (84%)	275 (97%)	9 (3%)	34 60
1	G	281/338 (83%)	277 (99%)	4 (1%)	62 82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	287/338 (85%)	280 (98%)	7 (2%)	44	70
1	K	291/338 (86%)	283 (97%)	8 (3%)	40	66
2	B	289/326 (89%)	276 (96%)	13 (4%)	23	47
2	D	293/326 (90%)	277 (94%)	16 (6%)	18	38
2	F	294/326 (90%)	280 (95%)	14 (5%)	21	44
2	H	288/326 (88%)	274 (95%)	14 (5%)	21	43
2	J	292/326 (90%)	277 (95%)	15 (5%)	20	42
2	L	296/326 (91%)	280 (95%)	16 (5%)	18	39
3	M	4/11 (36%)	4 (100%)	0	100	100
3	N	4/11 (36%)	4 (100%)	0	100	100
3	O	4/11 (36%)	4 (100%)	0	100	100
3	P	4/11 (36%)	4 (100%)	0	100	100
3	Q	4/11 (36%)	4 (100%)	0	100	100
3	R	5/11 (46%)	5 (100%)	0	100	100
All	All	3483/4050 (86%)	3353 (96%)	130 (4%)	29	55

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	33	LEU
2	L	216	LEU
1	E	214	ARG
1	E	191	ASP
2	L	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	195	GLN
2	J	246	ASN
1	I	201	HIS
2	J	30	GLN
1	K	201	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 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	M	1108	3	19,19,19	0.93	0	21,22,22	0.63	0
6	GRG	F	1503	-	27,28,28	0.81	0	33,37,37	0.90	1 (3%)
6	GRG	D	1502	-	27,28,28	0.82	0	33,37,37	0.89	1 (3%)
7	GER	O	1308	3	19,19,19	0.94	1 (5%)	21,22,22	0.63	0
6	GRG	L	1506	-	27,28,28	0.80	0	33,37,37	0.93	1 (3%)
6	GRG	J	1505	-	27,28,28	0.77	0	33,37,37	0.89	1 (3%)
6	GRG	H	1504	-	27,28,28	0.77	0	33,37,37	0.90	1 (3%)
7	GER	N	1208	3	19,19,19	0.92	0	21,22,22	0.63	0
6	GRG	B	1501	-	27,28,28	0.78	0	33,37,37	0.89	1 (3%)
7	GER	R	1608	3	19,19,19	0.91	0	21,22,22	0.65	0
7	GER	P	1408	3	19,19,19	0.93	0	21,22,22	0.61	0
7	GER	Q	1508	3	19,19,19	0.89	0	21,22,22	0.63	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
7	GER	M	1108	3	-	9/20/20/20	-
6	GRG	F	1503	-	-	7/31/31/31	-
6	GRG	D	1502	-	-	8/31/31/31	-
7	GER	O	1308	3	-	9/20/20/20	-
6	GRG	L	1506	-	-	8/31/31/31	-
6	GRG	J	1505	-	-	9/31/31/31	-
6	GRG	H	1504	-	-	8/31/31/31	-
7	GER	N	1208	3	-	10/20/20/20	-
6	GRG	B	1501	-	-	7/31/31/31	-
7	GER	R	1608	3	-	10/20/20/20	-
7	GER	P	1408	3	-	10/20/20/20	-
7	GER	Q	1508	3	-	9/20/20/20	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	1308	GER	C12-C13	2.04	1.37	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1504	GRG	O1B-PB-O3A	2.65	113.52	104.64
6	J	1505	GRG	O1B-PB-O3A	2.60	113.37	104.64
6	L	1506	GRG	O1B-PB-O3A	2.58	113.29	104.64
6	B	1501	GRG	O1B-PB-O3A	2.58	113.28	104.64
6	D	1502	GRG	O1B-PB-O3A	2.57	113.24	104.64

There are no chirality outliers.

5 of 104 torsion outliers are listed below:

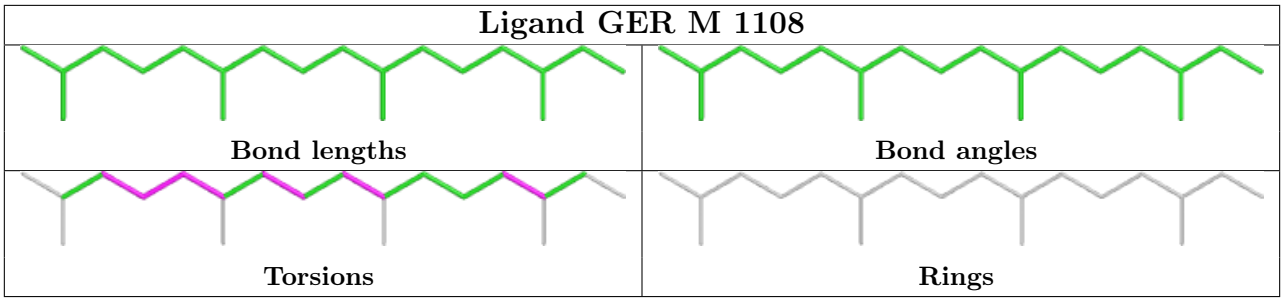
Mol	Chain	Res	Type	Atoms
6	B	1501	GRG	PA-O3A-PB-O1B
6	D	1502	GRG	PA-O3A-PB-O1B
6	F	1503	GRG	PA-O3A-PB-O1B
6	H	1504	GRG	PA-O3A-PB-O1B
6	J	1505	GRG	PA-O3A-PB-O1B

There are no ring outliers.

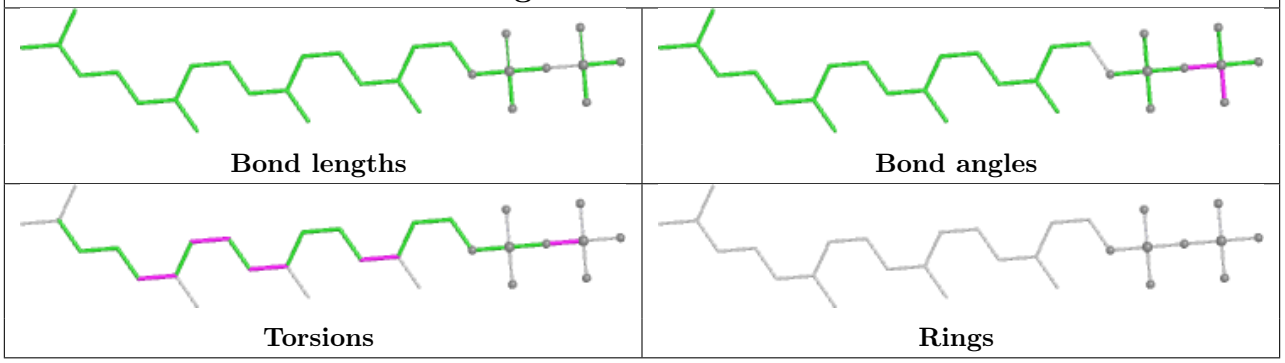
12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1108	GER	5	0
6	F	1503	GRG	2	0
6	D	1502	GRG	2	0
7	O	1308	GER	7	0
6	L	1506	GRG	2	0
6	J	1505	GRG	1	0
6	H	1504	GRG	1	0
7	N	1208	GER	6	0
6	B	1501	GRG	1	0
7	R	1608	GER	6	0
7	P	1408	GER	6	0
7	Q	1508	GER	4	0

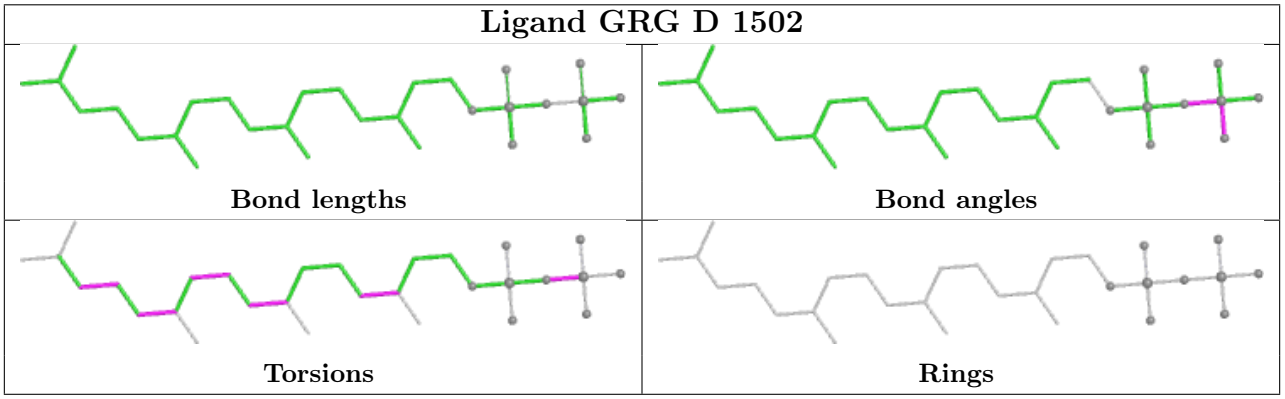
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



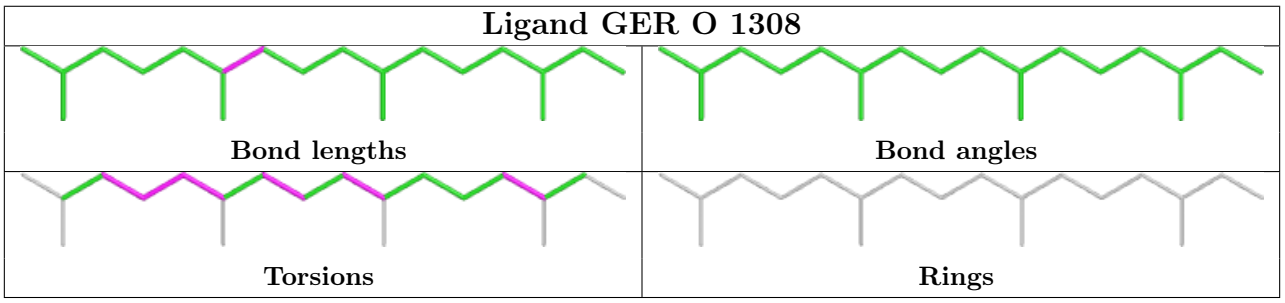
Ligand GRG F 1503



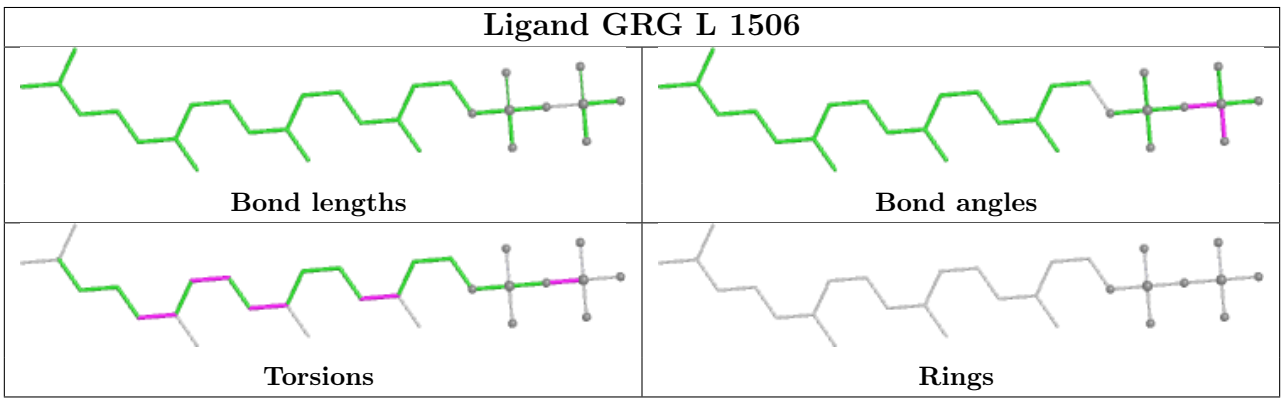
Ligand GRG D 1502



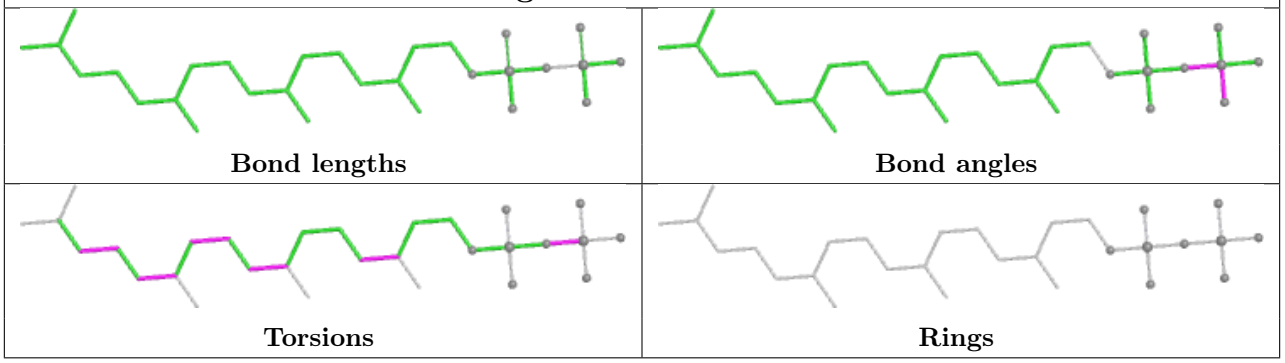
Ligand GER O 1308



Ligand GRG L 1506



Ligand GRG J 1505



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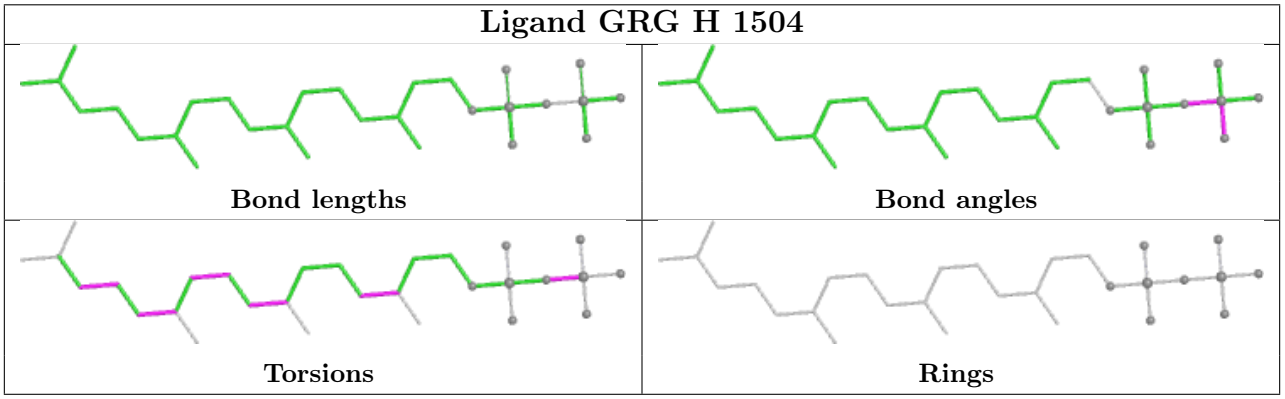
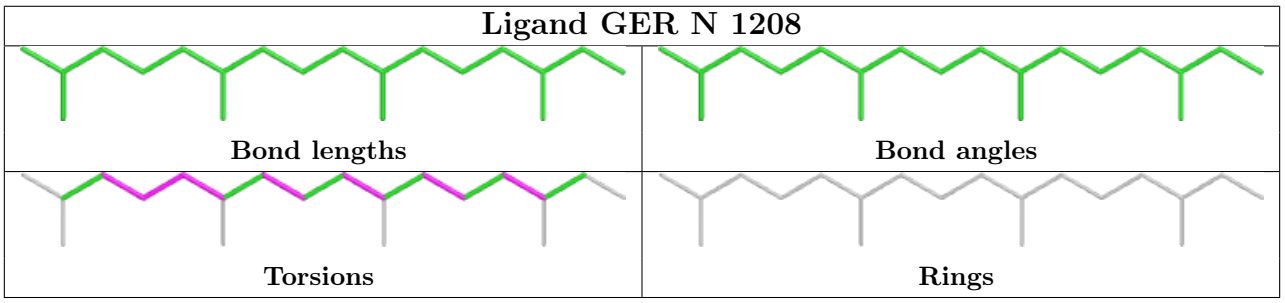


Ligand GER N 1208



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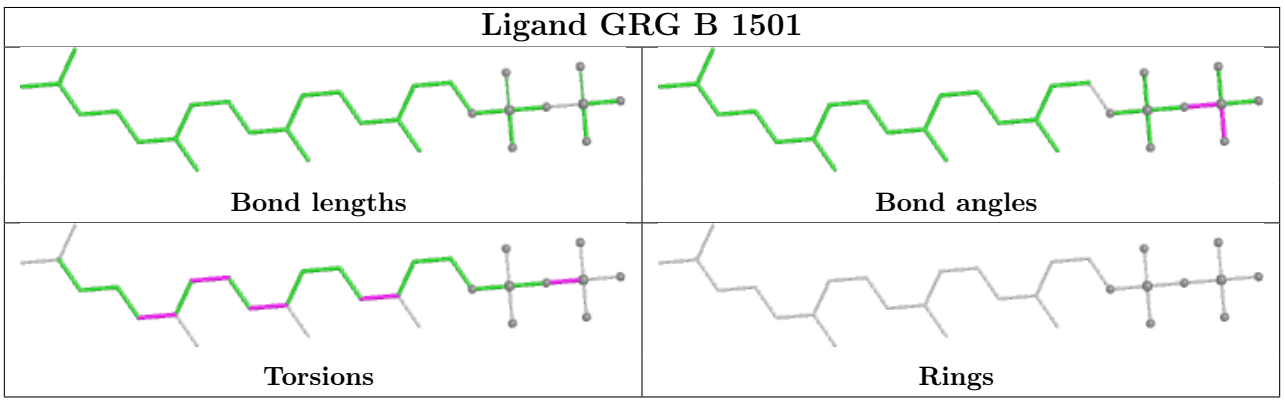

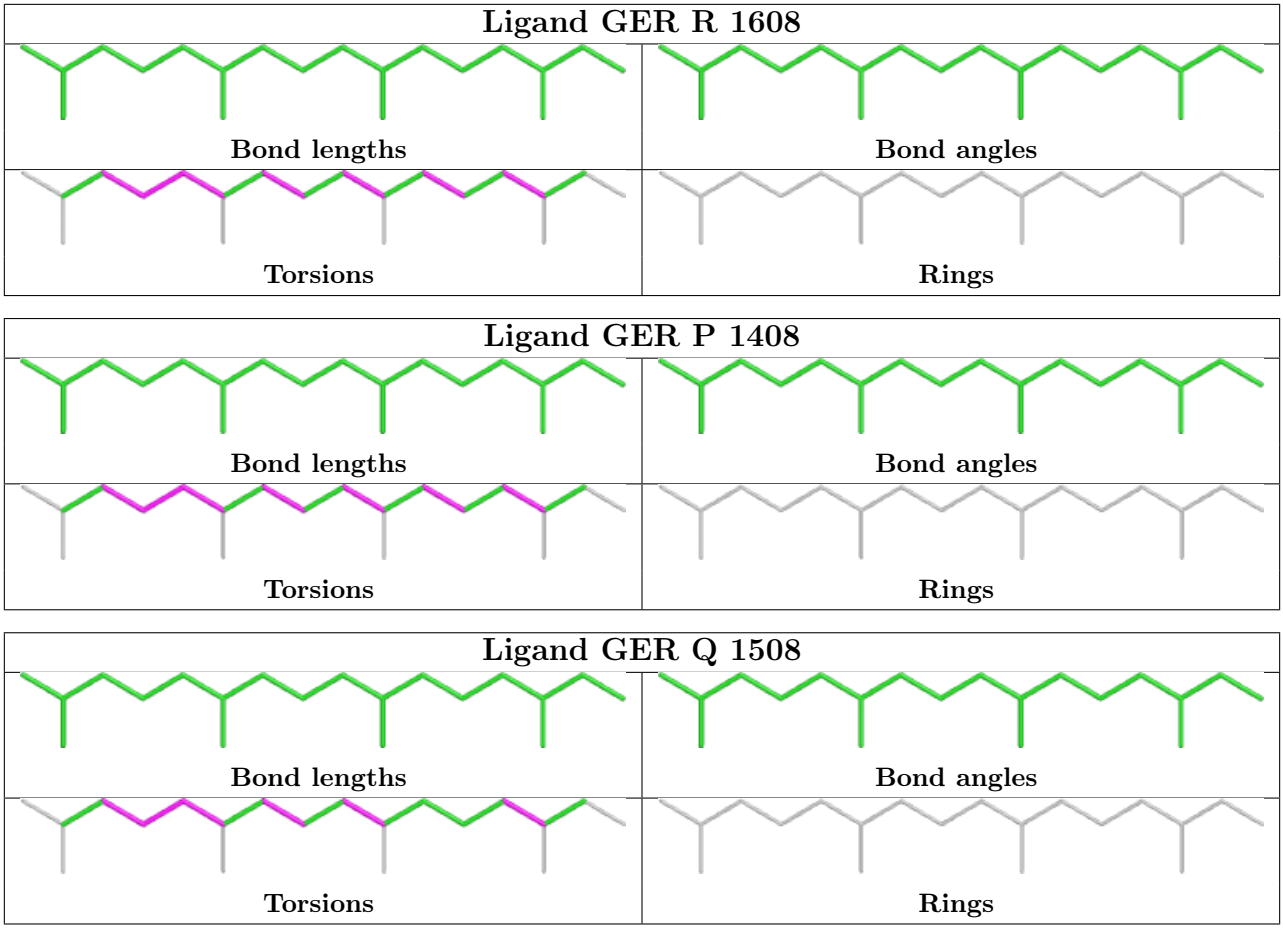

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	314/377 (83%)	0.24	15 (4%)	36	31	35, 57, 91, 109	0
1	C	314/377 (83%)	0.21	16 (5%)	34	29	33, 54, 82, 99	0
1	E	314/377 (83%)	0.36	13 (4%)	42	36	33, 58, 86, 104	0
1	G	314/377 (83%)	0.44	25 (7%)	20	16	36, 58, 88, 102	0
1	I	314/377 (83%)	0.14	11 (3%)	47	41	29, 53, 84, 95	0
1	K	314/377 (83%)	-0.30	5 (1%)	70	65	23, 43, 67, 82	0
2	B	346/377 (91%)	-0.06	12 (3%)	47	41	36, 51, 77, 102	0
2	D	346/377 (91%)	-0.19	11 (3%)	50	45	31, 47, 74, 94	0
2	F	346/377 (91%)	-0.15	16 (4%)	38	32	32, 47, 75, 100	0
2	H	346/377 (91%)	0.74	42 (12%)	10	8	37, 65, 95, 113	0
2	J	346/377 (91%)	0.04	16 (4%)	38	32	30, 50, 78, 104	0
2	L	346/377 (91%)	-0.40	9 (2%)	57	51	26, 41, 64, 95	0
3	M	4/11 (36%)	5.38	3 (75%)	0	0	45, 50, 55, 62	4 (100%)
3	N	4/11 (36%)	4.75	3 (75%)	0	0	47, 50, 55, 61	4 (100%)
3	O	4/11 (36%)	5.08	2 (50%)	0	0	43, 48, 53, 60	4 (100%)
3	P	4/11 (36%)	5.07	3 (75%)	0	0	43, 46, 50, 56	4 (100%)
3	Q	4/11 (36%)	3.43	2 (50%)	0	0	49, 54, 61, 69	4 (100%)
3	R	5/11 (45%)	3.53	3 (60%)	0	0	50, 54, 72, 73	5 (100%)
All	All	3985/4590 (86%)	0.11	207 (5%)	34	28	23, 52, 83, 113	25 (0%)

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	308	CYS	10.2
3	M	108	CYS	9.5
3	N	208	CYS	9.0

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Mol	Chain	Res	Type	RSRZ
3	P	408	CYS	9.0
3	M	109	VAL	7.8

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
7	GER	P	1408	20/20	0.73	0.51	72,78,81,82	20
7	GER	O	1308	20/20	0.76	0.47	71,78,83,83	20
7	GER	M	1108	20/20	0.76	0.49	69,76,83,84	20
7	GER	N	1208	20/20	0.77	0.44	67,76,84,84	20
7	GER	Q	1508	20/20	0.87	0.32	69,76,84,84	20
7	GER	R	1608	20/20	0.87	0.31	64,72,82,83	20
6	GRG	H	1504	29/29	0.93	0.16	61,65,75,77	0
6	GRG	B	1501	29/29	0.95	0.14	56,60,69,71	0
6	GRG	L	1506	29/29	0.95	0.12	40,45,53,58	0
6	GRG	D	1502	29/29	0.95	0.13	49,56,65,66	0
6	GRG	F	1503	29/29	0.95	0.13	50,58,70,71	0
6	GRG	J	1505	29/29	0.96	0.12	43,48,56,58	0
5	CL	H	1406	1/1	0.96	0.06	60,60,60,60	0
5	CL	J	1407	1/1	0.96	0.08	61,61,61,61	0
5	CL	C	1402	1/1	0.96	0.26	59,59,59,59	0
5	CL	B	1401	1/1	0.97	0.10	61,61,61,61	0
5	CL	D	1403	1/1	0.98	0.04	43,43,43,43	0
5	CL	G	1405	1/1	0.98	0.19	53,53,53,53	0
5	CL	F	1404	1/1	0.99	0.05	47,47,47,47	0
4	ZN	H	378	1/1	0.99	0.03	60,60,60,60	0
5	CL	K	1408	1/1	0.99	0.11	57,57,57,57	0

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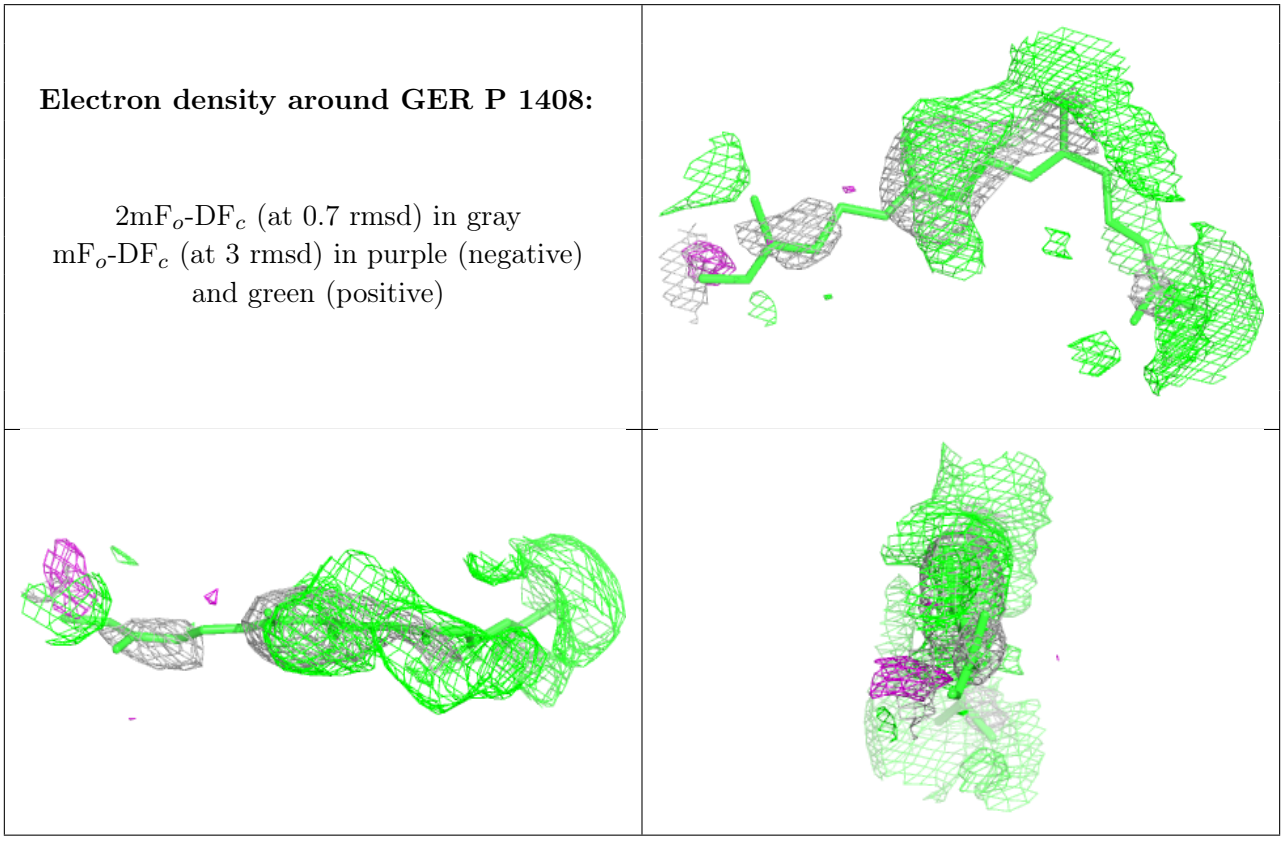
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	L	1409	1/1	0.99	0.04	45,45,45,45	0
4	ZN	F	378	1/1	1.00	0.03	47,47,47,47	0
4	ZN	B	378	1/1	1.00	0.02	47,47,47,47	0
4	ZN	J	378	1/1	1.00	0.02	42,42,42,42	0
4	ZN	L	378	1/1	1.00	0.01	34,34,34,34	0
4	ZN	D	378	1/1	1.00	0.01	45,45,45,45	0

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

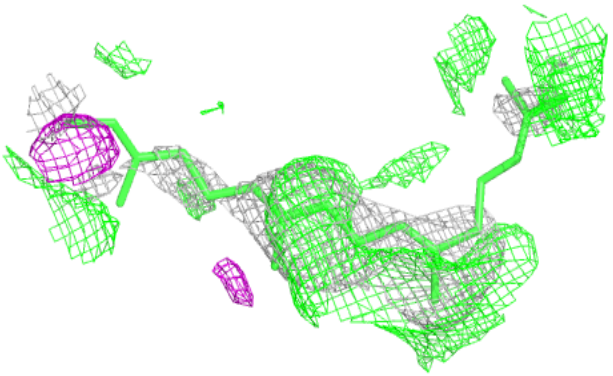
Electron density around GER P 1408:

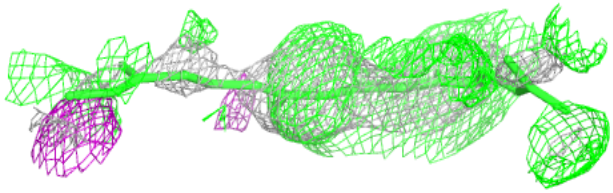
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

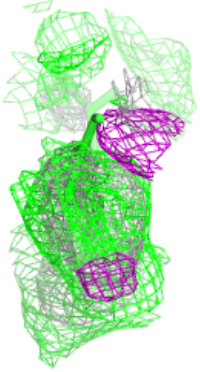


Electron density around GER O 1308:

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

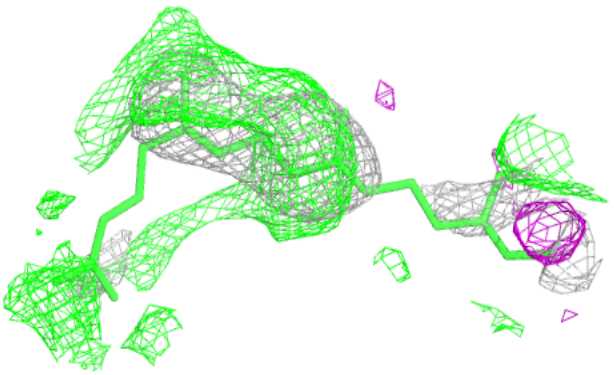


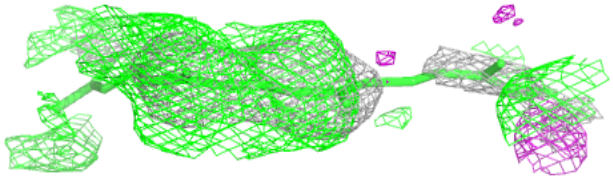


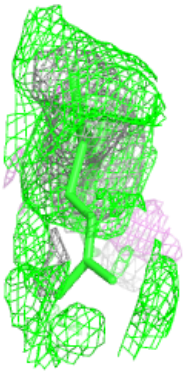


Electron density around GER M 1108:

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

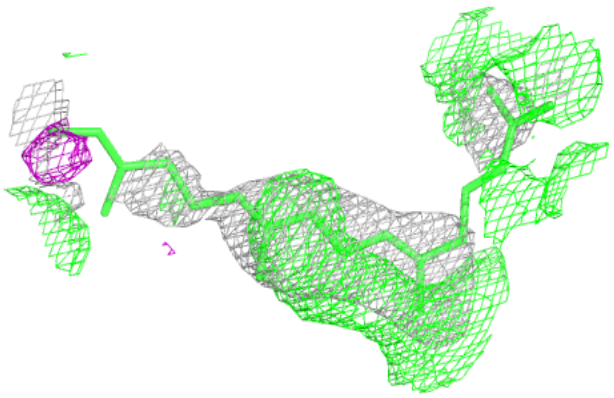


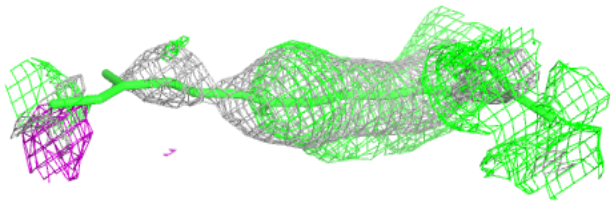


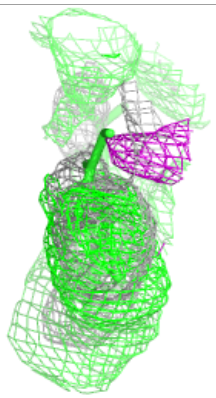


Electron density around GER N 1208:

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

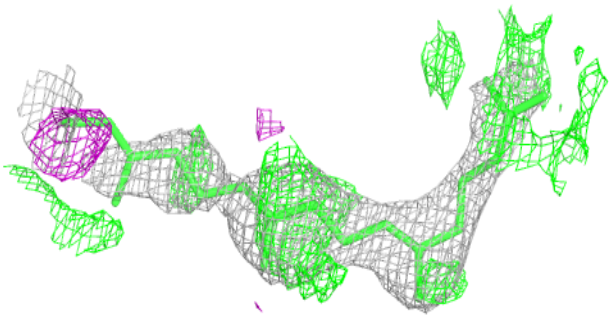


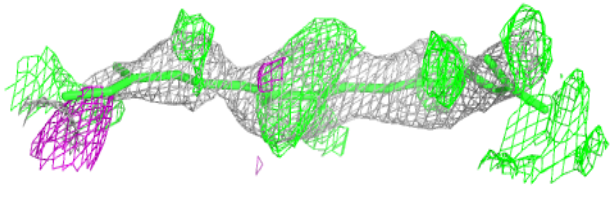


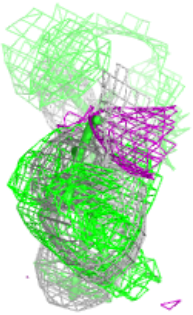


Electron density around GER Q 1508:

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

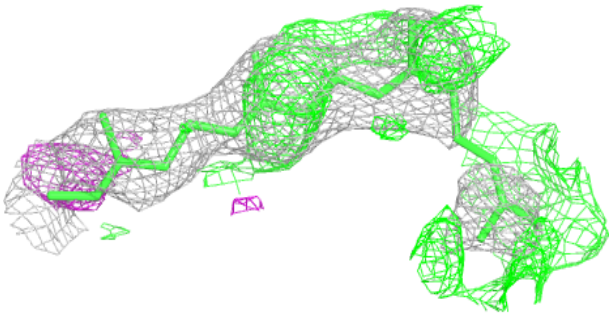


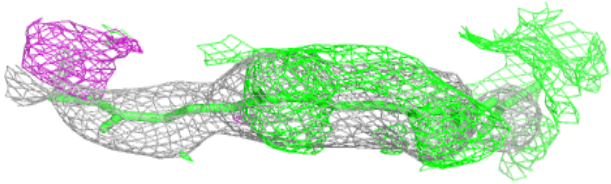


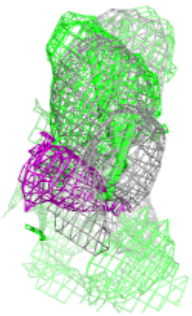


Electron density around GER R 1608:

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

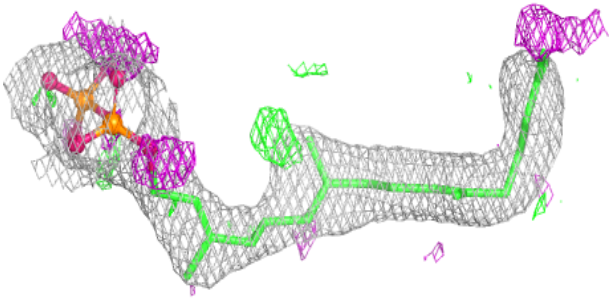


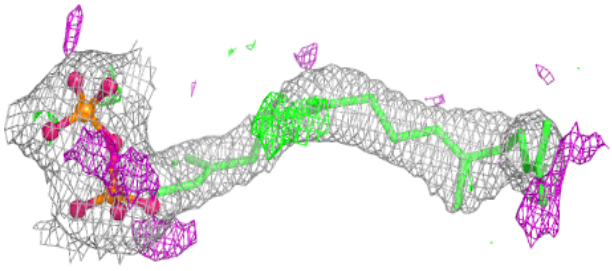


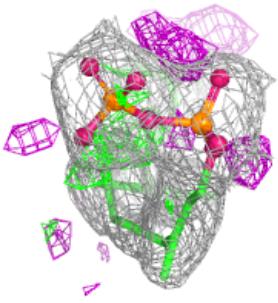


Electron density around GRG H 1504:

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

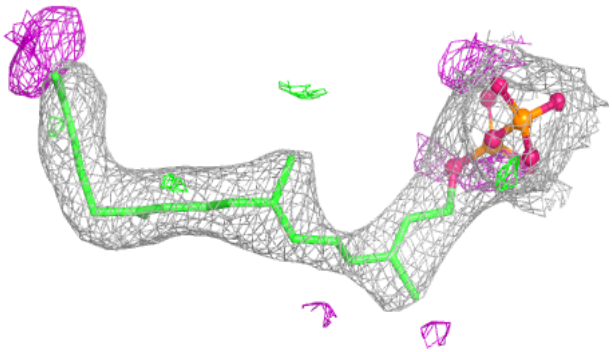


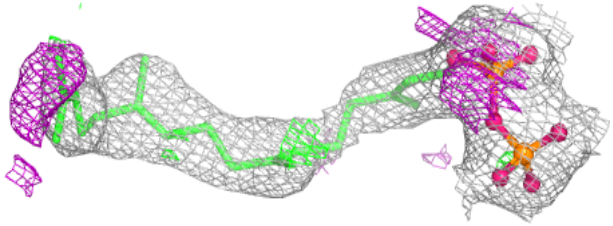


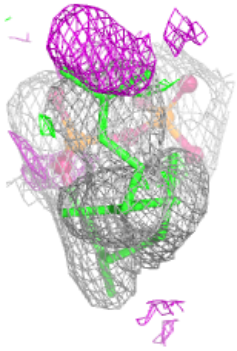


Electron density around GRG B 1501:

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

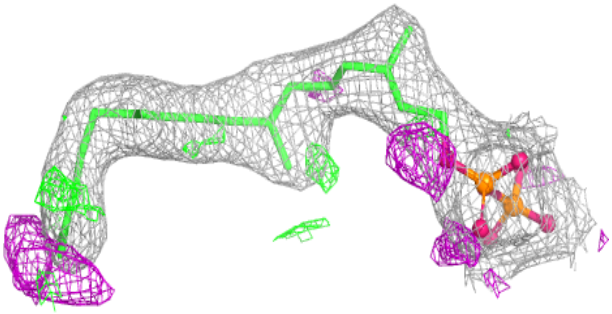


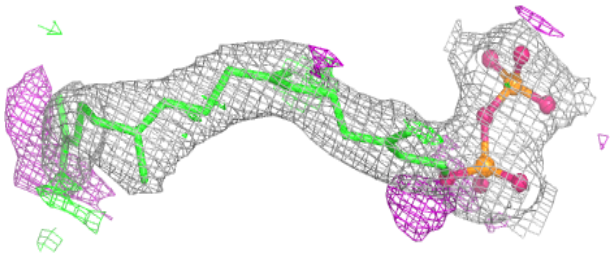


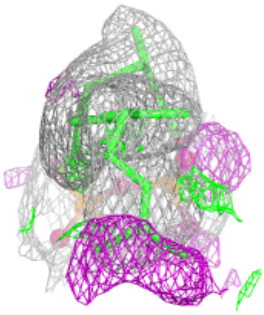


Electron density around GRG L 1506:

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

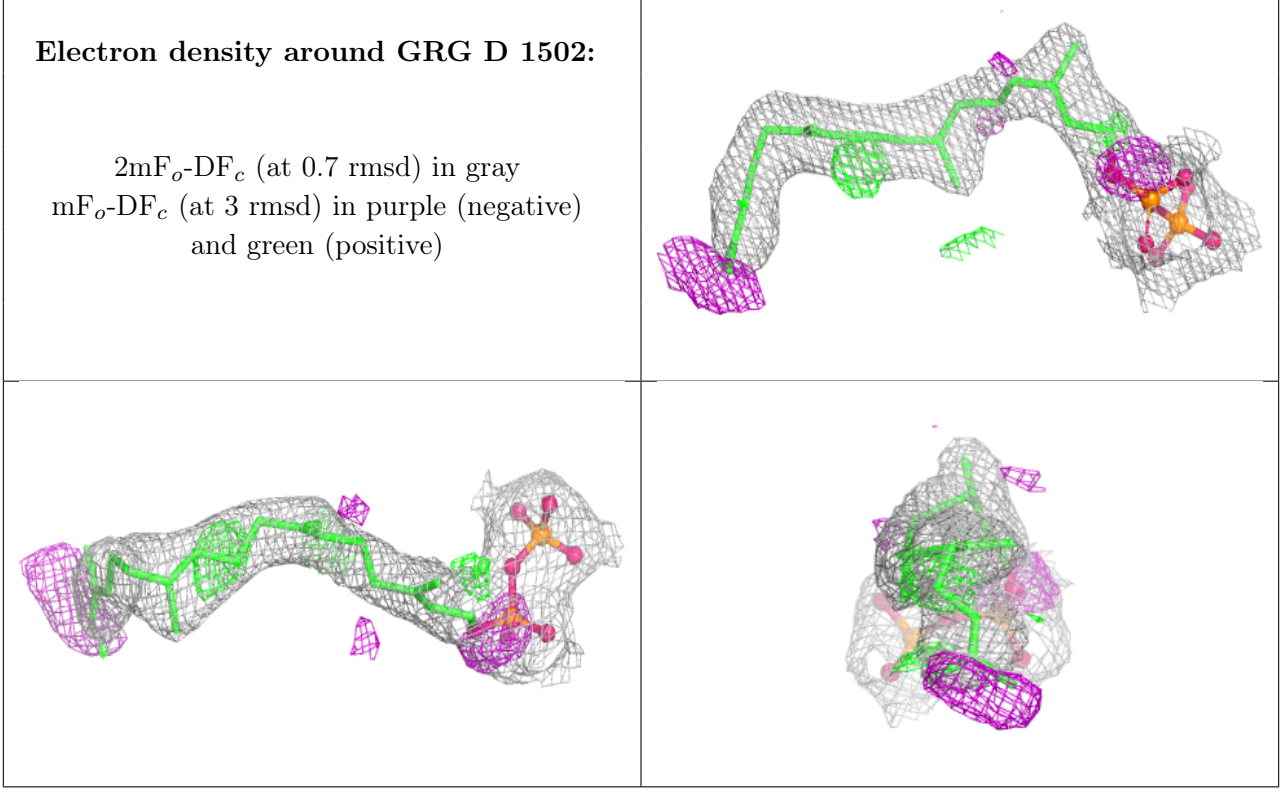






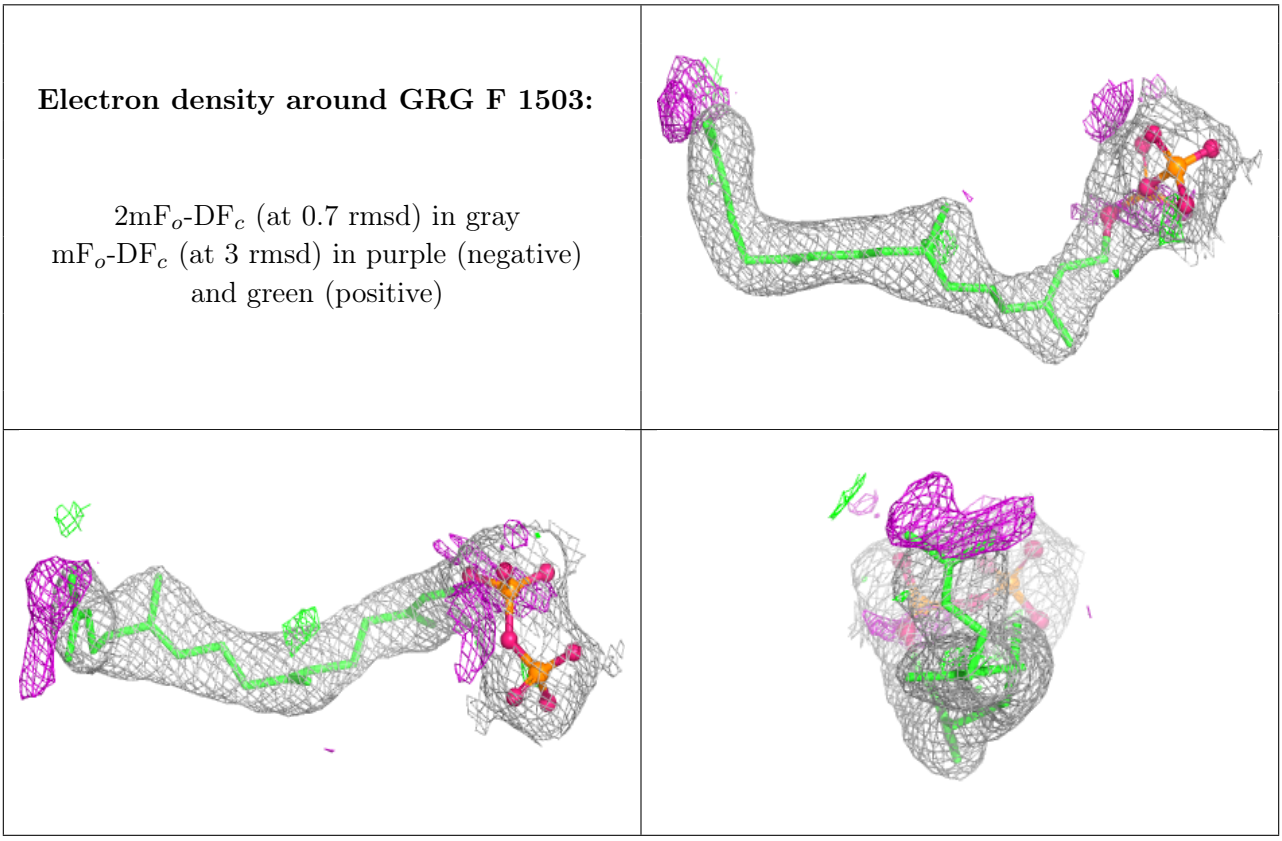
Electron density around GRG D 1502:

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



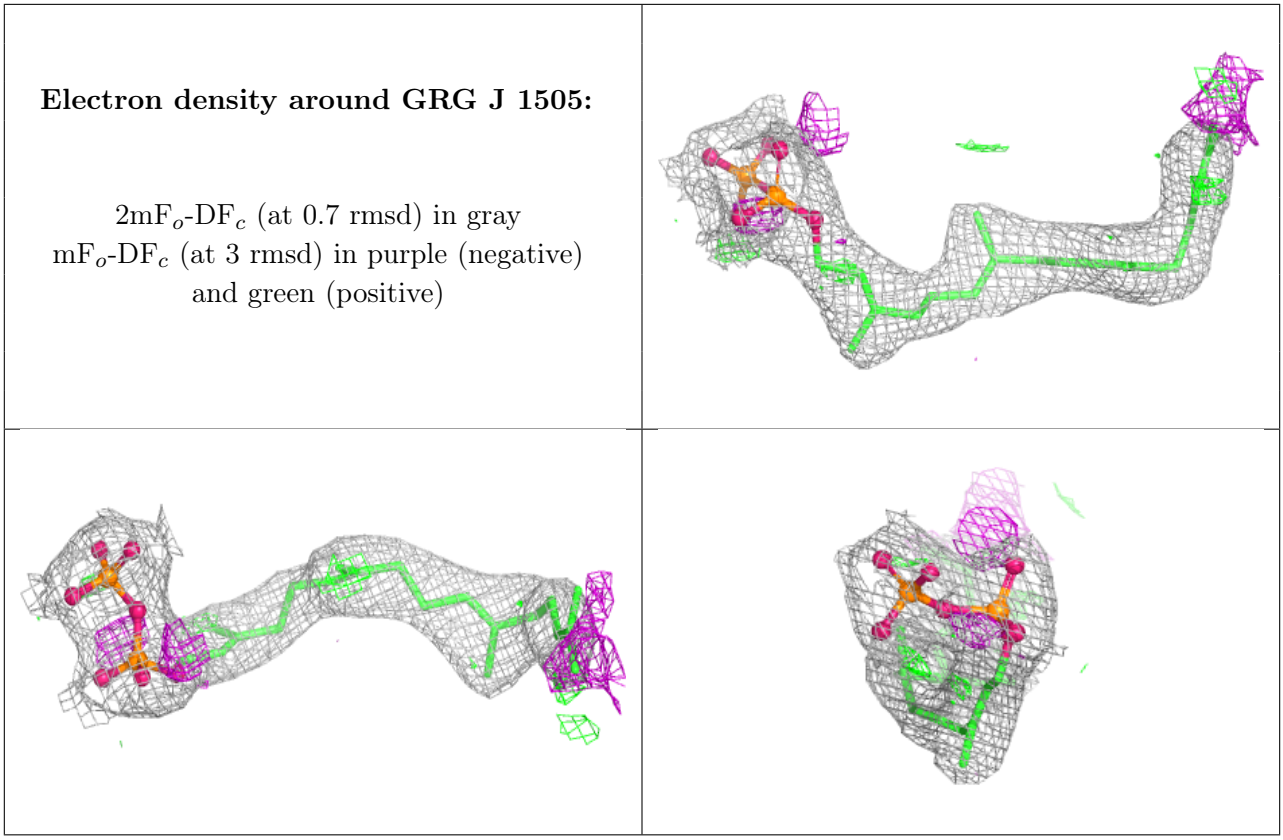
Electron density around GRG F 1503:

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



Electron density around GRG J 1505:

$2mF_o$-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.