



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 05:53 pm BST

PDB ID : 1N4S
Title : Protein Geranylgeranyltransferase type-I Complexed with GGPP and a Geranylgeranylated KKKSSTKCVIL 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

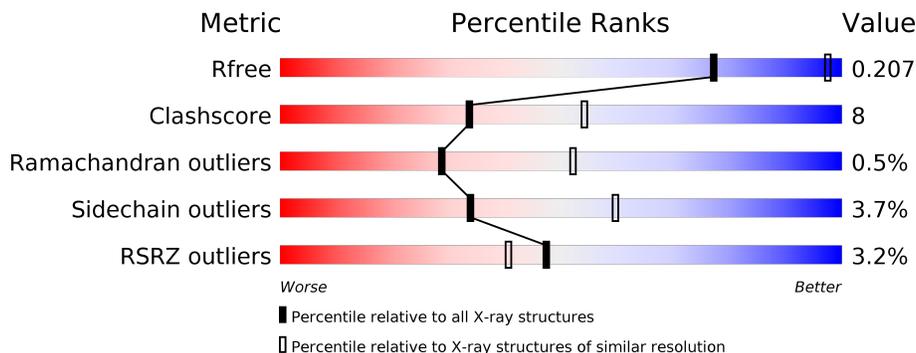
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	 2% 68% 14% 17%
1	C	377	 2% 67% 16% 17%
1	E	377	 2% 63% 19% 17%
1	G	377	 2% 66% 16% 17%
1	I	377	 2% 68% 15% 17%
1	K	377	 % 68% 15% 17%

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Mol	Chain	Length	Quality of chain
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
7	GER	Q	1508	-	-	-	X
7	GER	R	1608	-	-	-	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
			Total	C	N	O	S			
1	A	314	Total 2629	C 1679	N 463	O 482	S 5	0	0	0
1	C	314	Total 2643	C 1689	N 461	O 488	S 5	0	0	0
1	E	314	Total 2642	C 1686	N 461	O 490	S 5	0	0	0
1	G	314	Total 2633	C 1683	N 459	O 486	S 5	0	0	0
1	I	314	Total 2656	C 1694	N 465	O 492	S 5	0	0	0
1	K	314	Total 2671	C 1703	N 467	O 496	S 5	0	0	0

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

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

- Molecule 3 is a protein called 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	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

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

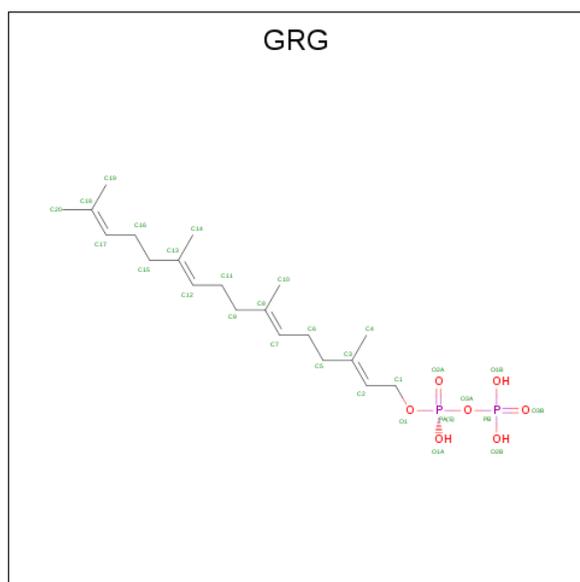
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		
5	J	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	K	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

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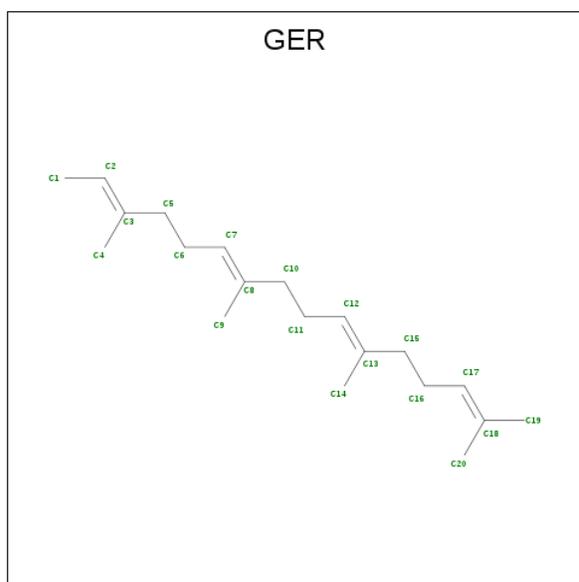
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0

- 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

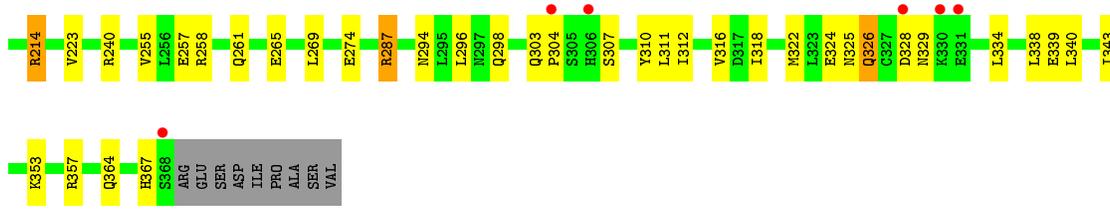
- Molecule 8 is water.

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

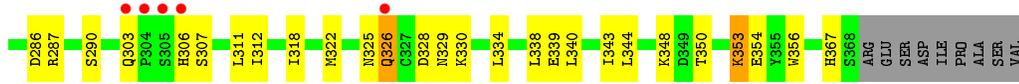
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	86	Total 86	O 86	0	0
8	H	56	Total 56	O 56	0	0
8	I	121	Total 121	O 121	0	0
8	J	88	Total 88	O 88	0	0
8	K	211	Total 211	O 211	0	0
8	L	157	Total 157	O 157	0	0
8	M	2	Total 2	O 2	0	0
8	N	2	Total 2	O 2	0	0
8	O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



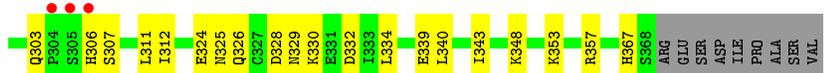
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



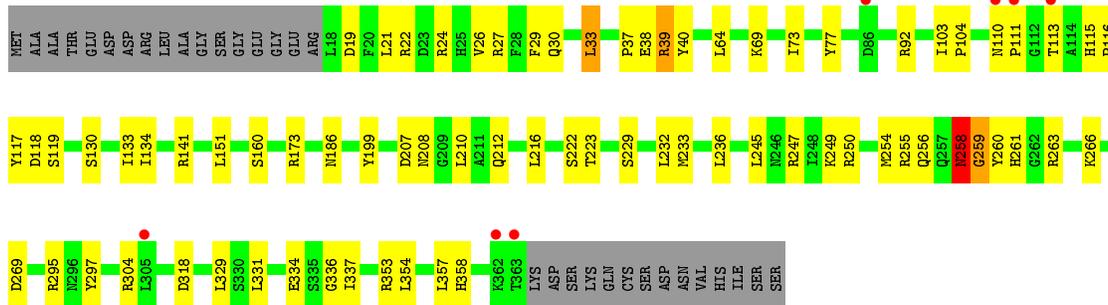
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



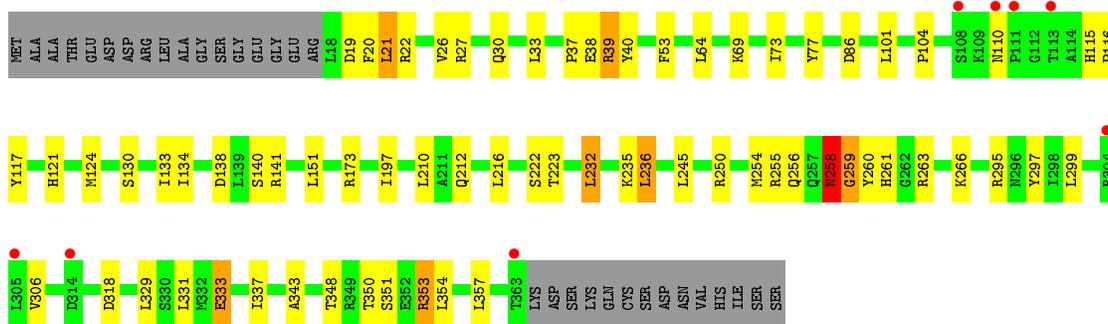
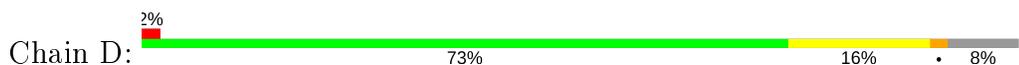
• Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



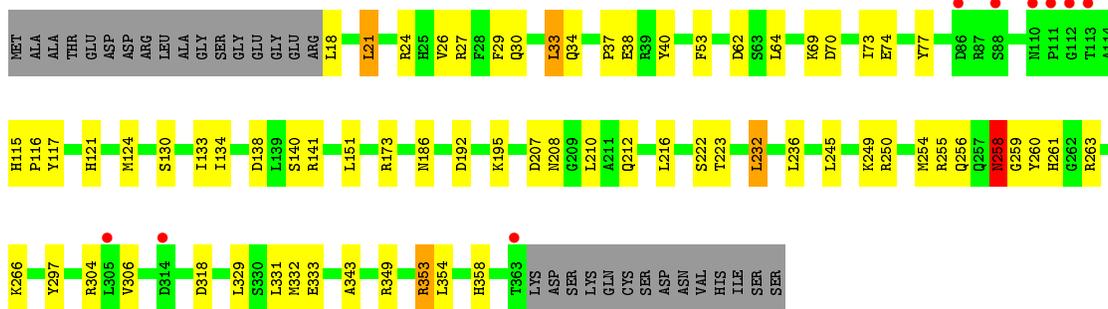
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta



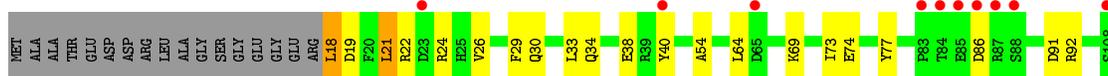
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

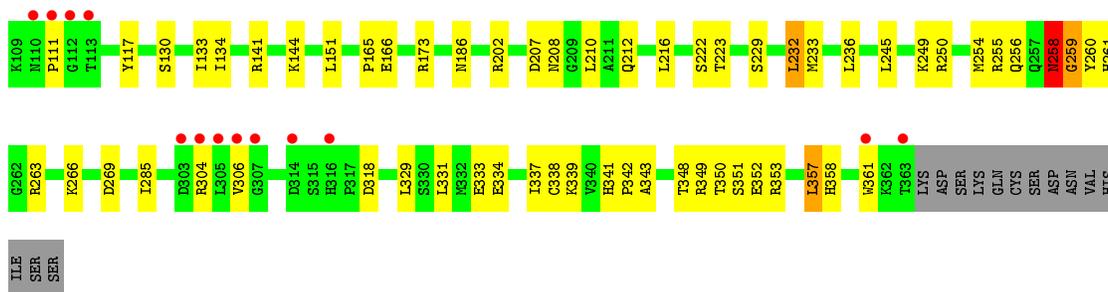


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

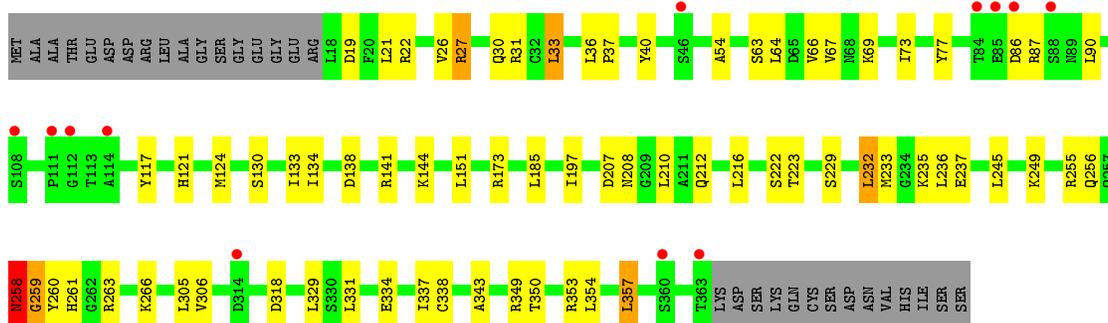


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

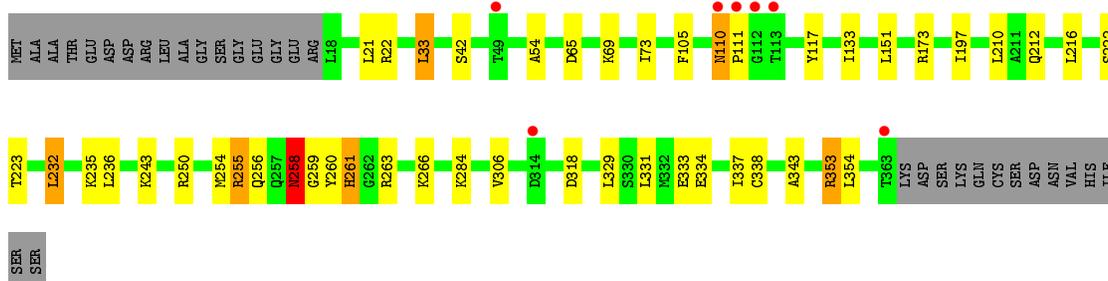
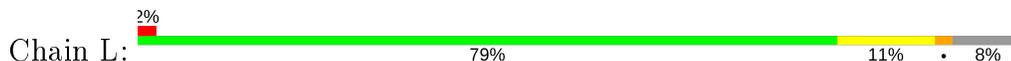




• Molecule 2: Geranylgeranyl transferase type-1 subunit beta



• Molecule 2: Geranylgeranyl transferase type-1 subunit beta



• 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



- 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

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 39.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.98-2.60) 99.7 (39.82-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.61Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.214 0.188 , 0.207	Depositor DCC
R_{free} test set	14968 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtrriage
Anisotropy	0.018	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.078 for -h-2*1,-k,l	Xtrriage
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

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GRG, ZN, CL, 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	0/2695	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(°)	Ideal(°)
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	1
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	1

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

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:433:HOH:O	8:I:433:HOH:O[2_657]	0.35	1.85

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%)	25 47
1	C	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	41 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	41	64
1	G	312/377 (83%)	294 (94%)	16 (5%)	2 (1%)	25	47
1	I	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	25	47
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	41	64
2	B	344/377 (91%)	334 (97%)	9 (3%)	1 (0%)	41	64
2	D	344/377 (91%)	333 (97%)	9 (3%)	2 (1%)	25	47
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	41	64
2	H	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	17	35
2	J	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	41	64
2	L	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	41	64
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%)	29	52

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%)	67	85
1	C	283/338 (84%)	273 (96%)	10 (4%)	36	62
1	E	284/338 (84%)	275 (97%)	9 (3%)	39	65
1	G	281/338 (83%)	277 (99%)	4 (1%)	67	85
1	I	287/338 (85%)	280 (98%)	7 (2%)	49	74
1	K	291/338 (86%)	283 (97%)	8 (3%)	44	71
2	B	289/326 (89%)	276 (96%)	13 (4%)	27	52
2	D	293/326 (90%)	277 (94%)	16 (6%)	21	43
2	F	294/326 (90%)	280 (95%)	14 (5%)	25	49
2	H	288/326 (88%)	274 (95%)	14 (5%)	25	48
2	J	292/326 (90%)	277 (95%)	15 (5%)	24	46
2	L	296/326 (91%)	280 (95%)	16 (5%)	22	44
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%)	34	60

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

Mol	Chain	Res	Type
2	F	236	LEU
2	H	91	ASP
2	L	232	LEU
2	F	258	ASN
1	G	71	GLU

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

Mol	Chain	Res	Type
2	F	212	GLN
1	G	153	ASN
1	K	201	HIS
2	F	246	ASN

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Mol	Chain	Res	Type
1	G	80	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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$
6	GRG	D	1502	-	26,28,28	0.80	0	33,37,37	0.82	1 (3%)
7	GER	M	1108	3	19,19,19	0.92	0	22,22,22	0.67	0
6	GRG	H	1504	-	26,28,28	0.77	0	33,37,37	0.83	1 (3%)
6	GRG	F	1503	-	26,28,28	0.77	0	33,37,37	0.82	1 (3%)
7	GER	Q	1508	3	19,19,19	0.89	0	22,22,22	0.67	0
7	GER	P	1408	3	19,19,19	0.92	0	22,22,22	0.64	0
6	GRG	J	1505	-	26,28,28	0.77	0	33,37,37	0.81	1 (3%)
7	GER	N	1208	3	19,19,19	0.91	0	22,22,22	0.66	0
6	GRG	B	1501	-	26,28,28	0.77	0	33,37,37	0.83	1 (3%)
6	GRG	L	1506	-	26,28,28	0.73	0	33,37,37	0.85	1 (3%)
7	GER	R	1608	3	19,19,19	0.91	0	22,22,22	0.69	0
7	GER	O	1308	3	19,19,19	0.93	0	22,22,22	0.67	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
6	GRG	D	1502	-	-	8/31/31/31	-
7	GER	M	1108	3	-	9/20/20/20	-
6	GRG	H	1504	-	-	8/31/31/31	-
6	GRG	F	1503	-	-	6/31/31/31	-
7	GER	Q	1508	3	-	9/20/20/20	-
7	GER	P	1408	3	-	10/20/20/20	-
6	GRG	J	1505	-	-	8/31/31/31	-
7	GER	N	1208	3	-	10/20/20/20	-
6	GRG	B	1501	-	-	8/31/31/31	-
6	GRG	L	1506	-	-	7/31/31/31	-
7	GER	R	1608	3	-	10/20/20/20	-
7	GER	O	1308	3	-	9/20/20/20	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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 102 torsion outliers are listed below:

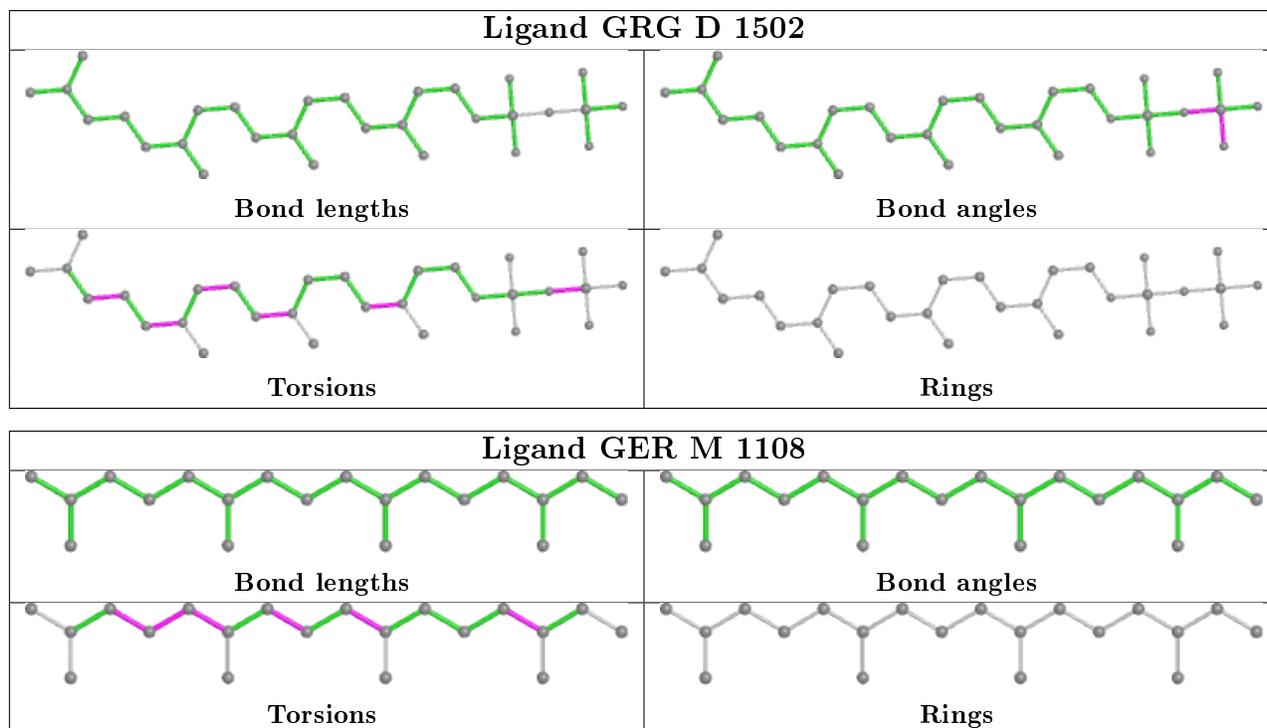
Mol	Chain	Res	Type	Atoms
6	F	1503	GRG	PA-O3A-PB-O1B
7	Q	1508	GER	C11-C10-C8-C7
7	Q	1508	GER	C11-C10-C8-C9
7	P	1408	GER	C11-C10-C8-C7
7	P	1408	GER	C11-C10-C8-C9

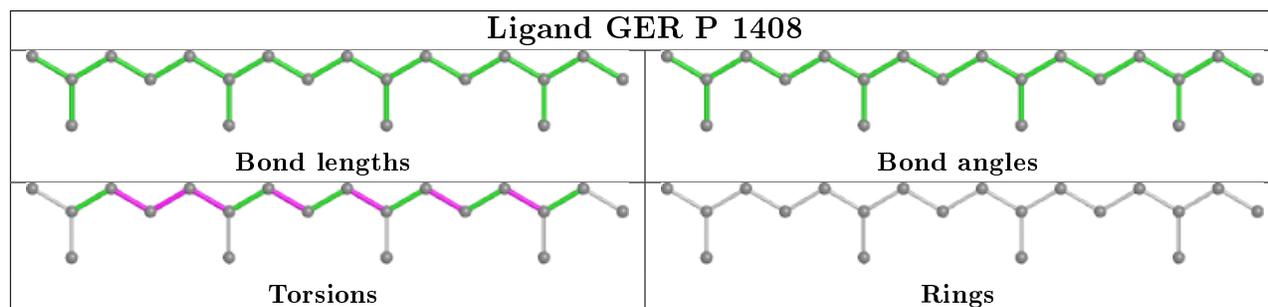
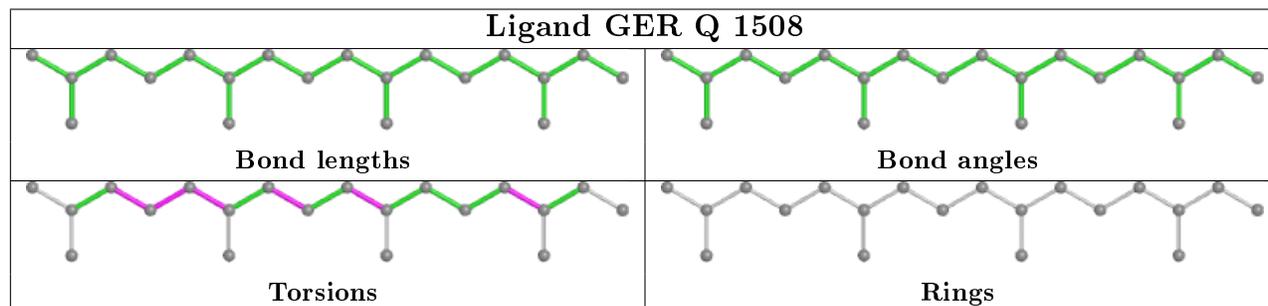
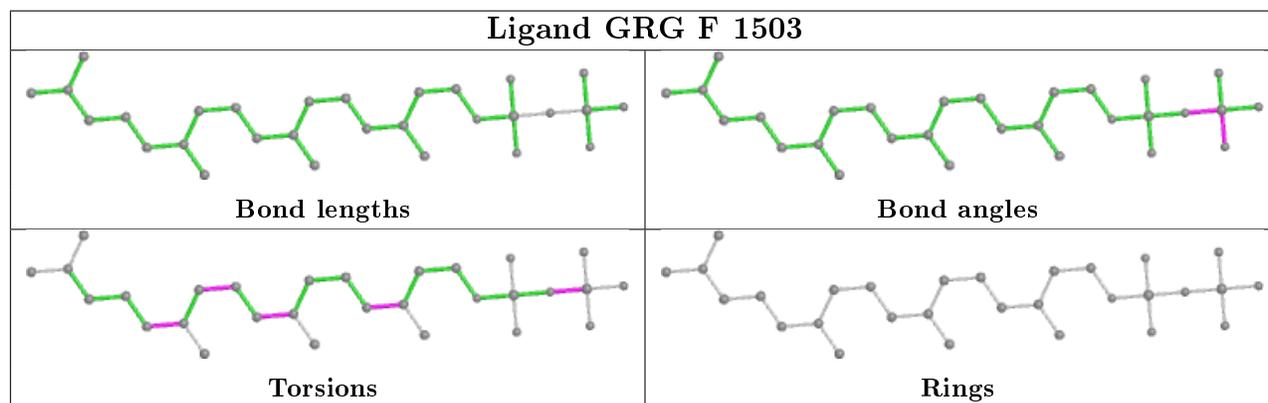
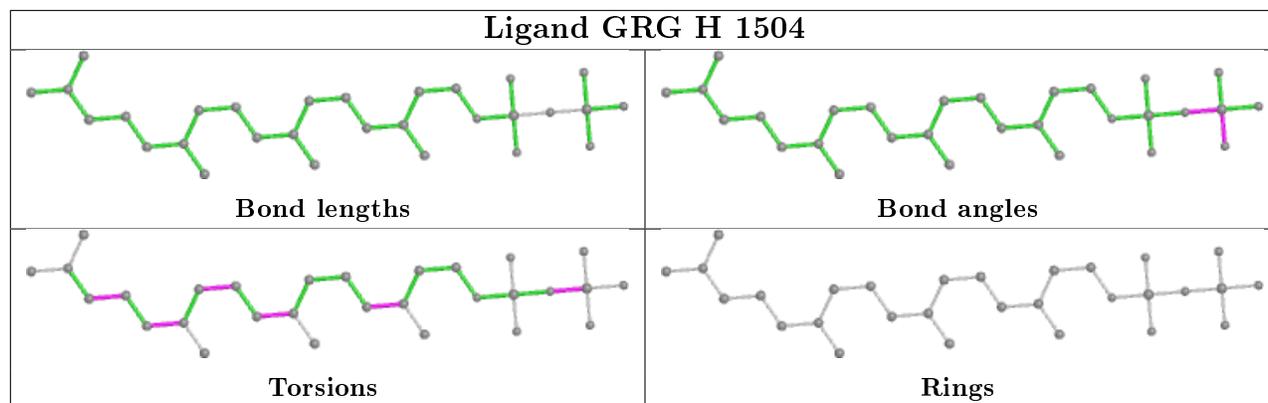
There are no ring outliers.

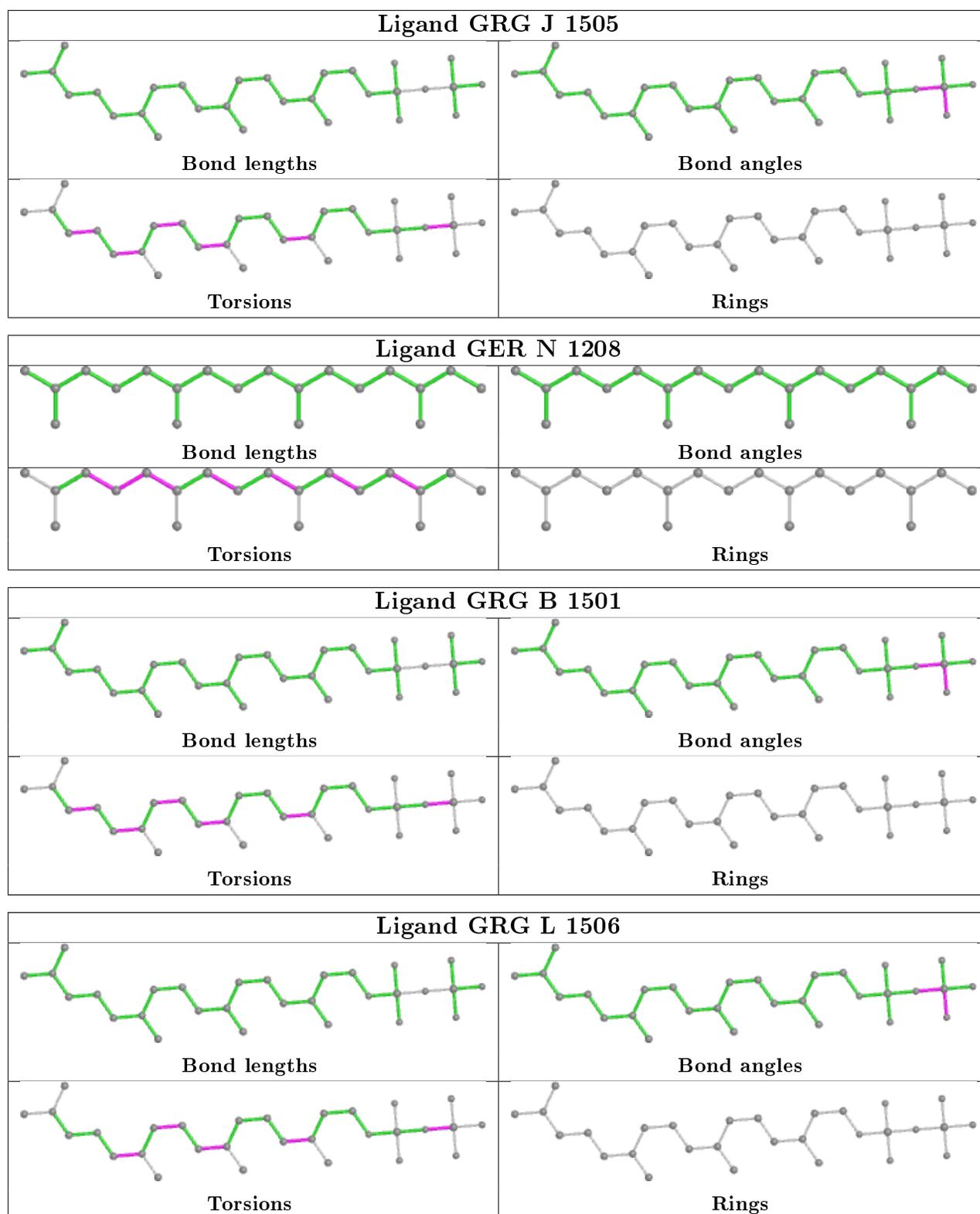
12 monomers are involved in 43 short contacts:

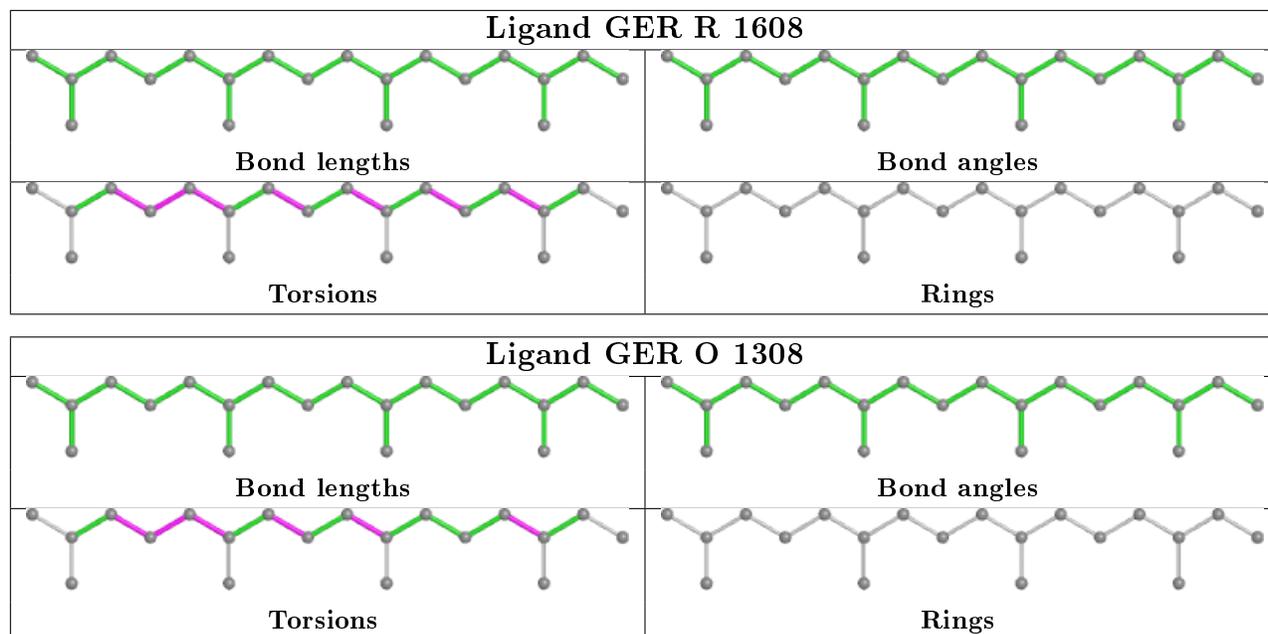
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1502	GRG	2	0
7	M	1108	GER	5	0
6	H	1504	GRG	1	0
6	F	1503	GRG	2	0
7	Q	1508	GER	4	0
7	P	1408	GER	6	0
6	J	1505	GRG	1	0
7	N	1208	GER	6	0
6	B	1501	GRG	1	0
6	L	1506	GRG	2	0
7	R	1608	GER	6	0
7	O	1308	GER	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.10	8 (2%) 57 51	35, 57, 91, 109	0
1	C	314/377 (83%)	-0.14	6 (1%) 66 62	33, 54, 82, 99	0
1	E	314/377 (83%)	-0.03	7 (2%) 62 56	33, 58, 86, 104	0
1	G	314/377 (83%)	-0.01	7 (2%) 62 56	36, 58, 88, 102	0
1	I	314/377 (83%)	-0.18	6 (1%) 66 62	29, 53, 84, 95	0
1	K	314/377 (83%)	-0.38	3 (0%) 82 80	23, 43, 67, 82	0
2	B	346/377 (91%)	-0.13	7 (2%) 65 60	36, 51, 77, 102	0
2	D	346/377 (91%)	-0.01	8 (2%) 60 54	31, 47, 74, 94	0
2	F	346/377 (91%)	-0.16	9 (2%) 56 50	32, 47, 75, 100	0
2	H	346/377 (91%)	0.34	23 (6%) 18 13	37, 65, 95, 113	0
2	J	346/377 (91%)	0.02	12 (3%) 44 36	30, 50, 78, 104	0
2	L	346/377 (91%)	-0.13	7 (2%) 65 60	26, 41, 64, 95	0
3	M	4/11 (36%)	6.70	4 (100%) 0 0	58, 64, 70, 80	4 (100%)
3	N	4/11 (36%)	6.17	4 (100%) 0 0	60, 64, 71, 78	4 (100%)
3	O	4/11 (36%)	7.91	4 (100%) 0 0	58, 64, 70, 80	4 (100%)
3	P	4/11 (36%)	6.15	4 (100%) 0 0	60, 64, 70, 78	4 (100%)
3	Q	4/11 (36%)	5.20	4 (100%) 0 0	58, 63, 72, 81	4 (100%)
3	R	5/11 (45%)	3.41	5 (100%) 0 0	57, 62, 83, 84	5 (100%)
All	All	3985/4590 (86%)	-0.04	128 (3%) 47 40	23, 52, 84, 113	25 (0%)

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	308	CYS	11.4
3	M	108	CYS	10.1
3	N	208	CYS	8.0

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Mol	Chain	Res	Type	RSRZ
3	M	109	VAL	7.6
3	O	310	ILE	7.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

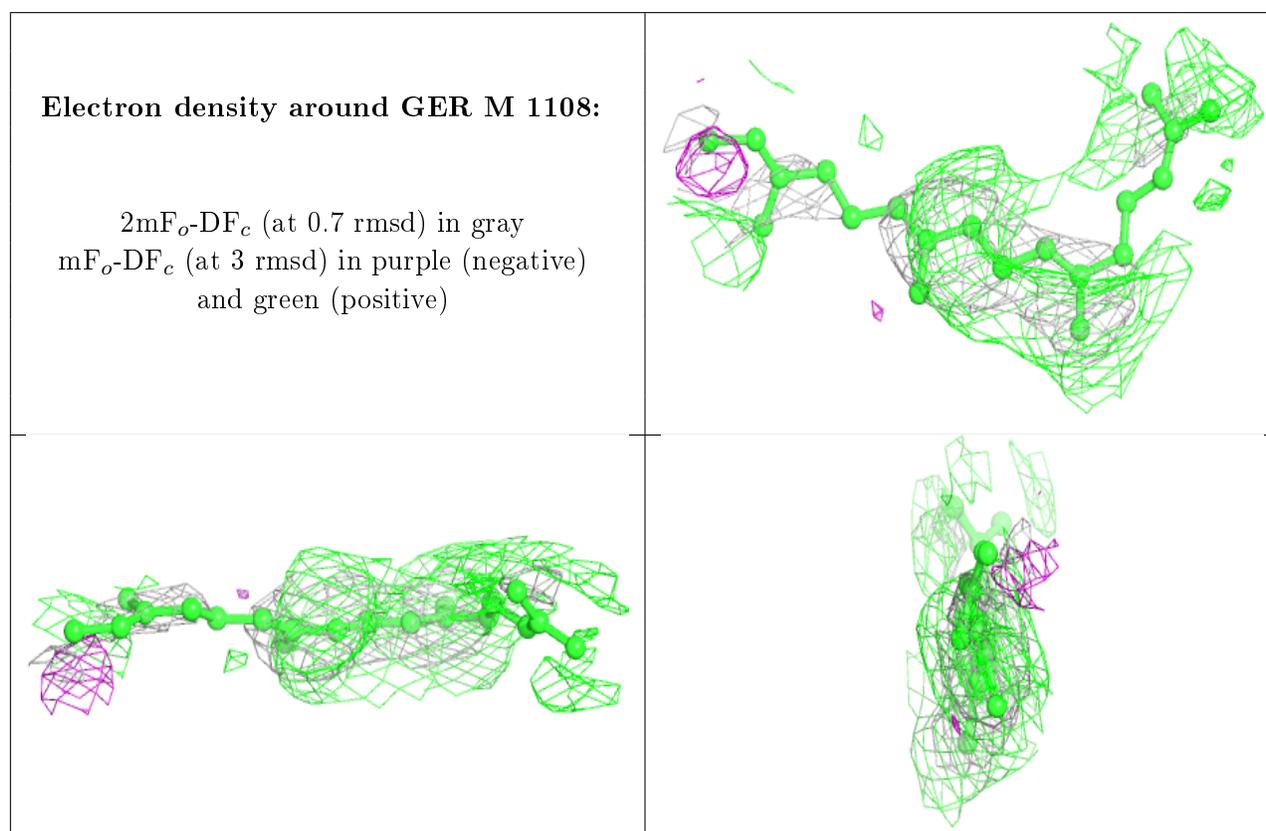
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GER	M	1108	20/20	0.50	0.58	69,76,83,84	20
7	GER	P	1408	20/20	0.52	0.57	72,78,81,82	20
7	GER	O	1308	20/20	0.54	0.56	71,78,83,83	20
7	GER	N	1208	20/20	0.62	0.51	67,76,84,84	20
7	GER	Q	1508	20/20	0.71	0.47	69,76,84,84	20
7	GER	R	1608	20/20	0.72	0.51	64,72,82,83	20
6	GRG	H	1504	29/29	0.94	0.27	61,65,75,77	0
6	GRG	D	1502	29/29	0.94	0.27	49,56,65,66	0
6	GRG	J	1505	29/29	0.95	0.25	43,48,56,58	0
6	GRG	F	1503	29/29	0.95	0.27	50,58,70,71	0
6	GRG	L	1506	29/29	0.95	0.26	40,45,53,58	0
6	GRG	B	1501	29/29	0.95	0.27	56,60,69,71	0
5	CL	J	1407	1/1	0.95	0.12	61,61,61,61	0
5	CL	H	1406	1/1	0.96	0.13	60,60,60,60	0
5	CL	G	1405	1/1	0.96	0.21	53,53,53,53	0
5	CL	C	1402	1/1	0.97	0.25	59,59,59,59	0
5	CL	K	1408	1/1	0.98	0.16	57,57,57,57	0
5	CL	B	1401	1/1	0.98	0.13	61,61,61,61	0
4	ZN	J	378	1/1	0.99	0.14	42,42,42,42	0
5	CL	F	1404	1/1	0.99	0.13	47,47,47,47	0
4	ZN	H	378	1/1	0.99	0.11	60,60,60,60	0

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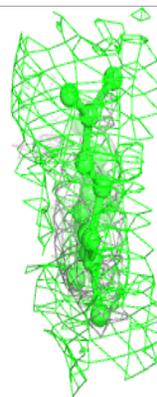
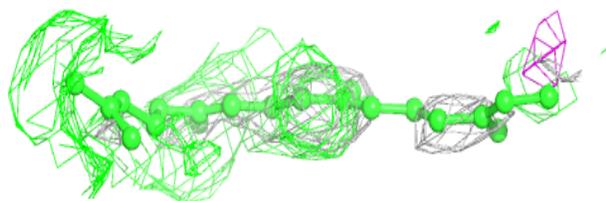
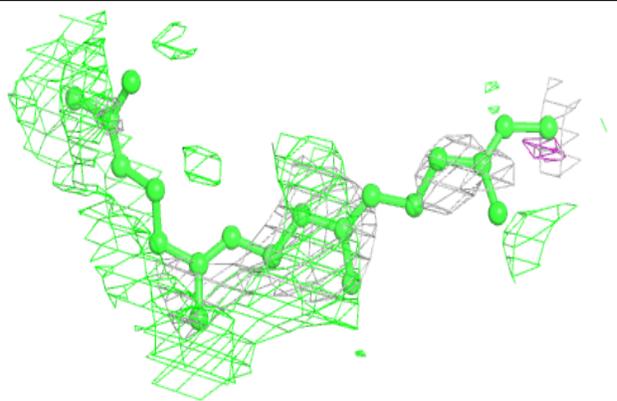
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	D	1403	1/1	0.99	0.13	43,43,43,43	0
5	CL	L	1409	1/1	0.99	0.07	45,45,45,45	0
4	ZN	D	378	1/1	1.00	0.14	45,45,45,45	0
4	ZN	F	378	1/1	1.00	0.10	47,47,47,47	0
4	ZN	B	378	1/1	1.00	0.11	47,47,47,47	0
4	ZN	L	378	1/1	1.00	0.12	34,34,34,34	0

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.

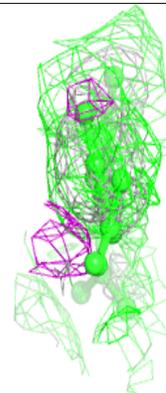
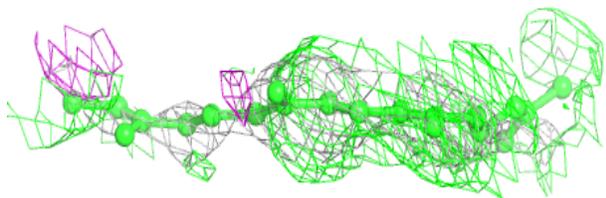
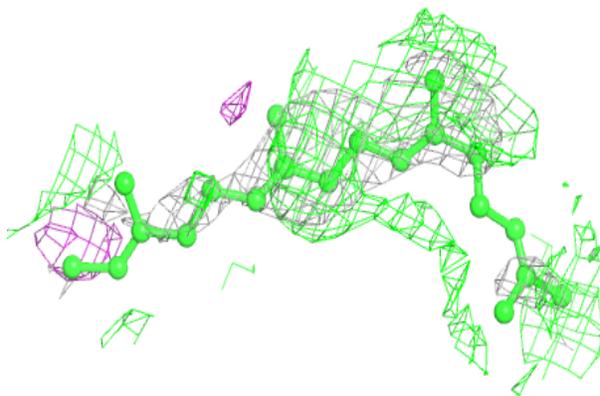


Electron density around GER P 1408:

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

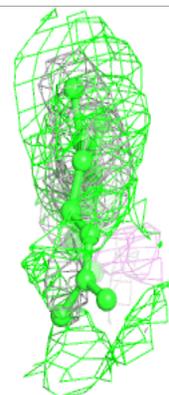
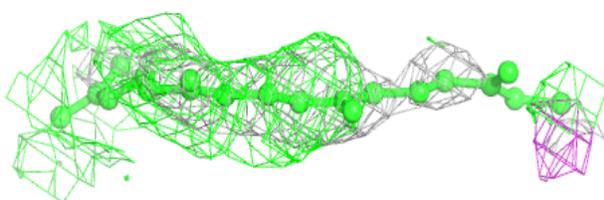
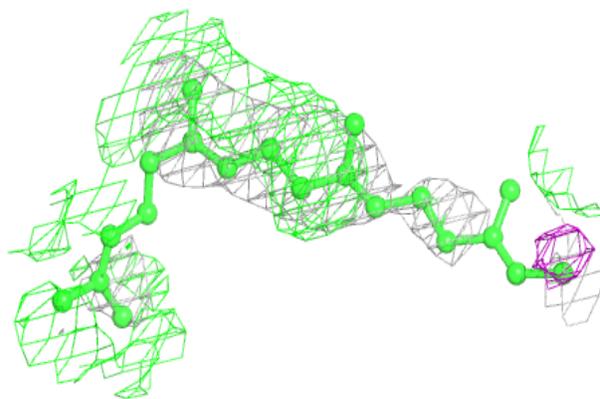
**Electron density around GER O 1308:**

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

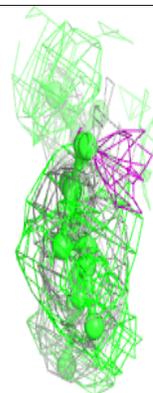
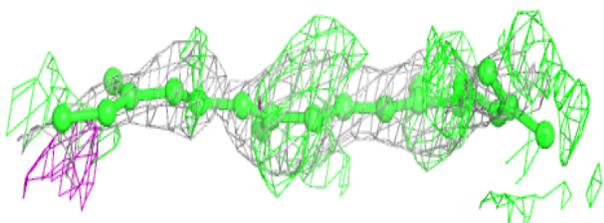
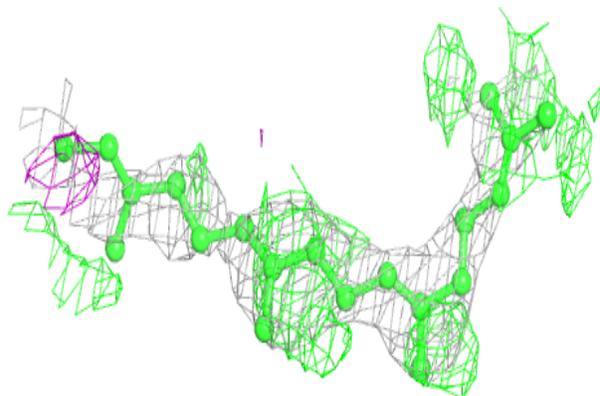


Electron density around GER N 1208:

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

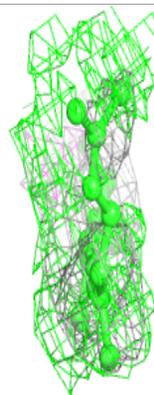
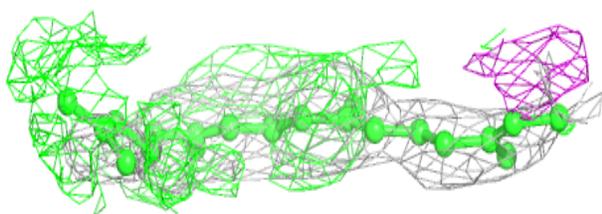
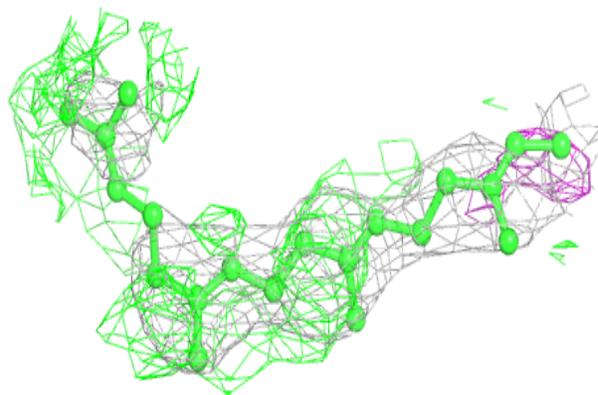
**Electron density around GER Q 1508:**

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

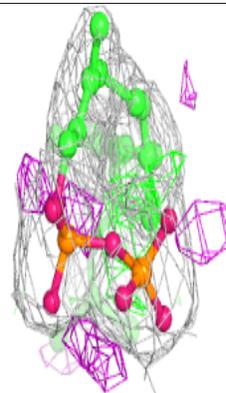
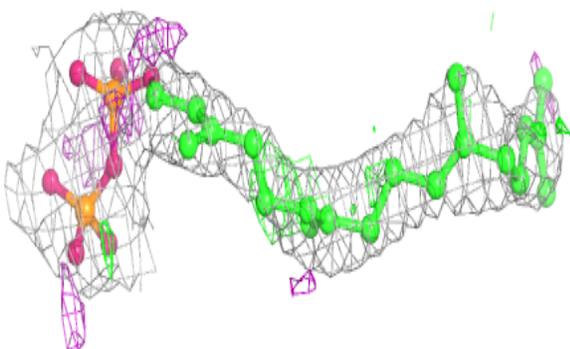
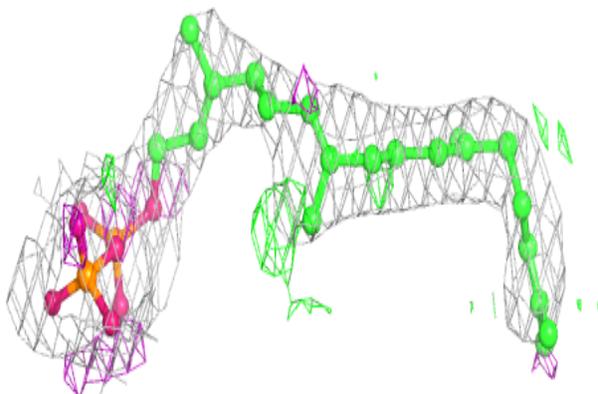


Electron density around GER R 1608:

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

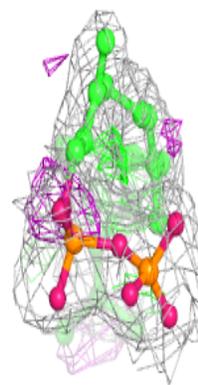
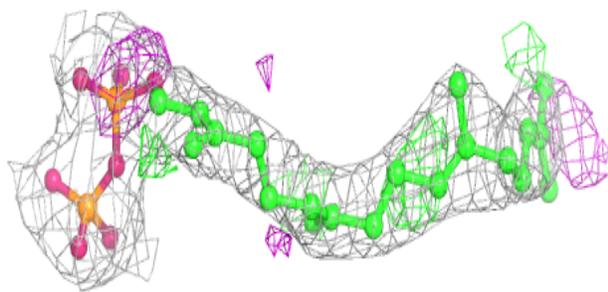
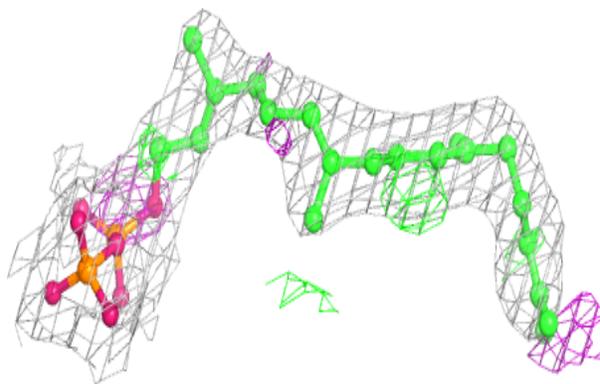
**Electron density around GRG H 1504:**

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

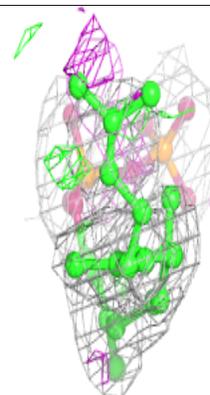
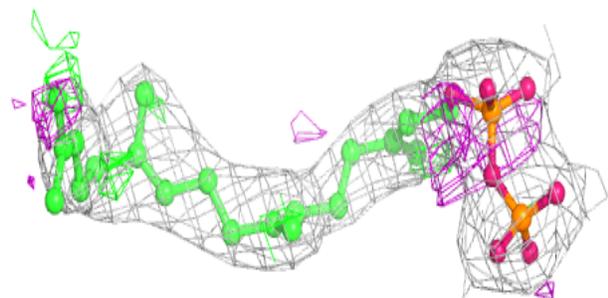
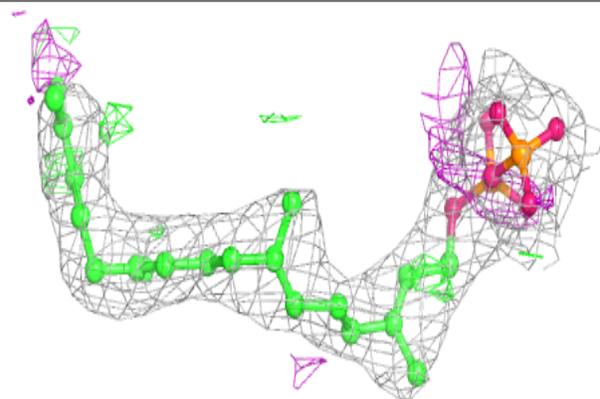


Electron density around GRG D 1502:

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

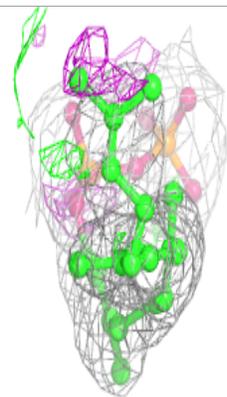
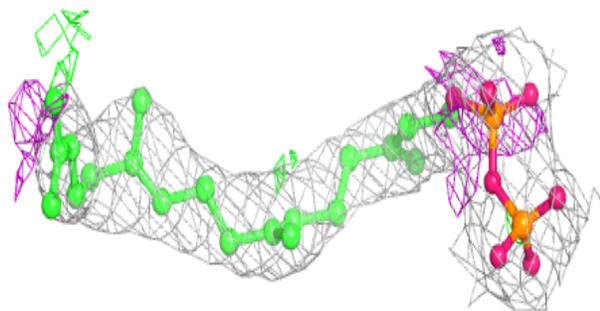
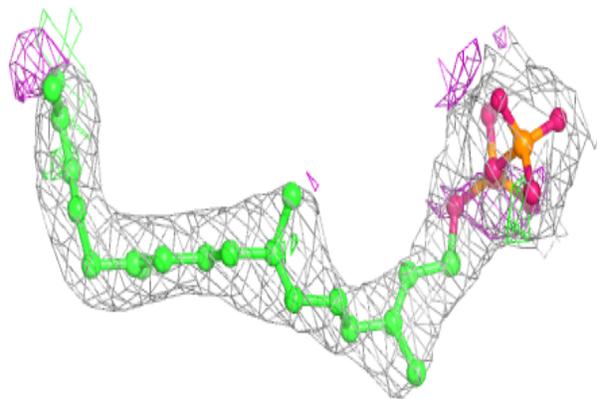
**Electron density around GRG J 1505:**

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

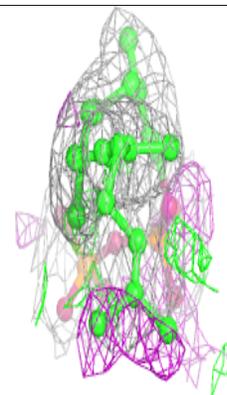
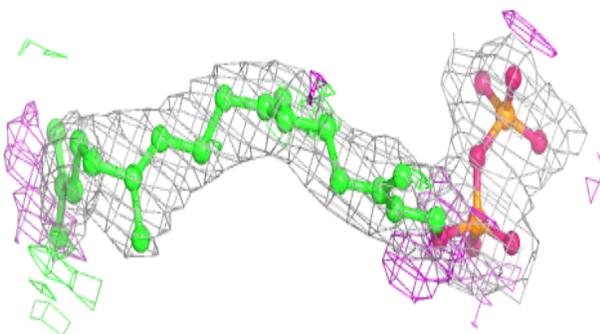
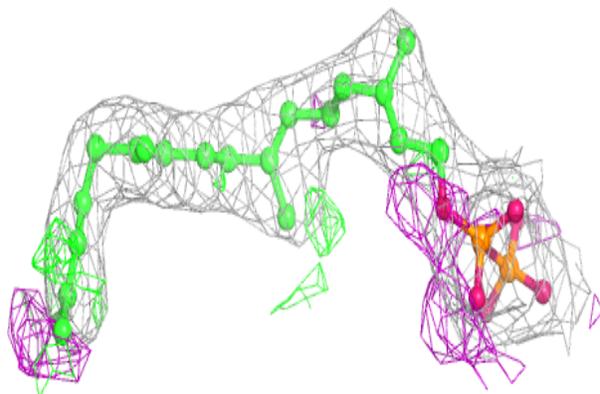


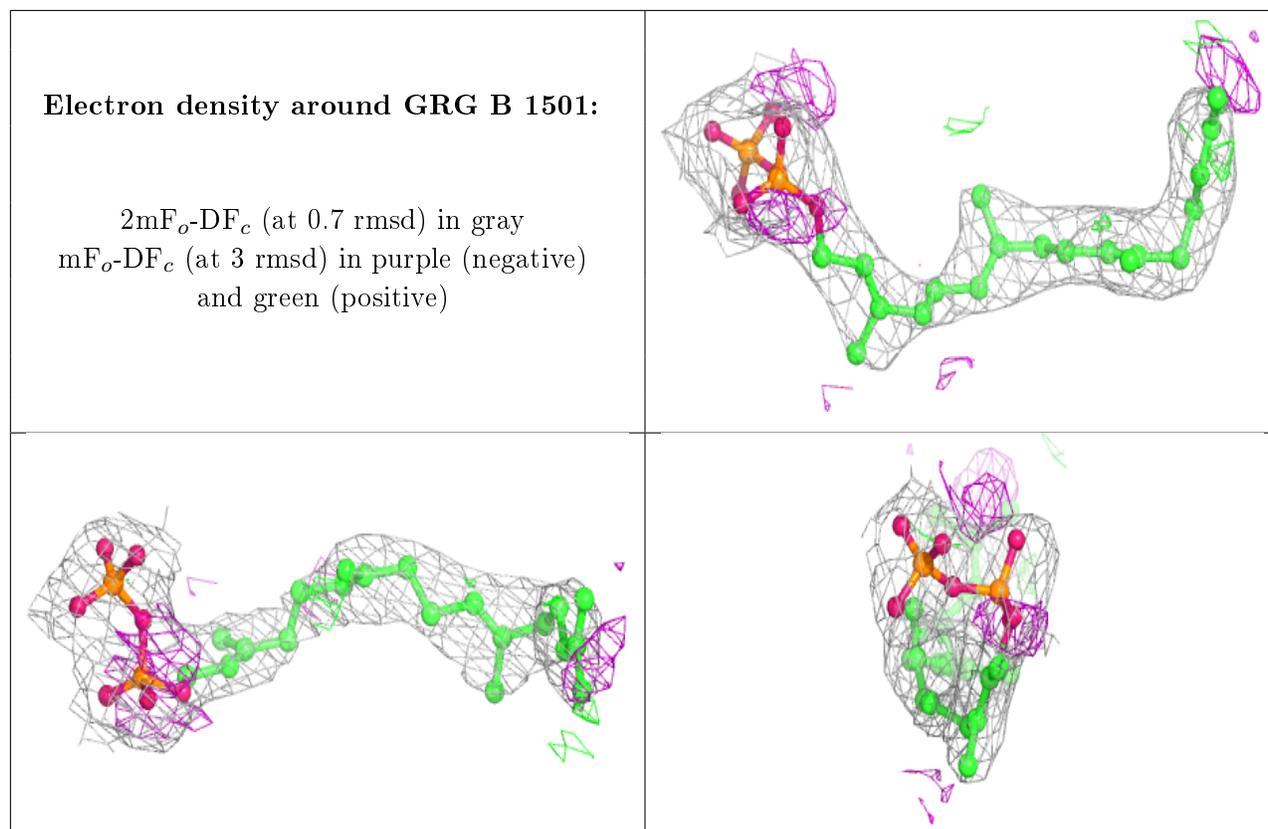
Electron density around GRG F 1503:

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

**Electron density around GRG 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.