



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:17 PM UTC

PDB ID : 1N4P / pdb_00001n4p
Title : Protein Geranylgeranyltransferase type-I Complexed with Geranylgeranyl Diphosphate
Authors : Taylor, J.S.; Reid, T.S.; Casey, P.J.; Beese, L.S.
Deposited on : 2002-11-01
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

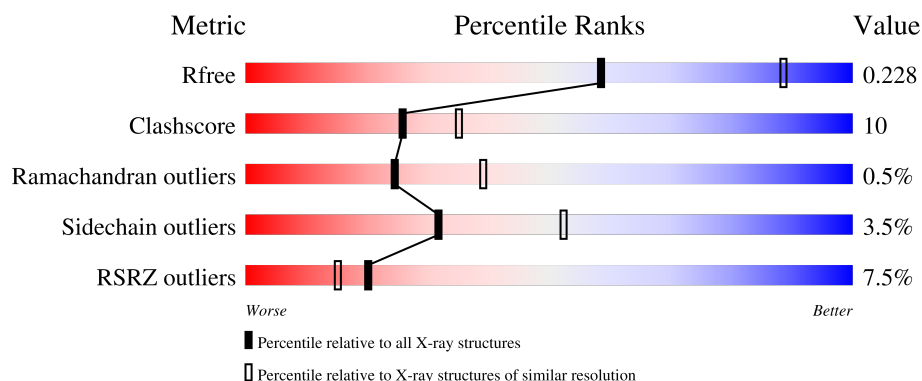
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	6% 66% 16% • 17%
1	C	377	6% 64% 19% • 17%
1	E	377	5% 63% 19% • 17%
1	G	377	10% 62% 21% • 17%
1	I	377	6% 63% 19% • 17%

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Mol	Chain	Length	Quality of chain
1	K	377	3% 67% 15% 17%
2	B	377	5% 71% 19% 8%
2	D	377	4% 70% 19% 8%
2	F	377	5% 74% 16% 8%
2	H	377	15% 67% 22% 8%
2	J	377	7% 68% 23% 8%
2	L	377	4% 71% 19% 8%
3	M	11	36% 9% 18% 9% 64%
3	N	11	36% 9% 18% 9% 64%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33443 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			

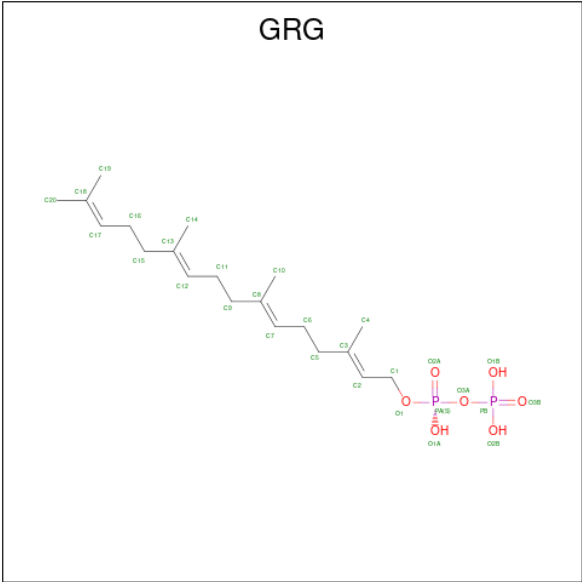
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: CL) (formula: Cl).

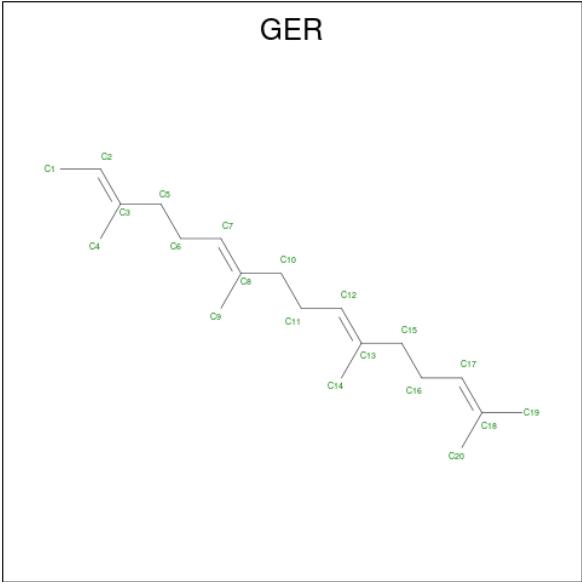
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		
5	J	1	Total	Cl	0	0
			1	1		
5	K	1	Total	Cl	0	0
			1	1		
5	L	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GERANYLGERANYL DIPHOSPHATE (CCD ID: GRG) (formula: C₂₀H₃₆O₇P₂).



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

- Molecule 7 is GERAN-8-YL GERAN (CCD ID: GER) (formula: C₂₀H₃₄).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	71	Total O 71 71	0	0
8	B	63	Total O 63 63	0	0
8	C	80	Total O 80 80	0	0
8	D	94	Total O 94 94	0	0
8	E	64	Total O 64 64	0	0
8	F	92	Total O 92 92	0	0
8	G	58	Total O 58 58	0	0
8	H	48	Total O 48 48	0	0
8	I	87	Total O 87 87	0	0
8	J	73	Total O 73 73	0	0

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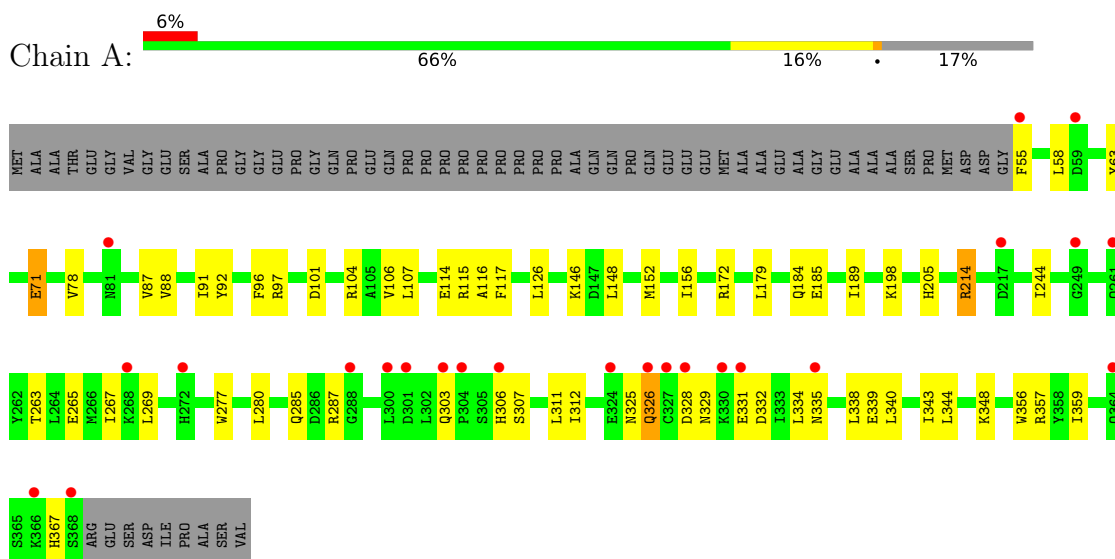
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	159	Total 159	O 159	0	0
8	L	134	Total 134	O 134	0	0
8	N	1	Total 1	O 1	0	0

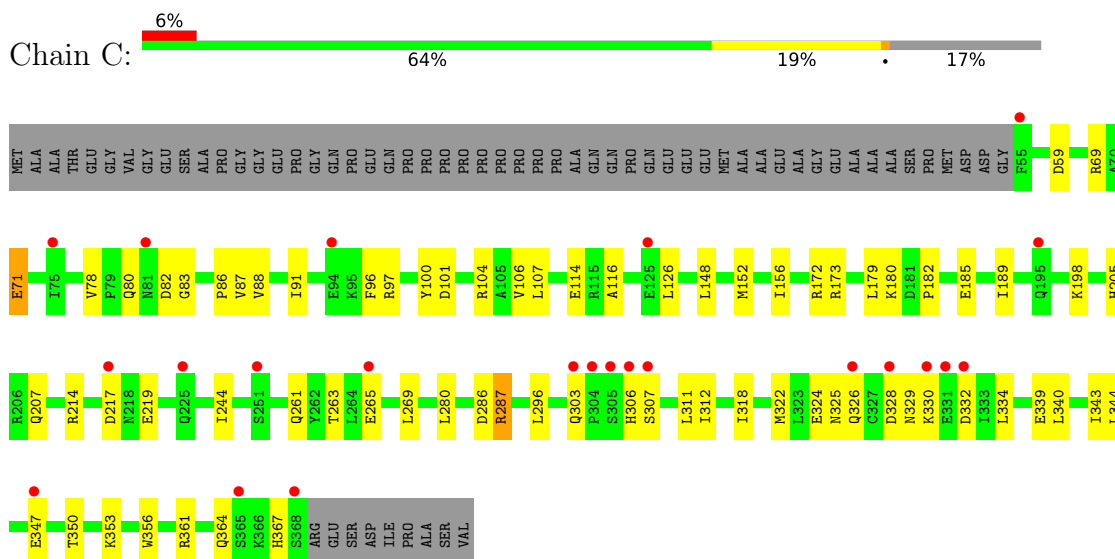
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

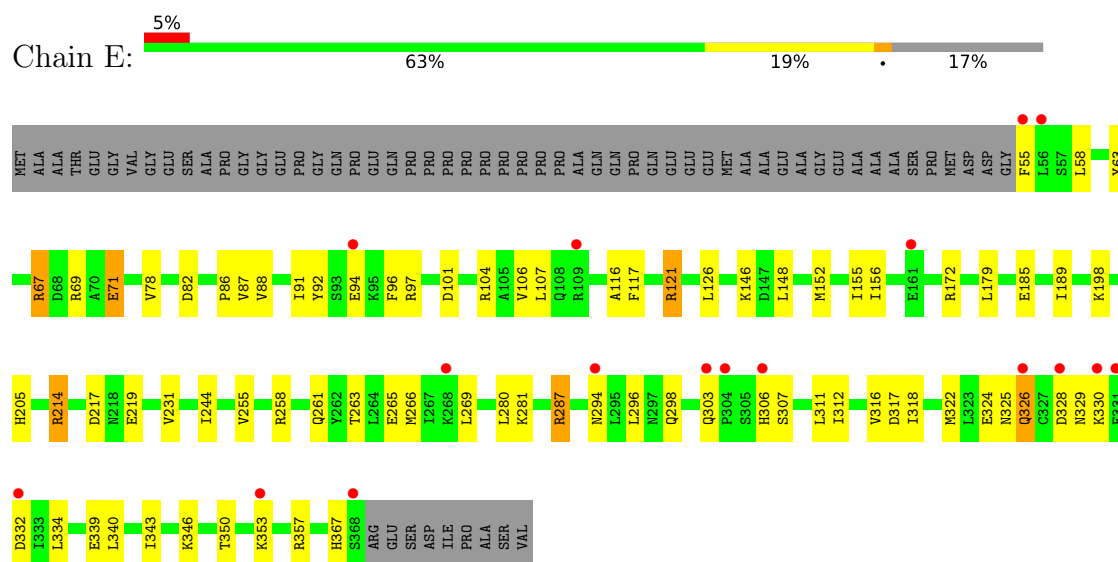
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



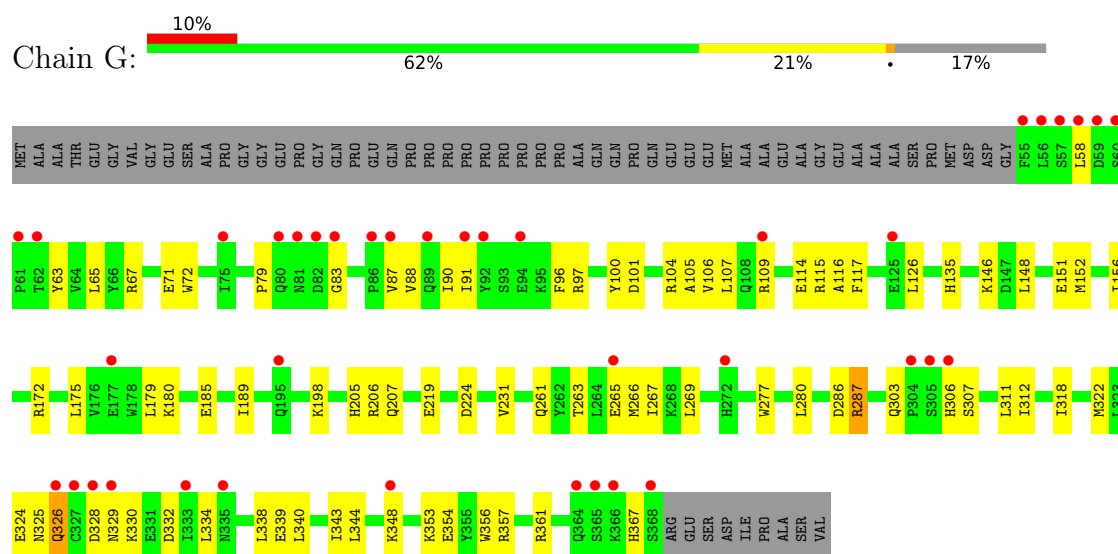
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



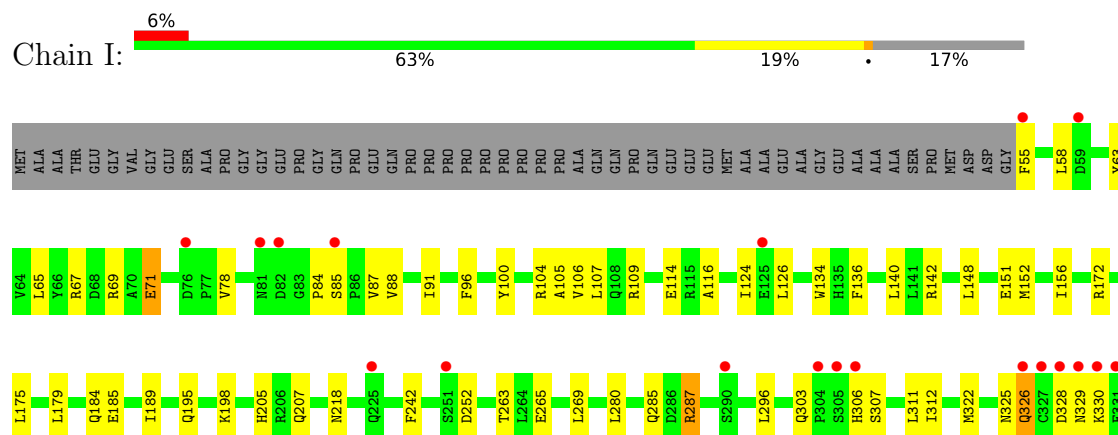
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



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

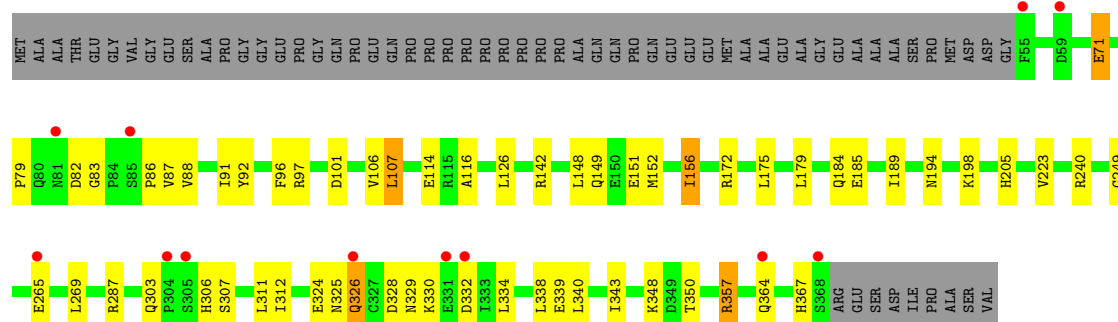


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

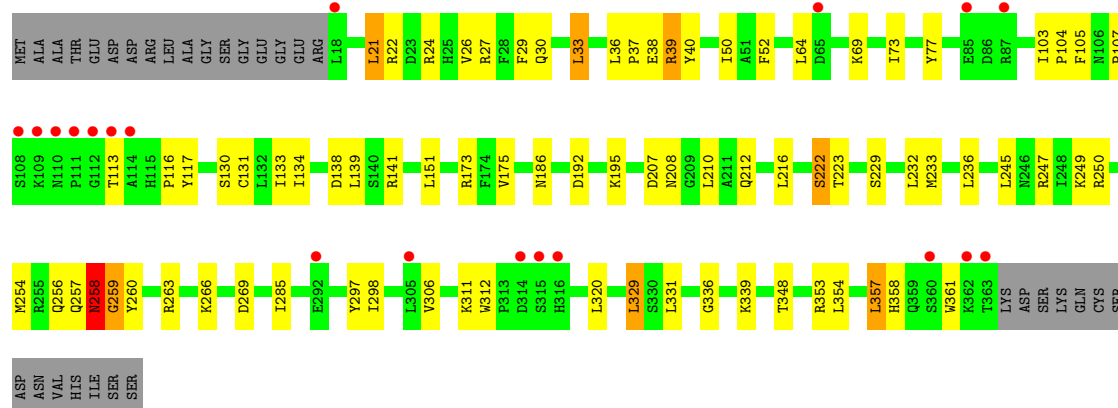




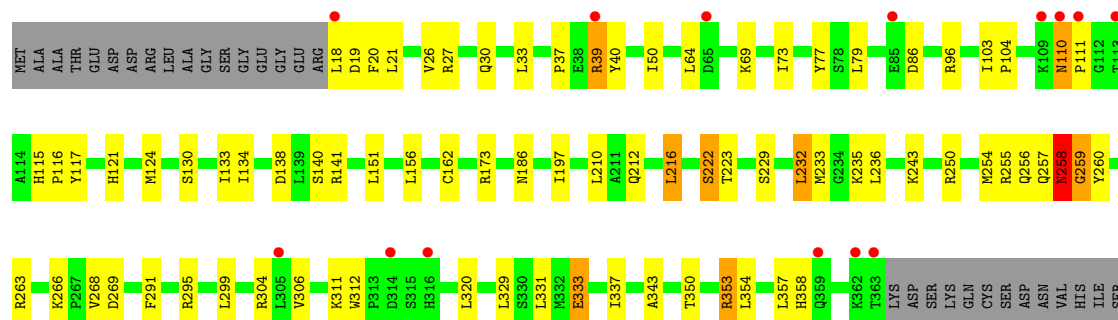
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



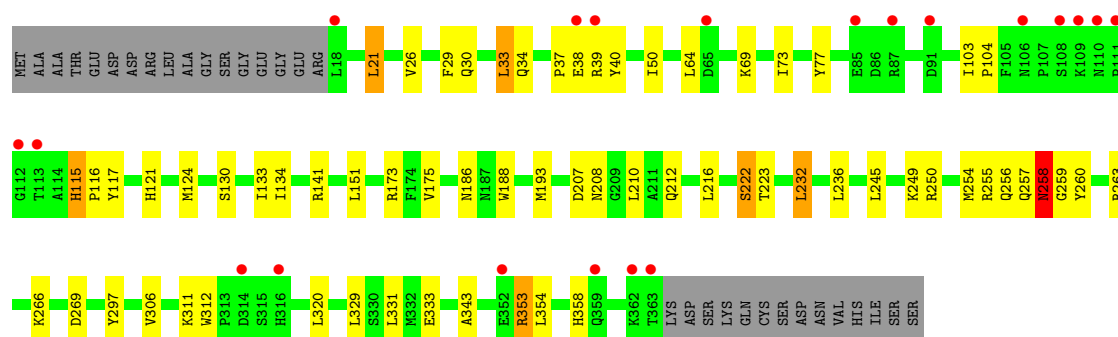
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



SER

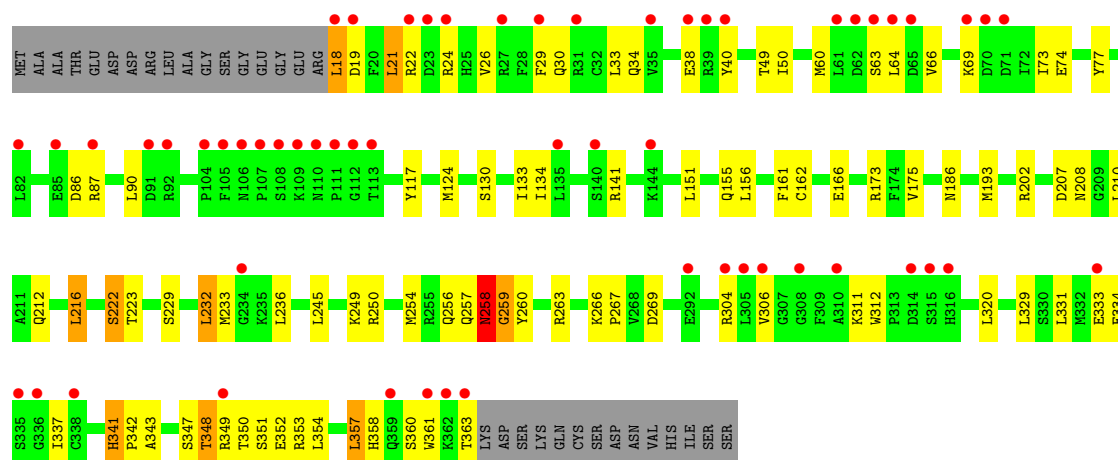
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain F: 



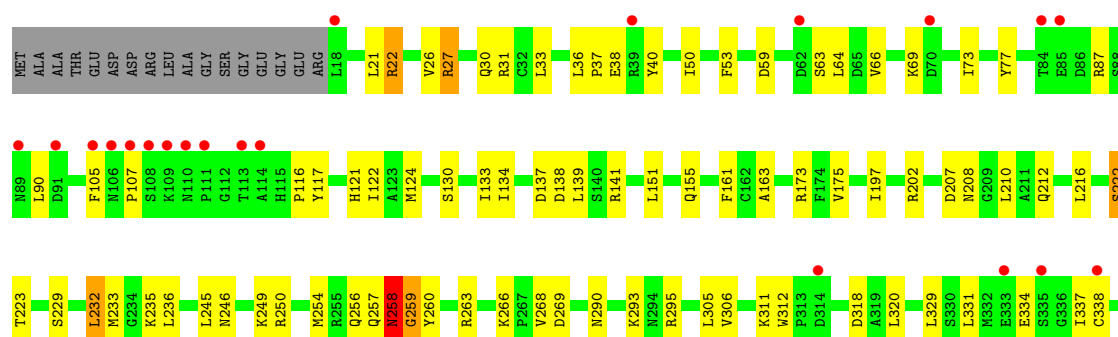
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

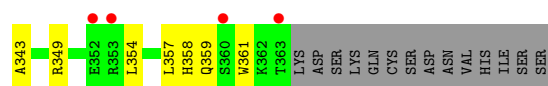
Chain H: 



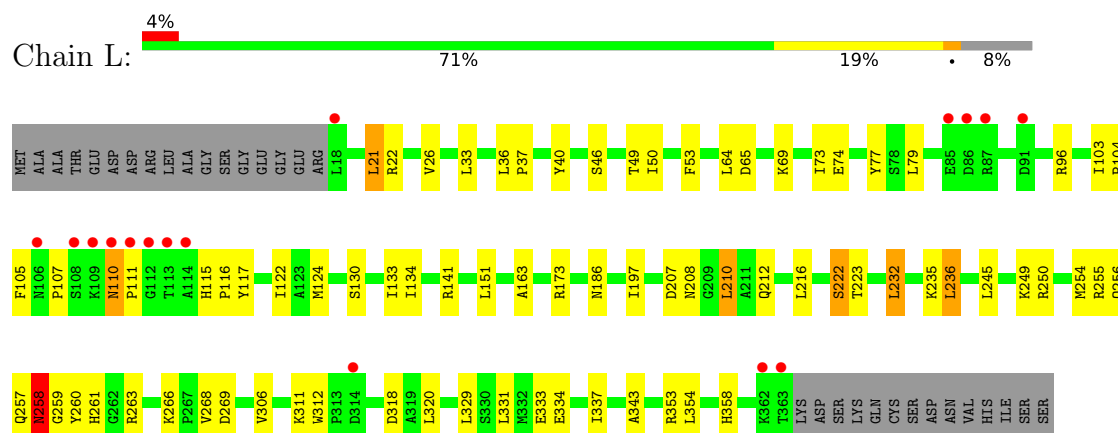
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain J: 

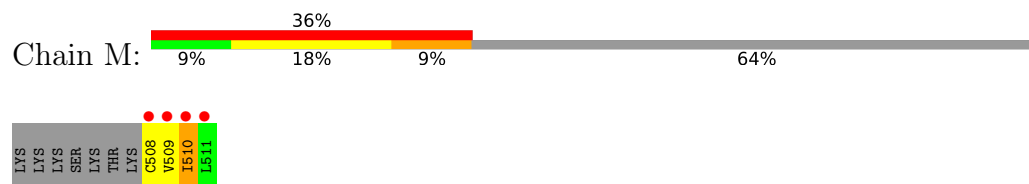




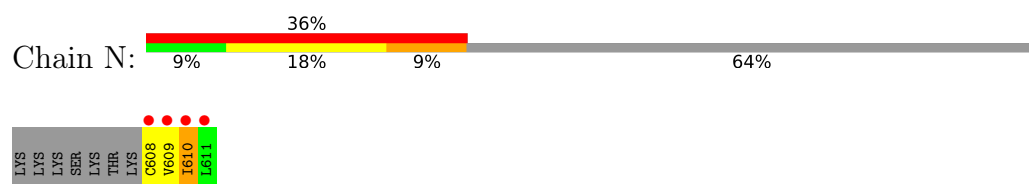
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



- 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	272.34Å 271.57Å 185.43Å 90.00° 131.56° 90.00°	Depositor
Resolution (Å)	29.92 – 2.65 29.92 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.92-2.65) 98.6 (29.92-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.228 0.205 , 0.228	Depositor DCC
R_{free} test set	14292 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.080 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33443	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.40	0/2695	0.84	2/3668 (0.1%)
1	C	0.42	0/2709	0.84	7/3684 (0.2%)
1	E	0.41	0/2708	0.83	5/3684 (0.1%)
1	G	0.42	0/2699	0.83	3/3672 (0.1%)
1	I	0.42	0/2722	0.84	2/3700 (0.1%)
1	K	0.45	0/2737	0.85	5/3717 (0.1%)
2	B	0.42	0/2759	0.90	7/3733 (0.2%)
2	D	0.42	0/2775	0.91	8/3752 (0.2%)
2	F	0.42	0/2780	0.90	8/3758 (0.2%)
2	H	0.39	0/2756	0.90	7/3729 (0.2%)
2	J	0.41	0/2773	0.90	6/3750 (0.2%)
2	L	0.45	0/2785	0.91	6/3764 (0.2%)
3	M	0.79	0/29	1.58	1/37 (2.7%)
3	N	0.77	0/29	1.32	1/37 (2.7%)
All	All	0.42	0/32956	0.87	68/44685 (0.2%)

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.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	259	GLY	N-CA-C	-10.16	98.07	112.60
2	F	259	GLY	N-CA-C	-10.07	98.20	112.60
2	D	259	GLY	N-CA-C	-9.87	98.49	112.60
2	J	259	GLY	N-CA-C	-9.85	98.51	112.60
2	L	259	GLY	N-CA-C	-9.73	98.68	112.60
2	B	259	GLY	N-CA-C	-9.72	98.70	112.60
1	K	185	GLU	N-CA-C	9.61	122.75	111.02
1	I	185	GLU	N-CA-C	9.57	122.69	111.02
1	A	185	GLU	N-CA-C	9.33	122.40	111.02
1	E	185	GLU	N-CA-C	9.18	122.21	111.02
1	C	185	GLU	N-CA-C	9.08	122.10	111.02
1	K	348	LYS	N-CA-C	6.95	121.51	112.89
2	L	258	ASN	N-CA-C	-6.83	96.25	110.80
2	J	258	ASN	N-CA-C	-6.78	96.36	110.80
1	C	83	GLY	CA-C-N	6.75	126.26	119.24
1	C	83	GLY	C-N-CA	6.75	126.26	119.24
2	B	258	ASN	N-CA-C	-6.65	96.63	110.80
2	D	258	ASN	N-CA-C	-6.63	96.67	110.80
2	H	258	ASN	N-CA-C	-6.61	96.72	110.80
2	F	257	GLN	N-CA-C	-6.58	105.26	113.55
2	F	258	ASN	N-CA-C	-6.56	96.84	110.80
2	D	257	GLN	N-CA-C	-6.38	105.52	113.55
3	M	510	ILE	N-CA-C	6.28	118.14	112.17
2	H	257	GLN	N-CA-C	-6.19	105.75	113.55
2	J	257	GLN	N-CA-C	-6.10	105.86	113.55
2	J	22	ARG	N-CA-C	6.09	118.42	111.11
2	J	50	ILE	N-CA-C	-6.08	104.58	110.72
2	F	50	ILE	N-CA-C	-6.08	104.58	110.72
2	B	257	GLN	N-CA-C	-6.04	105.94	113.55
2	D	353	ARG	N-CA-C	-5.97	104.77	111.28
2	D	50	ILE	N-CA-C	-5.75	104.91	110.72
2	L	257	GLN	N-CA-C	-5.73	106.33	113.55
1	C	347	GLU	N-CA-C	5.65	121.06	114.62
1	E	244	ILE	N-CA-C	5.63	115.83	110.42
2	H	50	ILE	N-CA-C	-5.57	105.09	110.72
2	H	341	HIS	CA-C-N	5.54	126.76	119.84
2	H	341	HIS	C-N-CA	5.54	126.76	119.84
2	B	50	ILE	N-CA-C	-5.52	105.14	110.72
2	F	175	VAL	N-CA-C	-5.44	105.22	110.72
1	C	350	THR	N-CA-C	5.42	118.69	111.75
2	H	175	VAL	N-CA-C	-5.40	105.27	110.72
3	N	610	ILE	N-CA-C	5.39	118.07	112.90
1	K	83	GLY	CA-C-N	5.38	124.84	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	83	GLY	C-N-CA	5.38	124.84	119.24
1	K	350	THR	N-CA-C	5.38	117.89	111.71
2	D	291	PHE	N-CA-C	5.25	116.81	111.14
2	L	115	HIS	CA-C-N	5.25	125.31	119.32
2	L	115	HIS	C-N-CA	5.25	125.31	119.32
1	C	244	ILE	N-CA-C	5.24	115.45	110.42
2	L	50	ILE	N-CA-C	-5.24	105.43	110.72
1	E	350	THR	N-CA-C	5.22	117.71	111.71
2	B	175	VAL	N-CA-C	-5.21	105.46	110.72
1	E	217	ASP	N-CA-C	5.18	119.92	111.37
2	F	115	HIS	CA-C-N	5.17	125.21	119.32
2	F	115	HIS	C-N-CA	5.17	125.21	119.32
1	G	185	GLU	N-CA-C	5.16	121.80	110.80
1	G	83	GLY	CA-C-N	5.15	124.59	119.24
1	G	83	GLY	C-N-CA	5.15	124.59	119.24
2	D	115	HIS	CA-C-N	5.08	125.11	119.32
2	D	115	HIS	C-N-CA	5.08	125.11	119.32
1	I	285	GLN	N-CA-C	5.05	117.44	111.33
1	A	244	ILE	N-CA-C	5.04	115.25	110.42
1	E	346	LYS	N-CA-C	5.03	118.56	112.23
2	J	175	VAL	N-CA-C	-5.01	105.66	110.72
2	B	36	LEU	CA-C-N	5.01	124.94	119.78
2	B	36	LEU	C-N-CA	5.01	124.94	119.78
1	C	217	ASP	N-CA-C	5.01	119.63	111.37
2	F	353	ARG	N-CA-C	-5.00	105.83	111.28

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

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	49	0
1	C	2643	0	2540	46	0
1	E	2642	0	2534	60	0
1	G	2633	0	2524	57	0
1	I	2656	0	2560	48	0
1	K	2671	0	2588	40	0
2	B	2697	0	2600	54	0
2	D	2713	0	2628	54	0
2	F	2718	0	2635	40	0
2	H	2694	0	2590	69	0
2	J	2711	0	2616	55	0
2	L	2723	0	2643	49	0
3	M	30	0	34	4	0
3	N	30	0	34	4	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	1	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	1	0
7	M	20	0	33	6	0
7	N	20	0	33	6	0
8	A	71	0	0	1	0
8	B	63	0	0	0	0
8	C	80	0	0	3	0
8	D	94	0	0	1	0
8	E	64	0	0	0	0
8	F	92	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	58	0	0	2	0
8	H	48	0	0	2	0
8	I	87	0	0	4	0
8	J	73	0	0	2	0
8	K	159	0	0	4	0
8	L	134	0	0	2	0
8	N	1	0	0	0	0
All	All	33443	0	31310	607	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.

All (607) 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:I:156:ILE:HG12	1:I:172:ARG:HH12	1.10	1.15
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.09	1.11
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.03	1.08
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.99	1.08
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.17	1.04
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.17	1.04
2:F:212:GLN:HE21	2:F:222:SER:HB3	1.21	1.01
2:J:212:GLN:HE21	2:J:222:SER:HB3	1.29	0.96
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.47	0.95
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.81	0.95
2:F:212:GLN:NE2	2:F:222:SER:HB3	1.86	0.90
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.86	0.90
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.38	0.87
5:G:1711:CL:CL	8:G:383:HOH:O	2.31	0.86
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.91	0.85
2:D:173:ARG:HG2	6:D:1722:GRG:H112	1.59	0.84
2:D:212:GLN:HE21	2:D:222:SER:HB3	1.41	0.84
2:L:173:ARG:HG2	6:L:1726:GRG:H112	1.59	0.83
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.42	0.83
2:B:212:GLN:HE21	2:B:222:SER:HB3	1.44	0.83
1:G:152:MET:O	1:G:156:ILE:HG13	1.79	0.83
2:D:39:ARG:H	2:D:39:ARG:HD2	1.42	0.82
2:D:212:GLN:NE2	2:D:222:SER:HB3	1.95	0.82
2:B:212:GLN:NE2	2:B:222:SER:HB3	1.95	0.82
2:H:348:THR:O	2:H:352:GLU:HG2	1.80	0.81
2:J:173:ARG:HG2	6:J:1725:GRG:H112	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:PRO:HB2	2:D:39:ARG:CD	2.11	0.81
1:A:152:MET:O	1:A:156:ILE:HG13	1.80	0.81
2:B:173:ARG:HG2	6:B:1721:GRG:H112	1.63	0.80
2:F:173:ARG:HG2	6:F:1723:GRG:H112	1.62	0.80
1:I:152:MET:O	1:I:156:ILE:HG13	1.82	0.79
1:E:152:MET:O	1:E:156:ILE:HG13	1.81	0.79
1:G:231:VAL:HG23	1:G:266:MET:HE3	1.67	0.77
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.66	0.77
2:D:37:PRO:HB2	2:D:39:ARG:HD2	1.67	0.77
2:H:173:ARG:HG2	6:H:1724:GRG:H112	1.67	0.76
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.20	0.76
1:C:152:MET:O	1:C:156:ILE:HG13	1.83	0.76
1:K:152:MET:O	1:K:156:ILE:HG13	1.85	0.76
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.94	0.75
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.01	0.75
2:H:212:GLN:NE2	2:H:222:SER:HB3	2.03	0.73
3:N:609:VAL:HG23	3:N:610:ILE:HG23	1.71	0.73
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.95	0.73
2:J:212:GLN:NE2	2:J:222:SER:HB3	2.02	0.73
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.89	0.72
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.90	0.72
2:H:229:SER:O	2:H:233:MET:HG3	1.90	0.71
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.56	0.71
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.98	0.71
5:K:1717:CL:CL	8:K:391:HOH:O	2.43	0.71
3:M:509:VAL:HG23	3:M:510:ILE:HG23	1.71	0.71
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.72	0.70
2:L:212:GLN:HE21	2:L:222:SER:HB3	1.56	0.70
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.57	0.69
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.73	0.69
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.57	0.69
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.58	0.69
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
2:D:69:LYS:O	2:D:73:ILE:HG13	1.93	0.68
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.76	0.68
2:B:69:LYS:O	2:B:73:ILE:HG13	1.93	0.67
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.75	0.67
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.75	0.67
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.75	0.66
2:H:19:ASP:HB2	8:H:1494:HOH:O	1.96	0.66
2:D:37:PRO:HB2	2:D:39:ARG:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:91:ILE:HD12	1:K:91:ILE:O	1.95	0.66
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.60	0.65
2:H:212:GLN:HE21	2:H:222:SER:HB3	1.61	0.65
2:H:69:LYS:O	2:H:73:ILE:HG13	1.97	0.65
2:H:18:LEU:HD22	2:H:18:LEU:N	2.11	0.65
1:I:91:ILE:HD12	1:I:91:ILE:O	1.96	0.65
2:B:245:LEU:O	2:B:249:LYS:HG3	1.97	0.64
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.78	0.64
1:C:318:ILE:HG22	1:C:322:MET:HE3	1.79	0.64
1:G:91:ILE:HD12	1:G:91:ILE:O	1.97	0.64
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.32	0.64
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.80	0.63
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.79	0.63
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.80	0.63
1:E:91:ILE:O	1:E:91:ILE:HD12	1.98	0.63
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.00	0.63
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.79	0.63
2:B:353:ARG:HG2	2:B:353:ARG:HH11	1.62	0.63
1:E:231:VAL:HG23	1:E:266:MET:HE3	1.81	0.63
1:G:261:GLN:O	1:G:265:GLU:HG2	1.99	0.63
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.62	0.63
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.80	0.63
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.80	0.62
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.29	0.62
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.25	0.62
2:F:69:LYS:O	2:F:73:ILE:HG13	1.99	0.62
1:A:91:ILE:HD12	1:A:91:ILE:O	2.00	0.62
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.81	0.62
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.65	0.62
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.82	0.61
1:E:353:LYS:CE	1:E:357:ARG:HH12	2.10	0.61
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.34	0.61
2:F:26:VAL:O	2:F:30:GLN:HG3	1.99	0.61
1:G:334:LEU:HD22	1:G:367:HIS:O	2.00	0.61
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.81	0.61
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.82	0.61
1:E:296:LEU:HD22	1:E:322:MET:HE1	1.82	0.61
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.65	0.61
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.83	0.61
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.83	0.61
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:O	1:C:91:ILE:HD12	2.01	0.60
1:G:100:TYR:O	1:G:104:ARG:HG3	2.01	0.60
1:G:198:LYS:HD3	2:H:266:LYS:HD3	1.81	0.60
1:C:330:LYS:HE2	1:C:367:HIS:HB3	1.83	0.60
1:A:78:VAL:O	1:A:104:ARG:HD2	2.01	0.60
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.82	0.60
1:G:357:ARG:O	1:G:361:ARG:HG3	2.01	0.60
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.84	0.60
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.67	0.59
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.67	0.59
1:A:339:GLU:O	1:A:343:ILE:HG13	2.02	0.59
2:D:39:ARG:H	2:D:39:ARG:CD	2.14	0.59
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.68	0.59
2:B:26:VAL:O	2:B:30:GLN:HG3	2.01	0.59
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.02	0.59
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.37	0.59
1:C:303:GLN:O	1:C:307:SER:HB2	2.03	0.58
1:I:207:GLN:HG2	1:I:242:PHE:CE2	2.38	0.58
2:H:210:LEU:HB2	2:H:223:THR:HA	1.85	0.58
2:J:22:ARG:O	2:J:26:VAL:HG23	2.03	0.58
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.85	0.58
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.85	0.58
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.85	0.58
2:J:210:LEU:HB2	2:J:223:THR:HA	1.84	0.58
1:E:78:VAL:O	1:E:104:ARG:HD2	2.03	0.57
2:L:353:ARG:HD3	2:L:353:ARG:O	2.04	0.57
2:L:210:LEU:HB2	2:L:223:THR:HA	1.86	0.57
2:H:245:LEU:O	2:H:249:LYS:HG3	2.04	0.57
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.87	0.57
1:G:334:LEU:O	1:G:338:LEU:HG	2.04	0.57
2:J:318:ASP:HB2	7:M:1727:GER:H71	1.87	0.57
1:A:328:ASP:O	1:A:329:ASN:HB2	2.05	0.57
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.87	0.57
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.87	0.56
1:A:214:ARG:HG3	1:A:214:ARG:O	2.05	0.56
2:D:210:LEU:HB2	2:D:223:THR:HA	1.86	0.56
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.69	0.56
2:H:22:ARG:HH11	2:H:22:ARG:HG2	1.70	0.56
1:K:311:LEU:C	1:K:311:LEU:HD23	2.30	0.56
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.78	0.56
1:K:265:GLU:O	1:K:269:LEU:HD13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:PRO:HB3	2:D:39:ARG:HH11	1.70	0.56
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.88	0.56
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.40	0.56
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.87	0.56
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.88	0.56
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.56
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.88	0.56
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.86	0.56
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.86	0.56
1:A:265:GLU:O	1:A:269:LEU:HD13	2.06	0.56
1:E:265:GLU:O	1:E:269:LEU:HD13	2.06	0.56
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.88	0.55
2:B:210:LEU:HB2	2:B:223:THR:HA	1.87	0.55
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.21	0.55
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.41	0.55
2:H:353:ARG:O	2:H:357:LEU:HB2	2.05	0.55
2:J:290:ASN:ND2	2:J:293:LYS:HD2	2.22	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55
1:G:90:ILE:HD13	2:H:40:TYR:O	2.07	0.55
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.41	0.55
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.89	0.55
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.87	0.55
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.88	0.55
1:I:311:LEU:HD23	1:I:311:LEU:C	2.32	0.55
1:C:334:LEU:HD22	1:C:367:HIS:O	2.07	0.55
2:F:210:LEU:HB2	2:F:223:THR:HA	1.88	0.55
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.89	0.55
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.89	0.55
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.55
1:E:261:GLN:O	1:E:265:GLU:HG2	2.06	0.55
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.89	0.55
1:E:121:ARG:NH1	1:E:121:ARG:HG3	2.21	0.55
1:E:353:LYS:HE2	1:E:357:ARG:NH1	2.17	0.55
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.07	0.55
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.22	0.54
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.72	0.54
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.73	0.54
1:G:311:LEU:HD23	1:G:311:LEU:C	2.32	0.54
2:L:212:GLN:NE2	2:L:222:SER:HB3	2.21	0.54
2:H:349:ARG:O	2:H:352:GLU:HB2	2.07	0.54
1:A:334:LEU:HD22	1:A:367:HIS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:318:ILE:HG22	1:E:322:MET:CE	2.38	0.54
2:H:348:THR:HA	2:H:351:SER:OG	2.07	0.54
1:K:334:LEU:HD22	1:K:367:HIS:O	2.07	0.54
1:E:339:GLU:O	1:E:343:ILE:HG13	2.08	0.54
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.89	0.54
1:A:303:GLN:O	1:A:307:SER:HB2	2.08	0.54
2:B:250:ARG:O	2:B:254:MET:HG2	2.07	0.54
1:I:198:LYS:HD3	2:J:266:LYS:HD3	1.89	0.54
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.89	0.54
1:I:195:GLN:NE2	8:I:1500:HOH:O	2.41	0.53
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.53
1:A:325:ASN:O	1:A:326:GLN:C	2.52	0.53
2:D:212:GLN:HE21	2:D:222:SER:CB	2.18	0.53
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.44	0.53
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.90	0.53
1:C:339:GLU:O	1:C:343:ILE:HG13	2.09	0.53
1:E:294:ASN:O	1:E:298:GLN:HG3	2.08	0.53
2:H:186:ASN:HB2	2:H:358:HIS:NE2	2.24	0.53
2:H:258:ASN:OD1	2:H:259:GLY:N	2.38	0.53
1:I:334:LEU:HD22	1:I:367:HIS:O	2.09	0.53
2:L:318:ASP:HB2	7:N:1727:GER:H71	1.90	0.53
1:G:328:ASP:O	1:G:329:ASN:HB2	2.09	0.53
1:K:311:LEU:HD23	1:K:311:LEU:O	2.09	0.53
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
1:I:339:GLU:O	1:I:343:ILE:HG13	2.08	0.52
3:N:609:VAL:N	7:N:1727:GER:H11	2.23	0.52
2:J:202:ARG:HD2	8:J:384:HOH:O	2.09	0.52
2:B:339:LYS:O	2:B:348:THR:HG23	2.10	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.92	0.52
2:B:24:ARG:HD3	2:B:27:ARG:HH22	1.74	0.52
2:B:229:SER:O	2:B:233:MET:HG3	2.09	0.52
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.22	0.52
1:C:311:LEU:C	1:C:311:LEU:HD23	2.34	0.52
2:H:130:SER:O	2:H:134:ILE:HG13	2.10	0.52
1:G:303:GLN:O	1:G:307:SER:HB2	2.10	0.52
1:I:67:ARG:HD2	8:I:927:HOH:O	2.09	0.52
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.11	0.51
1:K:338:LEU:HD11	1:K:364:GLN:HG2	1.92	0.51
2:J:87:ARG:HH12	2:J:90:LEU:HD11	1.75	0.51
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.51
1:C:78:VAL:O	1:C:104:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.92	0.51
1:I:265:GLU:O	1:I:269:LEU:HD13	2.10	0.51
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.41	0.51
2:H:267:PRO:HG2	8:H:1609:HOH:O	2.10	0.51
1:I:328:ASP:O	1:I:329:ASN:HB2	2.10	0.51
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.93	0.51
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.45	0.51
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.46	0.51
3:M:509:VAL:N	7:M:1727:GER:H11	2.25	0.51
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.93	0.51
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.93	0.51
2:F:250:ARG:O	2:F:254:MET:HG2	2.11	0.51
1:G:325:ASN:O	1:G:326:GLN:C	2.54	0.51
2:J:63:SER:O	2:J:66:VAL:HG22	2.11	0.51
1:K:71:GLU:CD	1:K:71:GLU:H	2.18	0.51
1:K:303:GLN:O	1:K:307:SER:HB2	2.11	0.51
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.45	0.51
1:I:151:GLU:HG3	1:I:175:LEU:HD11	1.93	0.51
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.46	0.50
2:H:60:MET:HE1	2:H:347:SER:N	2.25	0.50
1:A:58:LEU:HD23	1:A:63:TYR:CZ	2.46	0.50
1:I:78:VAL:O	1:I:104:ARG:HD2	2.11	0.50
1:I:325:ASN:O	1:I:326:GLN:C	2.54	0.50
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.46	0.50
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.94	0.50
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.12	0.50
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.92	0.50
2:L:212:GLN:HE21	2:L:212:GLN:HA	1.76	0.50
1:E:92:TYR:O	1:E:97:ARG:NH2	2.45	0.50
2:D:333:GLU:HA	8:D:740:HOH:O	2.11	0.49
2:D:333:GLU:O	1:K:357:ARG:NH2	2.45	0.49
2:F:207:ASP:O	2:F:208:ASN:HB2	2.11	0.49
2:B:130:SER:O	2:B:134:ILE:HG13	2.11	0.49
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.47	0.49
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.77	0.49
2:J:27:ARG:HH12	2:J:30:GLN:NE2	2.09	0.49
2:F:130:SER:O	2:F:134:ILE:HG13	2.12	0.49
1:K:325:ASN:O	1:K:326:GLN:C	2.55	0.49
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.95	0.49
2:B:29:PHE:O	2:B:33:LEU:HD22	2.12	0.49
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ARG:O	2:D:254:MET:HG2	2.13	0.49
2:F:38:GLU:O	2:F:38:GLU:HG2	2.13	0.49
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.93	0.49
1:G:135:HIS:CD2	2:H:166:GLU:HG2	2.48	0.49
2:B:207:ASP:O	2:B:208:ASN:HB2	2.13	0.49
2:L:333:GLU:HA	8:L:1050:HOH:O	2.13	0.49
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.77	0.49
2:D:186:ASN:HB2	2:D:358:HIS:CE1	2.48	0.49
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.45	0.49
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.94	0.49
1:C:296:LEU:HD22	1:C:322:MET:HE1	1.95	0.49
1:G:65:LEU:HD12	1:G:67:ARG:HH11	1.77	0.49
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.48	0.49
2:B:105:PHE:CE2	2:B:107:PRO:HD3	2.47	0.48
1:I:100:TYR:O	1:I:104:ARG:HG3	2.12	0.48
1:A:214:ARG:O	1:A:214:ARG:CG	2.59	0.48
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.78	0.48
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.43	0.48
1:E:303:GLN:O	1:E:307:SER:HB2	2.14	0.48
1:G:339:GLU:O	1:G:343:ILE:HG13	2.13	0.48
1:I:84:PRO:HG2	1:I:85:SER:H	1.79	0.48
1:I:296:LEU:CD2	1:I:322:MET:HE1	2.44	0.48
2:F:212:GLN:HE21	2:F:222:SER:CB	2.08	0.48
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.49	0.48
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.79	0.48
1:G:231:VAL:CG2	1:G:266:MET:HE3	2.42	0.48
2:H:22:ARG:O	2:H:26:VAL:HG23	2.14	0.48
1:I:303:GLN:O	1:I:307:SER:HB2	2.14	0.48
1:C:265:GLU:O	1:C:269:LEU:HD13	2.13	0.48
1:I:338:LEU:HD11	1:I:364:GLN:HG2	1.96	0.48
2:J:358:HIS:O	2:J:361:TRP:HB2	2.14	0.48
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.49	0.48
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.14	0.48
1:E:214:ARG:O	1:E:214:ARG:HG3	2.12	0.48
1:E:121:ARG:HG3	1:E:121:ARG:HH11	1.78	0.48
1:E:296:LEU:HD22	1:E:322:MET:CE	2.44	0.47
1:G:219:GLU:HA	1:G:219:GLU:OE1	2.14	0.47
1:A:184:GLN:HB2	8:A:379:HOH:O	2.14	0.47
2:D:79:LEU:O	2:D:96:ARG:HG3	2.14	0.47
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.95	0.47
2:J:130:SER:O	2:J:134:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.49	0.47
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.96	0.47
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.49	0.47
1:I:184:GLN:HB2	8:I:378:HOH:O	2.15	0.47
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.47	0.47
2:J:229:SER:O	2:J:233:MET:HG3	2.14	0.47
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.50	0.47
1:C:173:ARG:NH1	8:C:412:HOH:O	2.46	0.47
1:E:325:ASN:O	1:E:326:GLN:C	2.56	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.14	0.47
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.50	0.47
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.96	0.47
2:H:311:LYS:HG3	2:H:312:TRP:CD2	2.49	0.47
2:J:258:ASN:OD1	2:J:259:GLY:N	2.42	0.47
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.49	0.47
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.97	0.47
2:J:69:LYS:O	2:J:73:ILE:HG13	2.13	0.47
1:K:249:GLY:HA3	8:K:640:HOH:O	2.14	0.47
1:A:71:GLU:H	1:A:71:GLU:CD	2.17	0.47
2:F:311:LYS:HG3	2:F:312:TRP:CD2	2.50	0.47
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.80	0.47
2:H:193:MET:HE2	2:H:233:MET:HE2	1.96	0.47
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.27	0.47
1:A:311:LEU:C	1:A:311:LEU:HD23	2.40	0.46
1:E:312:ILE:O	1:E:316:VAL:HG23	2.15	0.46
1:C:214:ARG:O	1:C:214:ARG:HG2	2.14	0.46
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.79	0.46
2:D:130:SER:O	2:D:134:ILE:HG13	2.15	0.46
2:H:250:ARG:O	2:H:254:MET:HG2	2.16	0.46
2:B:212:GLN:HE21	2:B:222:SER:CB	2.20	0.46
1:E:334:LEU:HD22	1:E:367:HIS:O	2.15	0.46
2:H:30:GLN:OE1	2:H:66:VAL:HB	2.16	0.46
1:I:65:LEU:O	1:I:69:ARG:HG3	2.15	0.46
2:L:53:PHE:HE1	7:N:1727:GER:H42	1.80	0.46
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.50	0.46
2:B:22:ARG:O	2:B:26:VAL:HG23	2.16	0.46
2:B:38:GLU:O	2:B:38:GLU:HG2	2.14	0.46
1:E:311:LEU:C	1:E:311:LEU:HD23	2.41	0.46
2:H:29:PHE:O	2:H:33:LEU:HD22	2.15	0.46
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.44	0.46
1:C:325:ASN:O	1:C:326:GLN:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:LYS:HG3	2:D:312:TRP:CD2	2.50	0.46
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.97	0.46
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.42	0.46
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.51	0.46
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.15	0.46
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.29	0.46
1:A:198:LYS:HD3	2:B:266:LYS:HD3	1.97	0.46
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.51	0.46
2:B:311:LYS:HG3	2:B:312:TRP:CD2	2.51	0.46
1:E:263:THR:HG21	1:E:280:LEU:HB2	1.98	0.46
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
1:C:80:GLN:N	1:C:104:ARG:NH1	2.64	0.46
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.63	0.45
1:C:219:GLU:HA	1:C:219:GLU:OE1	2.16	0.45
2:H:74:GLU:CD	2:H:141:ARG:HH22	2.24	0.45
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.45
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.51	0.45
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.51	0.45
1:I:263:THR:HG21	1:I:280:LEU:HB2	1.98	0.45
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.30	0.45
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.15	0.45
2:H:26:VAL:O	2:H:30:GLN:HG3	2.17	0.45
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.51	0.45
2:F:245:LEU:O	2:F:249:LYS:HG3	2.16	0.45
1:G:58:LEU:HD23	1:G:63:TYR:CZ	2.51	0.45
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.51	0.45
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.31	0.45
1:E:287:ARG:H	1:E:287:ARG:HG2	1.49	0.45
1:A:263:THR:HG21	1:A:280:LEU:HB2	1.98	0.45
2:J:311:LYS:HE2	2:J:312:TRP:CZ2	2.52	0.45
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.52	0.45
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.98	0.45
1:G:105:ALA:O	1:G:109:ARG:HG3	2.16	0.45
2:L:22:ARG:HG2	2:L:22:ARG:HH11	1.81	0.45
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.98	0.45
1:E:281:LYS:NZ	1:E:317:ASP:OD1	2.37	0.45
2:H:21:LEU:CD1	2:H:21:LEU:N	2.79	0.45
1:I:218:ASN:HB3	8:I:1242:HOH:O	2.16	0.45
2:B:311:LYS:HE2	2:B:312:TRP:CZ2	2.51	0.45
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.52	0.45
1:E:296:LEU:CD2	1:E:322:MET:HE1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:ASP:HB2	8:G:618:HOH:O	2.16	0.45
1:G:318:ILE:HG22	1:G:322:MET:CE	2.47	0.45
2:H:156:LEU:HD21	2:H:162:CYS:SG	2.57	0.45
1:A:91:ILE:HD11	2:B:38:GLU:H	1.81	0.45
1:E:91:ILE:HD12	2:F:38:GLU:HB2	1.99	0.45
1:A:71:GLU:O	1:A:115:ARG:NH1	2.50	0.44
2:B:103:ILE:HG23	2:B:104:PRO:HD2	1.99	0.44
1:I:105:ALA:O	1:I:109:ARG:HG3	2.17	0.44
1:A:58:LEU:HD23	1:A:63:TYR:CE2	2.52	0.44
1:A:198:LYS:CD	2:B:266:LYS:HD3	2.47	0.44
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.98	0.44
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.52	0.44
2:J:359:GLN:C	2:J:361:TRP:H	2.24	0.44
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.52	0.44
2:D:19:ASP:OD2	2:D:19:ASP:N	2.44	0.44
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.44	0.44
1:E:328:ASP:O	1:E:329:ASN:HB2	2.18	0.44
1:C:263:THR:HG21	1:C:280:LEU:HB2	1.98	0.44
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.33	0.44
2:J:207:ASP:O	2:J:208:ASN:HB2	2.18	0.44
2:B:258:ASN:CG	2:B:259:GLY:H	2.25	0.44
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.99	0.44
2:D:229:SER:O	2:D:233:MET:HG3	2.18	0.44
1:I:58:LEU:HD23	1:I:63:TYR:CZ	2.52	0.44
3:N:608:CYS:HA	7:N:1727:GER:C2	2.48	0.44
2:B:269:ASP:OD1	2:B:269:ASP:C	2.61	0.44
1:G:353:LYS:HG2	1:G:354:GLU:N	2.32	0.44
1:G:318:ILE:HG22	1:G:322:MET:HE2	2.00	0.44
2:H:269:ASP:OD1	2:H:269:ASP:C	2.61	0.44
2:L:212:GLN:NE2	2:L:212:GLN:HA	2.33	0.44
3:M:508:CYS:HA	7:M:1727:GER:C2	2.48	0.44
1:A:334:LEU:O	1:A:338:LEU:HG	2.18	0.44
2:H:24:ARG:HG3	2:H:24:ARG:HH11	1.83	0.44
2:H:311:LYS:HE2	2:H:312:TRP:CZ2	2.52	0.44
2:J:116:PRO:HB2	2:J:117:TYR:CD2	2.53	0.44
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.53	0.44
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.53	0.44
2:H:360:SER:O	2:H:363:THR:HG23	2.18	0.44
2:J:359:GLN:C	2:J:361:TRP:N	2.76	0.44
2:L:207:ASP:O	2:L:208:ASN:HB2	2.18	0.44
2:J:38:GLU:HG2	2:J:38:GLU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:PRO:HB2	2:B:117:TYR:CD2	2.53	0.43
1:C:207:GLN:OE1	2:D:216:LEU:HD13	2.18	0.43
2:D:295:ARG:NH1	2:D:299:LEU:CD1	2.81	0.43
2:H:24:ARG:HG3	2:H:24:ARG:NH1	2.32	0.43
1:K:92:TYR:O	1:K:97:ARG:NH2	2.52	0.43
2:L:353:ARG:HD3	2:L:353:ARG:C	2.44	0.43
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.19	0.43
2:L:130:SER:O	2:L:134:ILE:HG13	2.18	0.43
1:G:263:THR:HG21	1:G:280:LEU:HB2	2.00	0.43
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.53	0.43
1:I:252:ASP:OD2	1:I:252:ASP:C	2.61	0.43
2:J:311:LYS:HG3	2:J:312:TRP:CD2	2.53	0.43
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.26	0.43
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.54	0.43
1:E:121:ARG:HH11	1:E:121:ARG:CG	2.32	0.43
2:F:29:PHE:O	2:F:33:LEU:HD22	2.19	0.43
2:F:333:GLU:HA	8:F:875:HOH:O	2.18	0.43
2:H:207:ASP:O	2:H:208:ASN:HB2	2.18	0.43
1:K:328:ASP:O	1:K:329:ASN:HB2	2.18	0.43
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.34	0.43
2:D:116:PRO:HB2	2:D:117:TYR:CD2	2.53	0.43
1:G:330:LYS:HE2	1:G:367:HIS:HB3	2.00	0.43
1:K:151:GLU:HG3	1:K:175:LEU:HD11	2.00	0.43
2:L:245:LEU:O	2:L:249:LYS:HG3	2.19	0.43
2:D:110:ASN:HB3	2:D:111:PRO:HD2	2.01	0.43
2:F:21:LEU:N	2:F:21:LEU:CD1	2.82	0.43
2:F:30:GLN:O	2:F:34:GLN:HG3	2.19	0.43
1:K:223:VAL:HG11	1:K:240:ARG:HB2	2.01	0.43
2:L:311:LYS:HG3	2:L:312:TRP:CD2	2.54	0.43
1:A:340:LEU:HD23	1:A:343:ILE:HD12	2.01	0.43
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.01	0.43
1:G:72:TRP:CZ2	1:G:115:ARG:HB2	2.53	0.43
2:H:18:LEU:N	2:H:18:LEU:CD2	2.81	0.43
2:J:53:PHE:HE1	7:M:1727:GER:H42	1.84	0.43
2:L:250:ARG:O	2:L:254:MET:HG2	2.19	0.43
2:B:192:ASP:OD1	2:B:195:LYS:HE3	2.18	0.43
2:F:103:ILE:HG23	2:F:104:PRO:HD2	2.00	0.43
2:J:320:LEU:C	2:J:320:LEU:HD23	2.44	0.43
1:K:339:GLU:O	1:K:343:ILE:HG13	2.19	0.43
2:L:21:LEU:HG	8:L:632:HOH:O	2.19	0.43
2:L:122:ILE:HG22	2:L:163:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ARG:HD3	8:C:1272:HOH:O	2.19	0.43
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.18	0.43
1:C:296:LEU:HD22	1:C:322:MET:CE	2.49	0.42
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.54	0.42
2:D:311:LYS:HE2	2:D:312:TRP:CZ2	2.54	0.42
2:F:116:PRO:HB2	2:F:117:TYR:CD2	2.54	0.42
2:F:269:ASP:OD1	2:F:269:ASP:C	2.62	0.42
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.54	0.42
2:J:295:ARG:HE	2:J:334:GLU:CD	2.26	0.42
1:C:286:ASP:HB2	8:C:621:HOH:O	2.18	0.42
1:C:296:LEU:CD2	1:C:322:MET:HE1	2.49	0.42
3:M:508:CYS:C	7:M:1727:GER:H11	2.44	0.42
2:D:86:ASP:OD2	2:D:86:ASP:N	2.48	0.42
1:E:329:ASN:HB3	1:E:332:ASP:HB3	2.00	0.42
2:H:354:LEU:HD11	2:H:358:HIS:NE2	2.34	0.42
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.89	0.42
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.53	0.42
2:D:243:LYS:HE2	2:D:243:LYS:HB3	1.87	0.42
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.53	0.42
2:L:22:ARG:O	2:L:26:VAL:HG23	2.18	0.42
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.84	0.42
6:F:1723:GRG:HC62	6:F:1723:GRG:H101	1.91	0.42
1:K:329:ASN:HB3	1:K:332:ASP:HB3	2.02	0.42
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.55	0.42
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.82	0.42
2:B:320:LEU:C	2:B:320:LEU:HD23	2.45	0.42
1:I:287:ARG:H	1:I:287:ARG:HG2	1.59	0.42
2:L:79:LEU:O	2:L:96:ARG:HG3	2.19	0.42
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.55	0.42
2:L:320:LEU:C	2:L:320:LEU:HD23	2.44	0.42
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.55	0.42
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.02	0.42
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.02	0.42
2:F:311:LYS:HE2	2:F:312:TRP:CZ2	2.54	0.42
2:B:21:LEU:N	2:B:21:LEU:CD1	2.83	0.42
2:F:353:ARG:NE	8:F:739:HOH:O	2.52	0.42
2:L:269:ASP:C	2:L:269:ASP:OD1	2.62	0.42
2:H:320:LEU:C	2:H:320:LEU:HD23	2.45	0.42
2:L:311:LYS:HE2	2:L:312:TRP:CZ2	2.55	0.42
1:A:359:ILE:HD13	1:A:359:ILE:HA	1.92	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:SER:O	2:H:66:VAL:HG22	2.20	0.42
2:H:87:ARG:HB3	2:H:87:ARG:NH1	2.35	0.42
2:J:122:ILE:HG22	2:J:163:ALA:HA	2.01	0.42
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.54	0.41
2:J:59:ASP:OD2	2:J:349:ARG:NH1	2.53	0.41
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.55	0.41
1:E:219:GLU:HA	1:E:219:GLU:OE1	2.19	0.41
1:K:91:ILE:HD12	1:K:91:ILE:C	2.44	0.41
2:L:69:LYS:O	2:L:73:ILE:HG13	2.20	0.41
1:E:214:ARG:O	1:E:214:ARG:CG	2.68	0.41
2:J:138:ASP:O	2:J:139:LEU:HB2	2.20	0.41
1:K:82:ASP:HB2	1:K:86:PRO:HB3	2.03	0.41
2:F:37:PRO:HD2	2:F:40:TYR:HD1	1.85	0.41
1:G:287:ARG:H	1:G:287:ARG:HG2	1.54	0.41
3:N:608:CYS:C	7:N:1727:GER:H11	2.44	0.41
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.55	0.41
2:B:77:TYR:CE1	2:B:141:ARG:HB2	2.55	0.41
1:E:329:ASN:O	1:E:330:LYS:C	2.63	0.41
2:F:188:TRP:CE3	2:F:193:MET:HE2	2.56	0.41
2:J:155:GLN:HB2	2:J:161:PHE:CE2	2.56	0.41
2:J:246:ASN:ND2	8:J:395:HOH:O	2.54	0.41
2:D:26:VAL:O	2:D:30:GLN:HG3	2.21	0.41
2:D:269:ASP:OD1	2:D:269:ASP:C	2.63	0.41
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.35	0.41
7:M:1727:GER:H112	7:M:1727:GER:H91	1.88	0.41
1:C:329:ASN:HB3	1:C:332:ASP:HB3	2.01	0.41
2:D:320:LEU:C	2:D:320:LEU:HD23	2.45	0.41
1:E:155:ILE:HD12	1:E:155:ILE:HA	1.94	0.41
1:I:136:PHE:CE2	1:I:140:LEU:HD11	2.55	0.41
1:I:344:LEU:HA	1:I:348:LYS:HB2	2.02	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.55	0.41
1:K:149:GLN:HG3	8:K:1048:HOH:O	2.20	0.41
2:L:116:PRO:HB2	2:L:117:TYR:CD2	2.56	0.41
1:A:92:TYR:O	1:A:97:ARG:NH2	2.54	0.41
2:B:208:ASN:CG	2:B:247:ARG:HB3	2.45	0.41
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.36	0.41
2:H:49:THR:HG23	2:H:124:MET:SD	2.61	0.41
1:I:71:GLU:H	1:I:71:GLU:CD	2.28	0.41
2:J:121:HIS:HB3	2:J:124:MET:HG2	2.03	0.41
2:J:269:ASP:C	2:J:269:ASP:OD1	2.63	0.41
2:L:37:PRO:HD2	2:L:40:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:ASP:O	2:B:139:LEU:HB2	2.20	0.41
1:C:353:LYS:HE3	1:K:339:GLU:HG3	2.03	0.41
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.55	0.41
1:E:353:LYS:CE	1:E:357:ARG:HH22	2.34	0.41
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.84	0.41
1:G:189:ILE:HG21	1:G:206:ARG:HB2	2.03	0.41
2:H:30:GLN:O	2:H:34:GLN:HG3	2.21	0.41
2:H:133:ILE:HG22	2:H:350:THR:HG23	2.02	0.41
2:H:193:MET:HE2	2:H:233:MET:CG	2.51	0.41
2:H:341:HIS:HA	2:H:342:PRO:HD2	1.81	0.41
2:H:352:GLU:OE2	2:H:352:GLU:HA	2.20	0.41
2:J:250:ARG:O	2:J:254:MET:HG2	2.20	0.41
2:L:36:LEU:HA	2:L:37:PRO:HD3	1.93	0.41
2:L:40:TYR:CE2	7:N:1727:GER:H101	2.56	0.41
2:L:236:LEU:HD22	2:L:245:LEU:HD21	2.03	0.41
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.55	0.41
1:A:331:GLU:O	1:A:335:ASN:ND2	2.54	0.41
2:B:52:PHE:HA	2:B:131:CYS:SG	2.61	0.41
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.04	0.41
2:J:245:LEU:O	2:J:249:LYS:HG3	2.21	0.41
1:K:184:GLN:HB2	8:K:382:HOH:O	2.20	0.41
1:A:87:VAL:O	1:A:88:VAL:C	2.64	0.40
2:B:249:LYS:HB3	2:B:285:ILE:HD13	2.03	0.40
2:D:156:LEU:HD21	2:D:162:CYS:SG	2.61	0.40
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.21	0.40
1:C:287:ARG:H	1:C:287:ARG:HG2	1.64	0.40
2:D:258:ASN:OD1	2:D:259:GLY:N	2.42	0.40
1:I:91:ILE:HD12	1:I:91:ILE:C	2.45	0.40
1:K:287:ARG:H	1:K:287:ARG:HG2	1.63	0.40
2:L:49:THR:HG23	2:L:124:MET:SD	2.61	0.40
2:B:64:LEU:HB3	2:B:69:LYS:HE2	2.03	0.40
1:G:58:LEU:HD23	1:G:63:TYR:CE2	2.56	0.40
1:I:350:THR:O	1:I:353:LYS:HB3	2.21	0.40
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.49	0.40
2:L:64:LEU:HA	2:L:64:LEU:HD23	1.90	0.40
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.35	0.40
2:B:298:ILE:HD12	2:B:329:LEU:HD13	2.04	0.40
1:G:151:GLU:HG3	1:G:175:LEU:HD11	2.02	0.40
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.56	0.40
2:F:64:LEU:HD11	2:F:134:ILE:HG22	2.04	0.40
2:F:320:LEU:HD23	2:F:320:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:ASP:N	2:H:86:ASP:OD2	2.50	0.40
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.56	0.40
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.56	0.40
1:I:124:ILE:HD13	1:I:134:TRP:CH2	2.57	0.40
2:J:30:GLN:HE21	2:J:30:GLN:HB3	1.65	0.40
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.57	0.40
2:J:64:LEU:HB3	2:J:69:LYS:HE2	2.03	0.40

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%)	287 (92%)	23 (7%)	2 (1%)	21	34
1	C	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	36	52
1	E	312/377 (83%)	289 (93%)	21 (7%)	2 (1%)	21	34
1	G	312/377 (83%)	291 (93%)	19 (6%)	2 (1%)	21	34
1	I	312/377 (83%)	289 (93%)	21 (7%)	2 (1%)	21	34
1	K	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	21	34
2	B	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	36	52
2	D	344/377 (91%)	329 (96%)	13 (4%)	2 (1%)	21	34
2	F	344/377 (91%)	328 (95%)	15 (4%)	1 (0%)	36	52
2	H	344/377 (91%)	323 (94%)	19 (6%)	2 (1%)	21	34
2	J	344/377 (91%)	324 (94%)	19 (6%)	1 (0%)	36	52
2	L	344/377 (91%)	330 (96%)	13 (4%)	1 (0%)	36	52
3	M	2/11 (18%)	2 (100%)	0	0	100	100
3	N	2/11 (18%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3940/4546 (87%)	3705 (94%)	216 (6%)	19 (0%)	24	39

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
1	G	306	HIS
1	G	326	GLN
2	H	258	ASN
1	I	306	HIS
2	J	258	ASN
1	K	306	HIS
2	L	258	ASN
1	A	306	HIS
1	A	326	GLN
2	D	258	ASN
2	F	258	ASN
1	I	326	GLN
1	K	326	GLN
1	C	306	HIS
2	D	333	GLU
1	E	306	HIS
2	H	333	GLU
1	E	326	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/338 (83%)	275 (98%)	5 (2%)	51	72
1	C	283/338 (84%)	276 (98%)	7 (2%)	42	64
1	E	284/338 (84%)	277 (98%)	7 (2%)	42	64
1	G	281/338 (83%)	276 (98%)	5 (2%)	51	72
1	I	287/338 (85%)	281 (98%)	6 (2%)	47	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	291/338 (86%)	283 (97%)	8 (3%)	39	61
2	B	289/326 (89%)	275 (95%)	14 (5%)	23	39
2	D	293/326 (90%)	277 (94%)	16 (6%)	19	33
2	F	294/326 (90%)	281 (96%)	13 (4%)	25	43
2	H	288/326 (88%)	276 (96%)	12 (4%)	26	45
2	J	292/326 (90%)	278 (95%)	14 (5%)	23	39
2	L	296/326 (91%)	280 (95%)	16 (5%)	20	35
3	M	4/11 (36%)	4 (100%)	0	100	100
3	N	4/11 (36%)	4 (100%)	0	100	100
All	All	3466/4006 (86%)	3343 (96%)	123 (4%)	32	52

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	PHE
1	A	71	GLU
1	A	114	GLU
1	A	214	ARG
1	A	287	ARG
2	B	21	LEU
2	B	33	LEU
2	B	39	ARG
2	B	113	THR
2	B	151	LEU
2	B	216	LEU
2	B	222	SER
2	B	232	LEU
2	B	236	LEU
2	B	258	ASN
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	59	ASP
1	C	71	GLU
1	C	114	GLU
1	C	182	PRO
1	C	287	ARG
1	C	324	GLU

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Mol	Chain	Res	Type
1	C	364	GLN
2	D	21	LEU
2	D	27	ARG
2	D	33	LEU
2	D	39	ARG
2	D	110	ASN
2	D	151	LEU
2	D	216	LEU
2	D	222	SER
2	D	232	LEU
2	D	236	LEU
2	D	255	ARG
2	D	258	ASN
2	D	268	VAL
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
1	E	55	PHE
1	E	67	ARG
1	E	71	GLU
1	E	121	ARG
1	E	214	ARG
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	33	LEU
2	F	39	ARG
2	F	151	LEU
2	F	216	LEU
2	F	222	SER
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	258	ASN
2	F	306	VAL
2	F	329	LEU
2	F	331	LEU
1	G	71	GLU
1	G	114	GLU
1	G	224	ASP
1	G	287	ARG
1	G	324	GLU

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Mol	Chain	Res	Type
2	H	18	LEU
2	H	21	LEU
2	H	151	LEU
2	H	216	LEU
2	H	222	SER
2	H	232	LEU
2	H	236	LEU
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	348	THR
2	H	357	LEU
1	I	55	PHE
1	I	71	GLU
1	I	114	GLU
1	I	142	ARG
1	I	287	ARG
1	I	364	GLN
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	33	LEU
2	J	151	LEU
2	J	216	LEU
2	J	222	SER
2	J	232	LEU
2	J	236	LEU
2	J	268	VAL
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	357	LEU
1	K	71	GLU
1	K	107	LEU
1	K	114	GLU
1	K	142	ARG
1	K	156	ILE
1	K	194	ASN
1	K	324	GLU
1	K	357	ARG
2	L	21	LEU
2	L	33	LEU

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Mol	Chain	Res	Type
2	L	46	SER
2	L	65	ASP
2	L	110	ASN
2	L	151	LEU
2	L	210	LEU
2	L	216	LEU
2	L	222	SER
2	L	232	LEU
2	L	236	LEU
2	L	258	ASN
2	L	268	VAL
2	L	306	VAL
2	L	329	LEU
2	L	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	89	GLN
1	A	135	HIS
1	A	149	GLN
1	A	285	GLN
1	A	303	GLN
1	A	329	ASN
1	A	335	ASN
1	A	367	HIS
2	B	208	ASN
2	B	212	GLN
2	B	257	GLN
1	C	81	ASN
1	C	108	GLN
1	C	135	HIS
1	C	149	GLN
1	C	184	GLN
1	C	218	ASN
1	C	261	GLN
1	C	285	GLN
1	C	298	GLN
1	C	303	GLN
1	C	367	HIS
2	D	30	GLN

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Mol	Chain	Res	Type
2	D	208	ASN
2	D	212	GLN
2	D	246	ASN
2	D	257	GLN
1	E	81	ASN
1	E	89	GLN
1	E	135	HIS
1	E	145	GLN
1	E	184	GLN
1	E	298	GLN
1	E	325	ASN
1	E	335	ASN
1	E	364	GLN
2	F	208	ASN
2	F	212	GLN
2	F	246	ASN
1	G	80	GLN
1	G	89	GLN
1	G	135	HIS
1	G	162	GLN
1	G	195	GLN
1	G	238	ASN
1	G	297	ASN
1	G	303	GLN
1	G	325	ASN
1	G	335	ASN
1	G	367	HIS
2	H	212	GLN
2	H	257	GLN
1	I	89	GLN
1	I	108	GLN
1	I	135	HIS
1	I	149	GLN
1	I	285	GLN
1	I	364	GLN
1	I	367	HIS
2	J	30	GLN
2	J	208	ASN
2	J	212	GLN
2	J	246	ASN
2	J	296	ASN
1	K	89	GLN

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Mol	Chain	Res	Type
1	K	135	HIS
1	K	238	ASN
1	K	285	GLN
1	K	298	GLN
2	L	208	ASN
2	L	212	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 15 are monoatomic - leaving 8 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	1727	-	19,19,19	0.85	0	21,22,22	0.62	0
7	GER	N	1727	-	19,19,19	0.88	0	21,22,22	0.64	0
6	GRG	H	1724	-	27,28,28	0.74	0	33,37,37	0.90	1 (3%)
6	GRG	F	1723	-	27,28,28	0.79	0	33,37,37	0.87	1 (3%)
6	GRG	B	1721	-	27,28,28	0.81	0	33,37,37	0.90	1 (3%)
6	GRG	L	1726	-	27,28,28	0.81	0	33,37,37	0.91	1 (3%)
6	GRG	D	1722	-	27,28,28	0.81	0	33,37,37	0.88	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GRG	J	1725	-	27,28,28	0.78	0	33,37,37	0.87	1 (3%)

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	1727	-	-	9/20/20/20	-
7	GER	N	1727	-	-	9/20/20/20	-
6	GRG	H	1724	-	-	8/31/31/31	-
6	GRG	F	1723	-	-	6/31/31/31	-
6	GRG	B	1721	-	-	7/31/31/31	-
6	GRG	L	1726	-	-	7/31/31/31	-
6	GRG	D	1722	-	-	6/31/31/31	-
6	GRG	J	1725	-	-	8/31/31/31	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1726	GRG	O1B-PB-O3A	2.61	113.40	104.64
6	B	1721	GRG	O1B-PB-O3A	2.58	113.30	104.64
6	H	1724	GRG	O1B-PB-O3A	2.56	113.24	104.64
6	D	1722	GRG	O1B-PB-O3A	2.53	113.12	104.64
6	J	1725	GRG	O1B-PB-O3A	2.45	112.86	104.64
6	F	1723	GRG	O1B-PB-O3A	2.38	112.61	104.64

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1721	GRG	PA-O3A-PB-O1B
6	D	1722	GRG	PA-O3A-PB-O1B
6	F	1723	GRG	PA-O3A-PB-O1B
6	H	1724	GRG	PA-O3A-PB-O1B
6	J	1725	GRG	PA-O3A-PB-O1B
6	L	1726	GRG	PA-O3A-PB-O1B
7	M	1727	GER	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
7	N	1727	GER	C11-C10-C8-C9
7	M	1727	GER	C11-C10-C8-C7
7	N	1727	GER	C11-C10-C8-C7
7	M	1727	GER	C4-C3-C5-C6
7	N	1727	GER	C4-C3-C5-C6
7	M	1727	GER	C2-C3-C5-C6
7	N	1727	GER	C14-C13-C15-C16
7	M	1727	GER	C12-C13-C15-C16
7	N	1727	GER	C12-C13-C15-C16
7	M	1727	GER	C14-C13-C15-C16
7	M	1727	GER	C13-C15-C16-C17
7	N	1727	GER	C13-C15-C16-C17
7	N	1727	GER	C2-C3-C5-C6
6	L	1726	GRG	C14-C13-C15-C16
6	F	1723	GRG	C14-C13-C15-C16
6	F	1723	GRG	C10-C8-C9-C11
6	J	1725	GRG	C14-C13-C15-C16
6	B	1721	GRG	C14-C13-C15-C16
6	D	1722	GRG	C14-C13-C15-C16
6	H	1724	GRG	C14-C13-C15-C16
6	B	1721	GRG	C10-C8-C9-C11
6	D	1722	GRG	C10-C8-C9-C11
6	H	1724	GRG	C10-C8-C9-C11
6	J	1725	GRG	C10-C8-C9-C11
6	L	1726	GRG	C10-C8-C9-C11
6	H	1724	GRG	C12-C13-C15-C16
6	B	1721	GRG	PA-O3A-PB-O3B
6	H	1724	GRG	PA-O3A-PB-O3B
6	J	1725	GRG	PA-O3A-PB-O3B
6	L	1726	GRG	PA-O3A-PB-O3B
6	B	1721	GRG	C12-C13-C15-C16
6	D	1722	GRG	C12-C13-C15-C16
6	B	1721	GRG	PA-O3A-PB-O2B
6	D	1722	GRG	PA-O3A-PB-O2B
6	F	1723	GRG	PA-O3A-PB-O2B
6	H	1724	GRG	PA-O3A-PB-O2B
6	J	1725	GRG	PA-O3A-PB-O2B
6	L	1726	GRG	PA-O3A-PB-O2B
6	J	1725	GRG	C12-C13-C15-C16
6	F	1723	GRG	C12-C13-C15-C16
6	H	1724	GRG	C4-C3-C5-C6
6	L	1726	GRG	C12-C13-C15-C16

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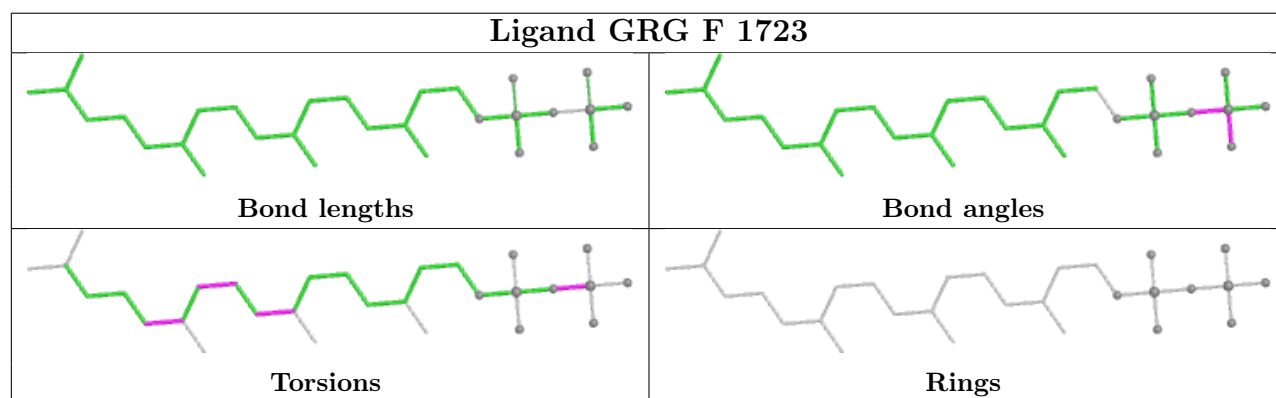
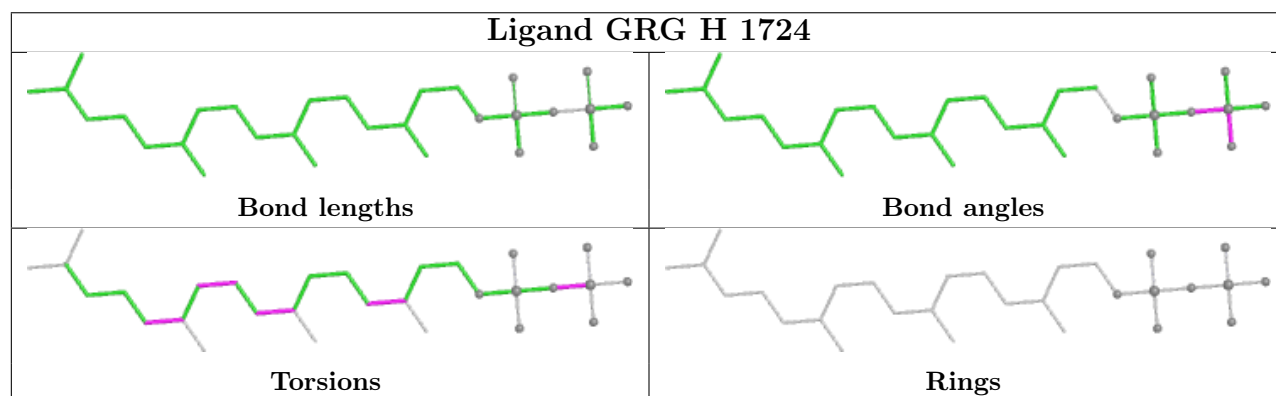
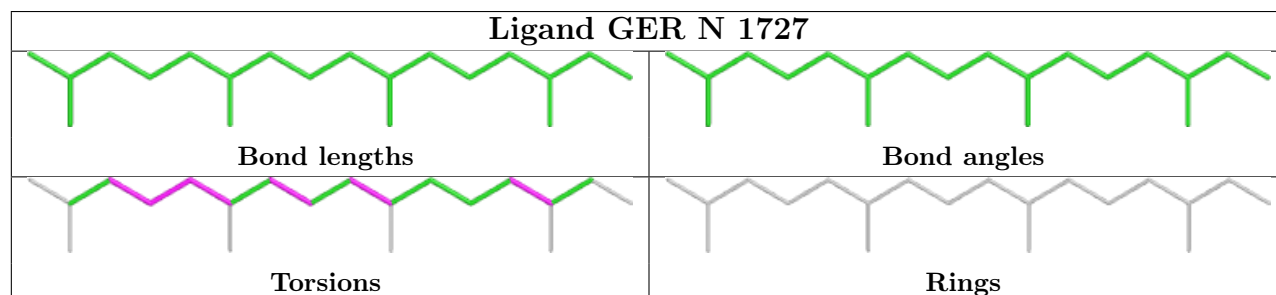
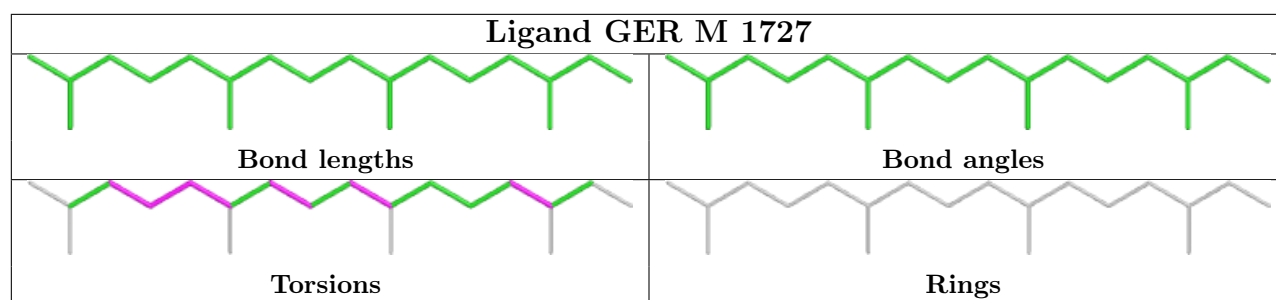
Mol	Chain	Res	Type	Atoms
6	J	1725	GRG	C9-C11-C12-C13
6	L	1726	GRG	C9-C11-C12-C13
7	M	1727	GER	C10-C11-C12-C13
7	M	1727	GER	C15-C16-C17-C18
7	N	1727	GER	C10-C11-C12-C13
7	N	1727	GER	C15-C16-C17-C18
6	B	1721	GRG	C9-C11-C12-C13
6	D	1722	GRG	C9-C11-C12-C13
6	F	1723	GRG	C9-C11-C12-C13
6	H	1724	GRG	C9-C11-C12-C13
6	J	1725	GRG	C4-C3-C5-C6

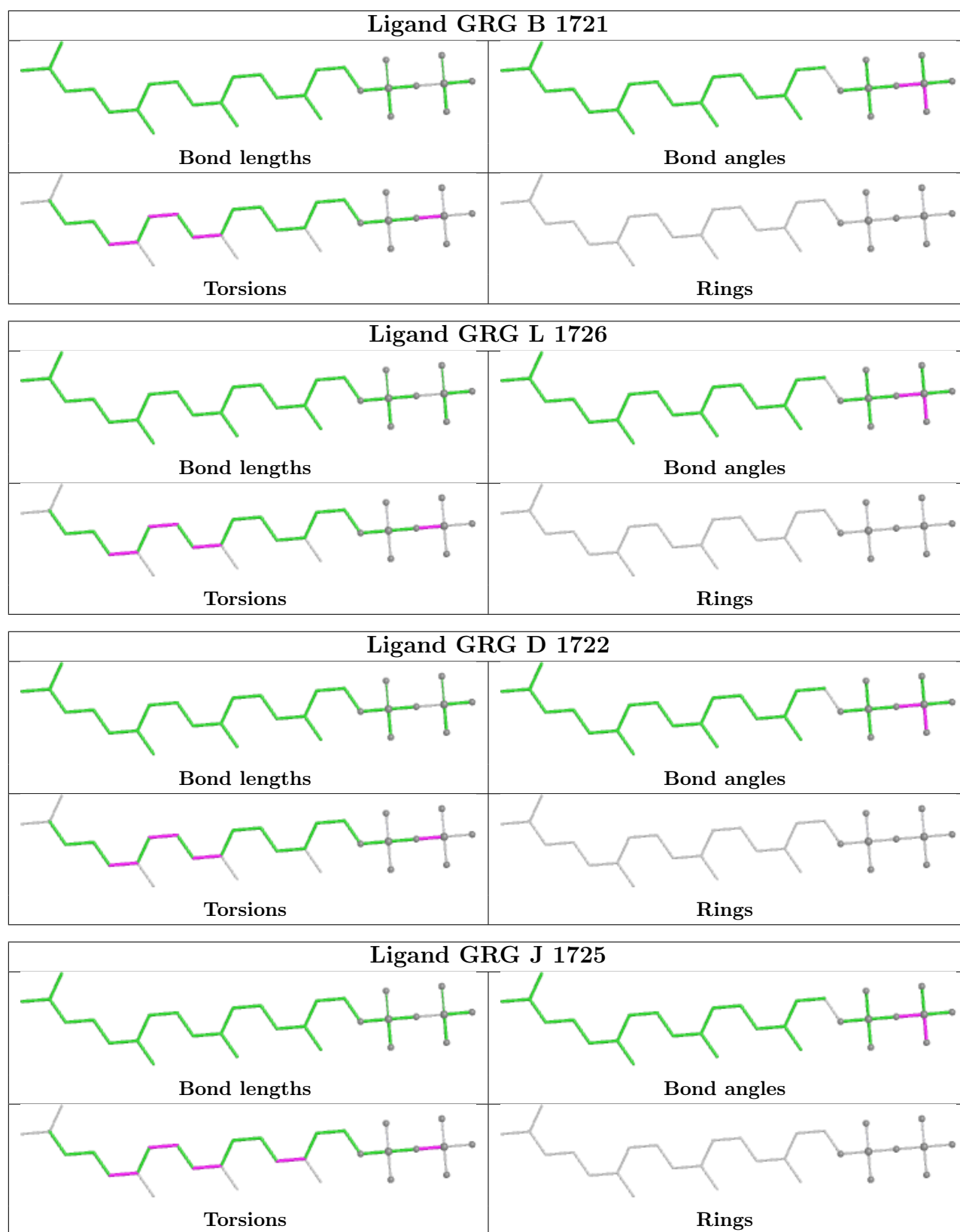
There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1727	GER	6	0
7	N	1727	GER	6	0
6	H	1724	GRG	1	0
6	F	1723	GRG	2	0
6	B	1721	GRG	1	0
6	L	1726	GRG	1	0
6	D	1722	GRG	1	0
6	J	1725	GRG	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	314/377 (83%)	0.41	24 (7%)	20	15	35, 57, 92, 110	0
1	C	314/377 (83%)	0.43	23 (7%)	21	15	33, 54, 80, 97	0
1	E	314/377 (83%)	0.61	17 (5%)	31	25	35, 59, 86, 103	0
1	G	314/377 (83%)	0.66	39 (12%)	8	7	35, 59, 87, 102	0
1	I	314/377 (83%)	0.37	24 (7%)	20	15	29, 52, 84, 95	0
1	K	314/377 (83%)	-0.11	12 (3%)	44	36	23, 41, 67, 81	0
2	B	346/377 (91%)	0.19	19 (5%)	30	24	35, 52, 75, 100	0
2	D	346/377 (91%)	0.00	14 (4%)	42	34	32, 46, 71, 95	0
2	F	346/377 (91%)	0.05	20 (5%)	29	22	34, 47, 74, 101	0
2	H	346/377 (91%)	0.98	57 (16%)	4	3	36, 65, 95, 112	0
2	J	346/377 (91%)	0.24	25 (7%)	21	16	30, 50, 80, 104	0
2	L	346/377 (91%)	-0.20	16 (4%)	37	29	25, 40, 65, 93	0
3	M	4/11 (36%)	4.69	4 (100%)	0	0	51, 55, 61, 66	4 (100%)
3	N	4/11 (36%)	4.54	4 (100%)	0	0	51, 56, 63, 69	4 (100%)
All	All	3968/4546 (87%)	0.31	298 (7%)	20	15	23, 52, 84, 112	8 (0%)

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	18	LEU	7.3
1	C	55	PHE	7.1
3	M	509	VAL	7.1
1	G	55	PHE	6.9
1	E	55	PHE	6.8
3	N	609	VAL	6.5
2	J	110	ASN	6.2
3	M	508	CYS	6.2

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Mol	Chain	Res	Type	RSRZ
2	H	18	LEU	6.0
2	H	362	LYS	6.0
1	I	55	PHE	5.6
2	B	110	ASN	5.5
2	H	113	THR	5.4
2	B	18	LEU	5.4
2	H	85	GLU	5.4
2	F	363	THR	5.0
2	L	363	THR	4.9
2	J	18	LEU	4.9
2	B	113	THR	4.9
3	N	608	CYS	4.9
1	G	368	SER	4.9
2	H	110	ASN	4.9
2	H	111	PRO	4.9
2	F	113	THR	4.8
2	F	110	ASN	4.8
2	D	363	THR	4.6
2	J	363	THR	4.6
1	K	55	PHE	4.5
2	H	363	THR	4.5
2	J	108	SER	4.5
1	I	368	SER	4.4
2	J	113	THR	4.4
2	B	363	THR	4.3
1	G	326	GLN	4.3
2	H	314	ASP	4.2
2	H	335	SER	4.2
1	C	368	SER	4.2
1	A	55	PHE	4.2
2	L	111	PRO	4.1
1	E	332	ASP	4.1
1	G	304	PRO	4.1
2	L	18	LEU	4.0
2	J	111	PRO	4.0
1	C	306	HIS	4.0
2	H	359	GLN	4.0
2	B	362	LYS	4.0
2	H	65	ASP	3.9
1	A	368	SER	3.9
1	A	331	GLU	3.9
1	E	368	SER	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	304	ARG	3.9
2	H	108	SER	3.8
2	H	316	HIS	3.8
1	A	328	ASP	3.8
2	D	111	PRO	3.8
2	D	314	ASP	3.8
1	G	57	SER	3.8
2	F	111	PRO	3.7
2	H	315	SER	3.7
1	G	364	GLN	3.7
2	D	109	LYS	3.7
1	A	364	GLN	3.7
2	D	113	THR	3.6
3	N	611	LEU	3.6
1	A	326	GLN	3.6
2	F	362	LYS	3.6
2	H	305	LEU	3.6
1	E	306	HIS	3.5
2	H	112	GLY	3.5
2	B	111	PRO	3.5
1	C	331	GLU	3.4
2	L	85	GLU	3.4
1	G	305	SER	3.3
2	L	108	SER	3.3
1	K	332	ASP	3.3
1	G	91	ILE	3.3
1	C	304	PRO	3.3
2	B	85	GLU	3.3
1	I	327	CYS	3.2
2	J	85	GLU	3.2
3	N	610	ILE	3.2
2	L	362	LYS	3.2
2	F	112	GLY	3.2
2	J	338	CYS	3.2
2	H	336	GLY	3.1
1	G	92	TYR	3.1
2	D	18	LEU	3.1
2	J	106	ASN	3.1
3	M	511	LEU	3.0
1	E	331	GLU	3.0
2	F	314	ASP	3.0
1	G	195	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	85	GLU	3.0
2	L	106	ASN	3.0
2	H	144	LYS	3.0
1	C	328	ASP	3.0
2	H	39	ARG	3.0
1	I	305	SER	2.9
2	H	24	ARG	2.9
2	L	110	ASN	2.9
1	G	328	ASP	2.9
2	L	113	THR	2.9
1	G	56	LEU	2.9
1	C	265	GLU	2.9
2	F	316	HIS	2.9
1	G	365	SER	2.9
2	D	65	ASP	2.9
1	G	125	GLU	2.9
1	I	85	SER	2.9
1	K	326	GLN	2.8
2	L	314	ASP	2.8
1	A	327	CYS	2.8
1	G	306	HIS	2.8
2	H	107	PRO	2.8
2	H	361	TRP	2.8
1	A	59	ASP	2.8
2	B	360	SER	2.8
1	C	332	ASP	2.8
2	B	316	HIS	2.8
1	G	61	PRO	2.7
2	H	109	LYS	2.7
1	E	330	LYS	2.7
1	G	366	LYS	2.7
2	H	71	ASP	2.7
1	I	81	ASN	2.7
1	I	328	ASP	2.7
2	F	109	LYS	2.7
1	E	109	ARG	2.7
1	C	81	ASN	2.7
1	I	251	SER	2.7
2	F	39	ARG	2.6
2	H	308	GLY	2.6
2	F	108	SER	2.6
1	A	366	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	307	SER	2.6
1	E	326	GLN	2.6
1	K	305	SER	2.6
1	G	59	ASP	2.6
1	E	268	LYS	2.6
2	B	109	LYS	2.6
2	H	338	CYS	2.6
1	I	335	ASN	2.6
2	B	314	ASP	2.5
1	I	306	HIS	2.5
1	C	326	GLN	2.5
2	H	105	PHE	2.5
2	H	310	ALA	2.5
1	C	251	SER	2.5
2	J	335	SER	2.5
1	K	59	ASP	2.5
2	H	70	ASP	2.5
1	C	94	GLU	2.5
1	C	305	SER	2.5
1	G	58	LEU	2.5
1	I	332	ASP	2.5
2	H	27	ARG	2.5
2	J	62	ASP	2.5
1	A	272	HIS	2.5
1	C	195	GLN	2.5
1	C	303	GLN	2.5
2	F	359	GLN	2.5
2	H	306	VAL	2.5
3	M	510	ILE	2.5
2	F	65	ASP	2.5
2	H	19	ASP	2.5
1	A	268	LYS	2.4
2	D	110	ASN	2.4
2	J	89	ASN	2.4
1	I	59	ASP	2.4
1	K	304	PRO	2.4
2	F	87	ARG	2.4
2	H	87	ARG	2.4
2	H	63	SER	2.4
1	I	331	GLU	2.4
2	J	107	PRO	2.4
2	D	362	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	87	ARG	2.4
2	B	305	LEU	2.4
1	A	301	ASP	2.4
1	C	125	GLU	2.4
2	J	91	ASP	2.4
2	H	29	PHE	2.4
1	E	56	LEU	2.4
1	I	329	ASN	2.4
1	K	81	ASN	2.4
2	F	91	ASP	2.4
2	J	314	ASP	2.4
2	H	234	GLY	2.4
2	H	35	VAL	2.4
1	G	62	THR	2.3
1	E	94	GLU	2.3
1	I	290	SER	2.3
2	B	315	SER	2.3
1	A	300	LEU	2.3
2	F	85	GLU	2.3
1	C	217	ASP	2.3
1	E	303	GLN	2.3
1	I	364	GLN	2.3
2	B	112	GLY	2.3
2	H	82	LEU	2.3
1	I	330	LYS	2.3
1	G	81	ASN	2.3
1	K	368	SER	2.3
1	C	225	GLN	2.3
1	G	80	GLN	2.3
1	G	83	GLY	2.3
2	D	359	GLN	2.3
1	G	348	LYS	2.3
1	G	94	GLU	2.3
2	H	92	ARG	2.3
2	J	360	SER	2.3
2	J	105	PHE	2.3
1	G	333	ILE	2.2
2	B	114	ALA	2.2
2	L	114	ALA	2.2
1	K	331	GLU	2.2
1	A	304	PRO	2.2
2	H	140	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	2.2
2	H	64	LEU	2.2
2	H	135	LEU	2.2
2	J	109	LYS	2.2
2	F	38	GLU	2.2
1	A	81	ASN	2.2
1	A	335	ASN	2.2
1	G	335	ASN	2.2
2	H	104	PRO	2.2
1	A	303	GLN	2.2
1	I	326	GLN	2.2
1	K	364	GLN	2.2
1	E	328	ASP	2.2
1	I	365	SER	2.2
2	D	316	HIS	2.2
1	E	161	GLU	2.2
2	H	38	GLU	2.2
2	H	292	GLU	2.2
2	H	349	ARG	2.2
2	H	40	TYR	2.2
2	L	109	LYS	2.2
2	L	112	GLY	2.2
1	C	75	ILE	2.2
1	I	125	GLU	2.2
2	D	39	ARG	2.2
1	E	294	ASN	2.2
1	E	353	LYS	2.2
2	H	69	LYS	2.2
1	A	217	ASP	2.2
1	G	75	ILE	2.2
2	J	114	ALA	2.1
2	B	292	GLU	2.1
2	H	333	GLU	2.1
1	G	109	ARG	2.1
2	H	31	ARG	2.1
2	L	87	ARG	2.1
1	A	261	GLN	2.1
1	A	249	GLY	2.1
1	G	82	ASP	2.1
1	G	87	VAL	2.1
2	B	65	ASP	2.1
1	G	265	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	352	GLU	2.1
2	J	333	GLU	2.1
2	J	353	ARG	2.1
2	J	84	THR	2.1
1	A	330	LYS	2.1
1	C	330	LYS	2.1
1	G	86	PRO	2.1
1	G	327	CYS	2.1
2	H	61	LEU	2.1
1	I	82	ASP	2.1
2	H	91	ASP	2.1
2	L	91	ASP	2.1
1	G	60	SER	2.1
1	G	177	GLU	2.1
1	G	89	GLN	2.1
2	H	106	ASN	2.1
1	I	76	ASP	2.1
2	H	23	ASP	2.1
2	H	62	ASP	2.1
2	J	70	ASP	2.1
2	B	108	SER	2.1
1	A	324	GLU	2.1
1	C	347	GLU	2.1
2	J	39	ARG	2.1
1	I	304	PRO	2.1
2	L	86	ASP	2.0
2	J	352	GLU	2.0
1	K	85	SER	2.0
1	I	225	GLN	2.0
2	D	305	LEU	2.0
1	G	272	HIS	2.0
2	F	106	ASN	2.0
1	K	265	GLU	2.0
1	C	365	SER	2.0
1	E	304	PRO	2.0
1	A	306	HIS	2.0
1	G	329	ASN	2.0
2	H	22	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

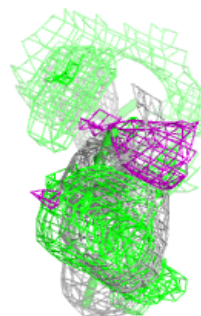
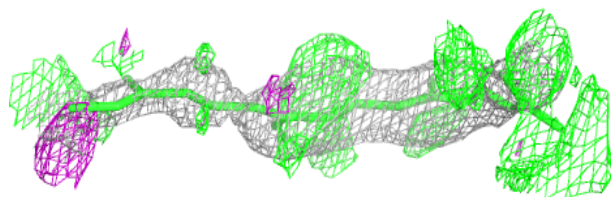
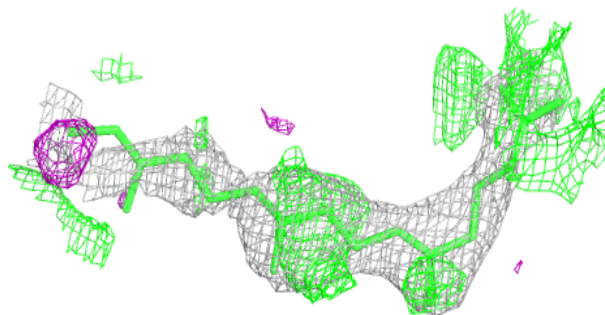
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GER	M	1727	20/20	0.87	0.31	67,74,81,82	20
7	GER	N	1727	20/20	0.87	0.32	63,70,82,82	20
5	CL	C	1705	1/1	0.95	0.23	55,55,55,55	0
6	GRG	H	1724	29/29	0.95	0.13	52,57,72,73	0
6	GRG	F	1723	29/29	0.96	0.11	47,52,59,59	0
5	CL	J	1715	1/1	0.96	0.07	58,58,58,58	0
6	GRG	L	1726	29/29	0.96	0.11	37,42,53,58	0
6	GRG	B	1721	29/29	0.96	0.12	48,53,59,60	0
6	GRG	D	1722	29/29	0.96	0.11	42,48,55,57	0
5	CL	B	1702	1/1	0.97	0.11	64,64,64,64	0
5	CL	K	1717	1/1	0.97	0.12	55,55,55,55	0
6	GRG	J	1725	29/29	0.97	0.10	38,44,55,58	0
5	CL	D	1706	1/1	0.98	0.05	41,41,41,41	0
5	CL	H	1712	1/1	0.98	0.05	58,58,58,58	0
4	ZN	H	378	1/1	0.99	0.04	54,54,54,54	0
5	CL	F	1709	1/1	0.99	0.06	46,46,46,46	0
5	CL	G	1711	1/1	0.99	0.19	55,55,55,55	0
5	CL	L	1718	1/1	0.99	0.04	43,43,43,43	0
4	ZN	B	378	1/1	1.00	0.01	38,38,38,38	0
4	ZN	J	378	1/1	1.00	0.01	35,35,35,35	0
4	ZN	L	378	1/1	1.00	0.01	27,27,27,27	0
4	ZN	D	378	1/1	1.00	0.01	37,37,37,37	0
4	ZN	F	378	1/1	1.00	0.01	40,40,40,40	0

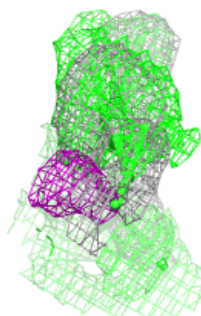
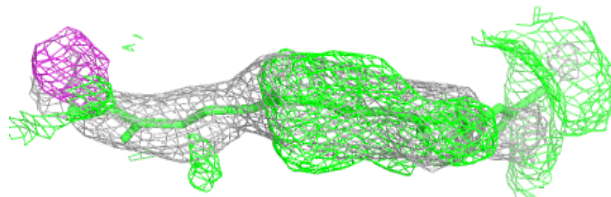
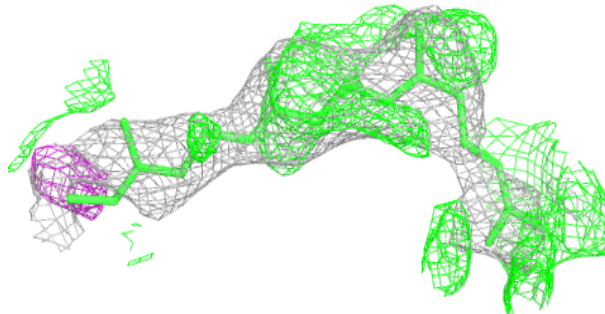
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GER M 1727:

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

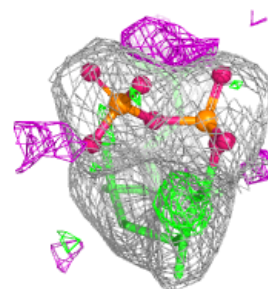
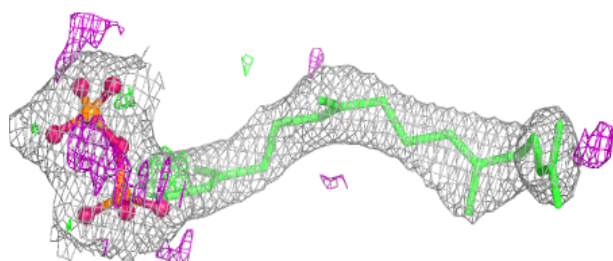
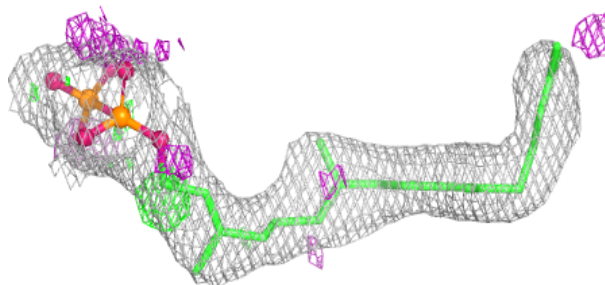
**Electron density around GER N 1727:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

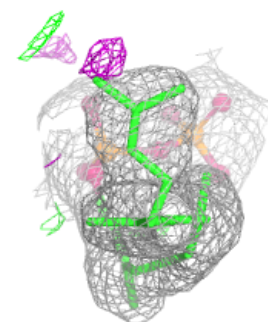
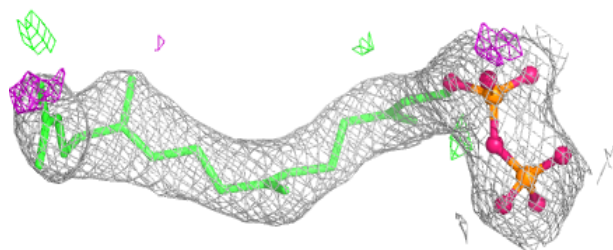
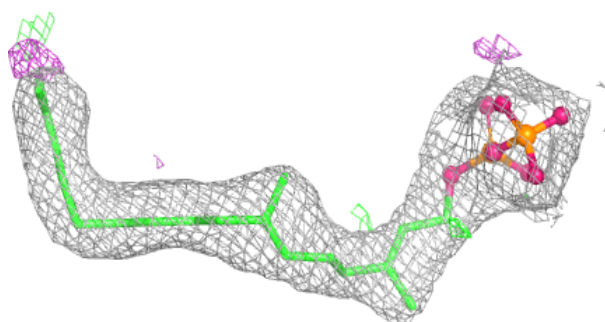


Electron density around GRG H 1724:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

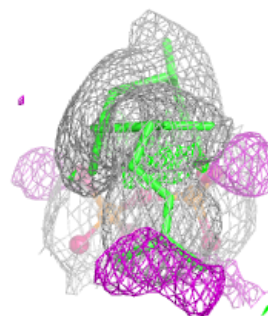
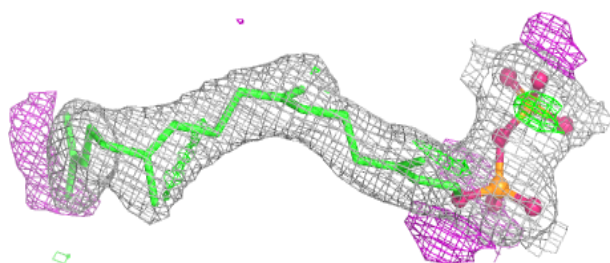
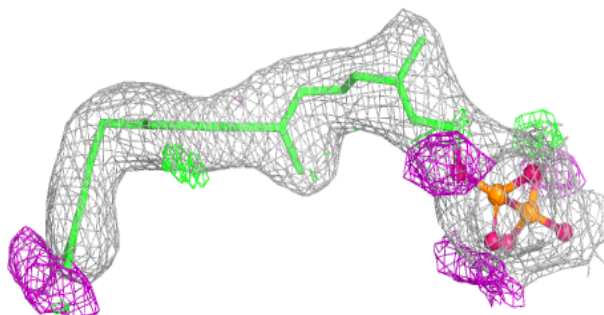
**Electron density around GRG F 1723:**

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

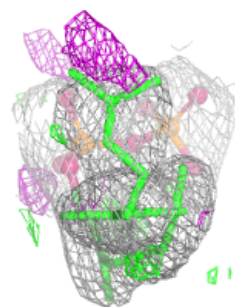
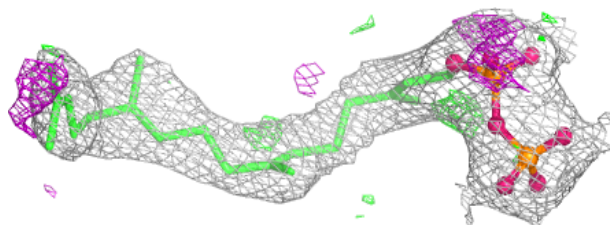
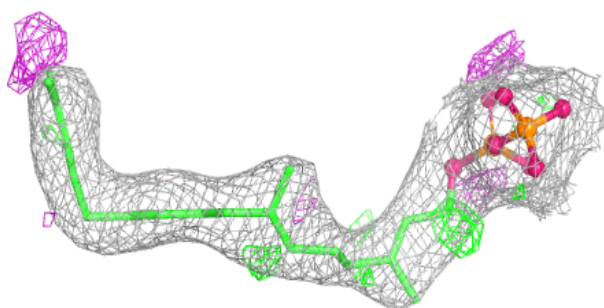


Electron density around GRG L 1726:

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

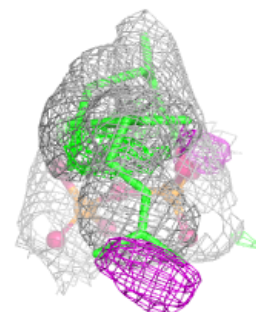
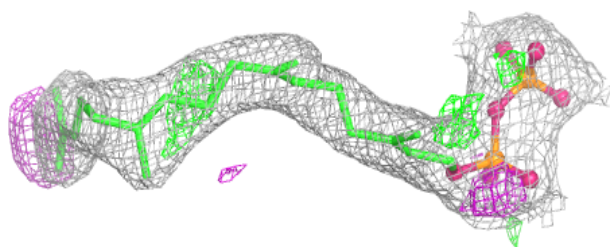
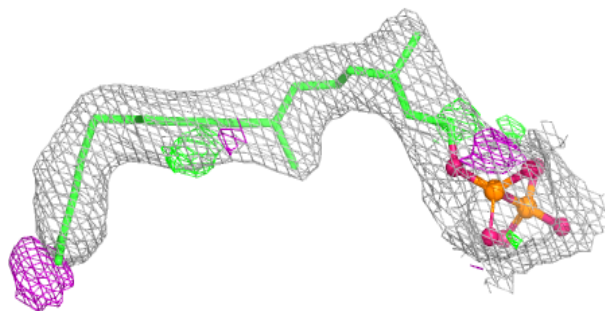
**Electron density around GRG B 1721:**

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

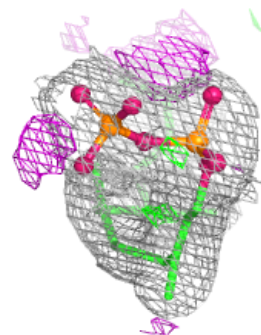
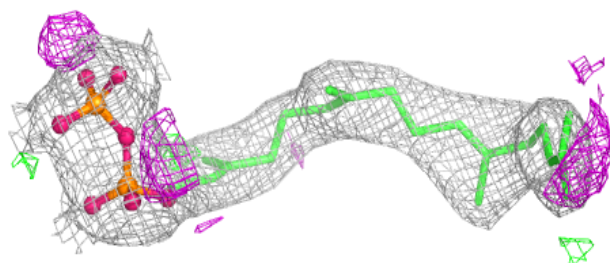
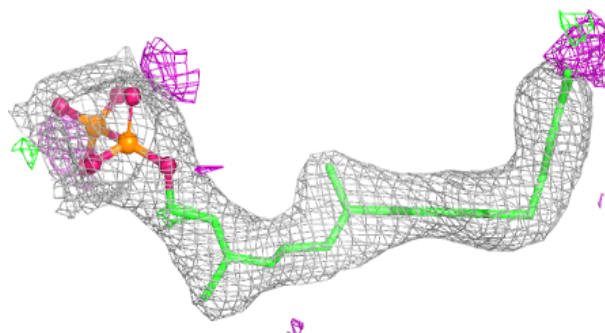


Electron density around GRG D 1722:

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

**Electron density around GRG J 1725:**

$2mF_o-DF_c$ (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.