



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:52 AM UTC

PDB ID : 1N4S / pdb_00001n4s
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 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

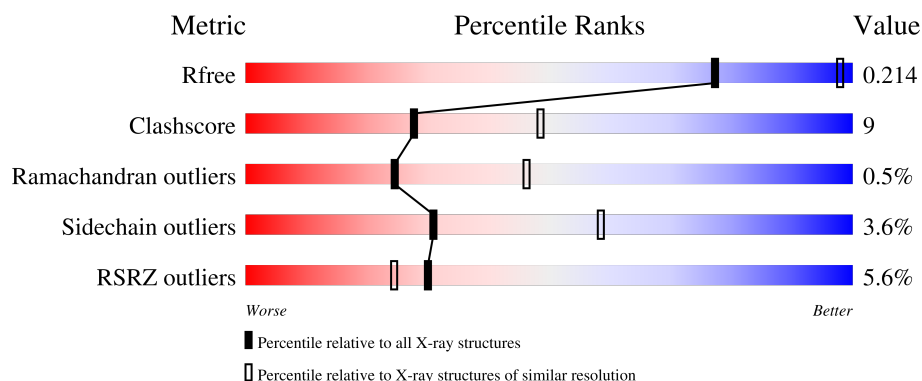
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 67% 15% • 17%
1	C	377	5% 66% 16% • 17%
1	E	377	4% 62% 20% • 17%
1	G	377	7% 65% 17% • 17%
1	I	377	3% 65% 17% • 17%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GER	M	1108	-	-	-	X
7	GER	N	1208	-	-	-	X
7	GER	O	1308	-	-	-	X
7	GER	P	1408	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33924 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2643	1689	461	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2656	1694	465	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2671	1703	467	496	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	N	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	O	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	P	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	Q	4	Total	C	N	O	S	0	0	0
			30	20	4	5	1			
3	R	5	Total	C	N	O	S	0	0	0
			39	26	6	6	1			

- Molecule 4 is ZINC ION (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).

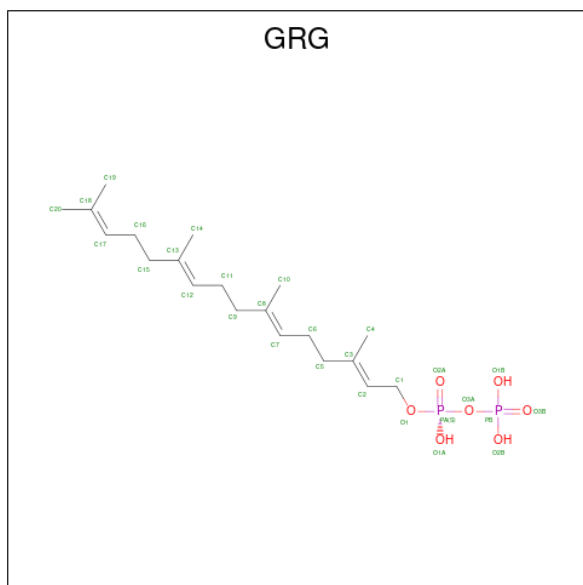
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		
5	G	1	Total	Cl	0	0
			1	1		
5	H	1	Total	Cl	0	0
			1	1		

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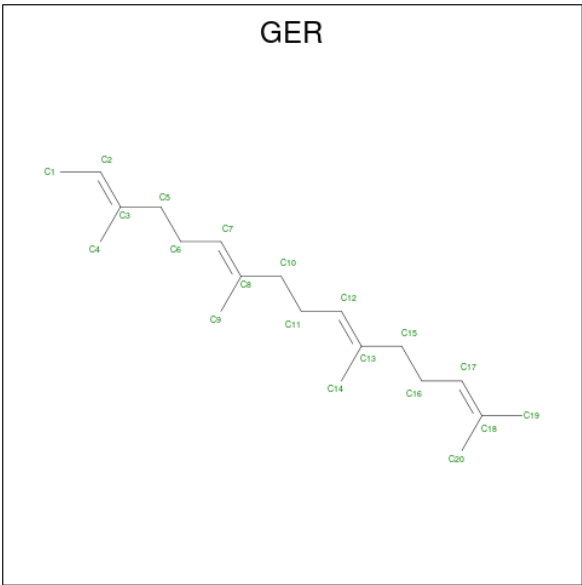
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Cl	0	0
			1	1		
5	K	1	Total	Cl	0	0
			1	1		
5	L	1	Total	Cl	0	0
			1	1		

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



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: $C_{20}H_{34}$).



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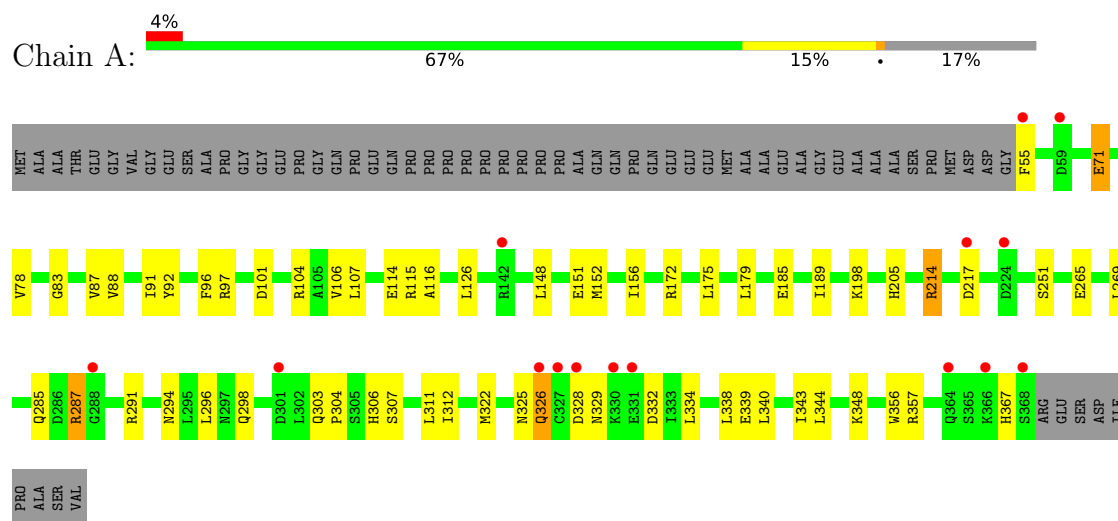
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	86	Total 86	O 86	0	0
8	H	56	Total 56	O 56	0	0
8	I	121	Total 121	O 121	0	0
8	J	88	Total 88	O 88	0	0
8	K	211	Total 211	O 211	0	0
8	L	157	Total 157	O 157	0	0
8	M	2	Total 2	O 2	0	0
8	N	2	Total 2	O 2	0	0
8	O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

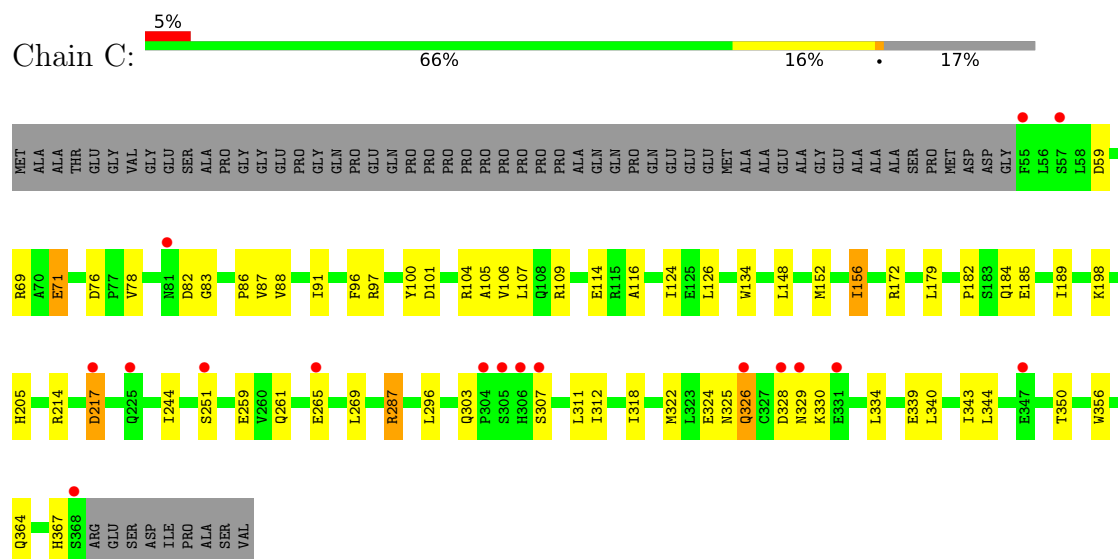
3 Residue-property plots [i](#)

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

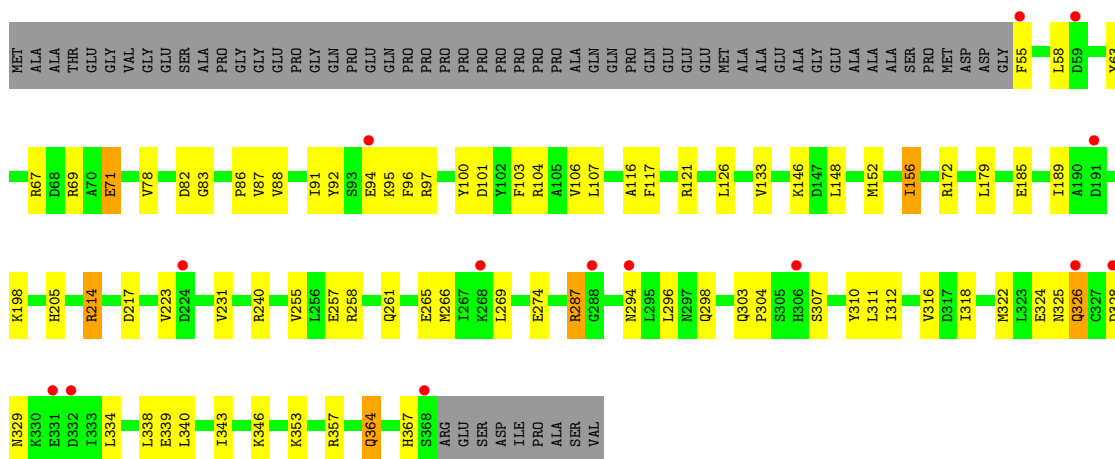


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

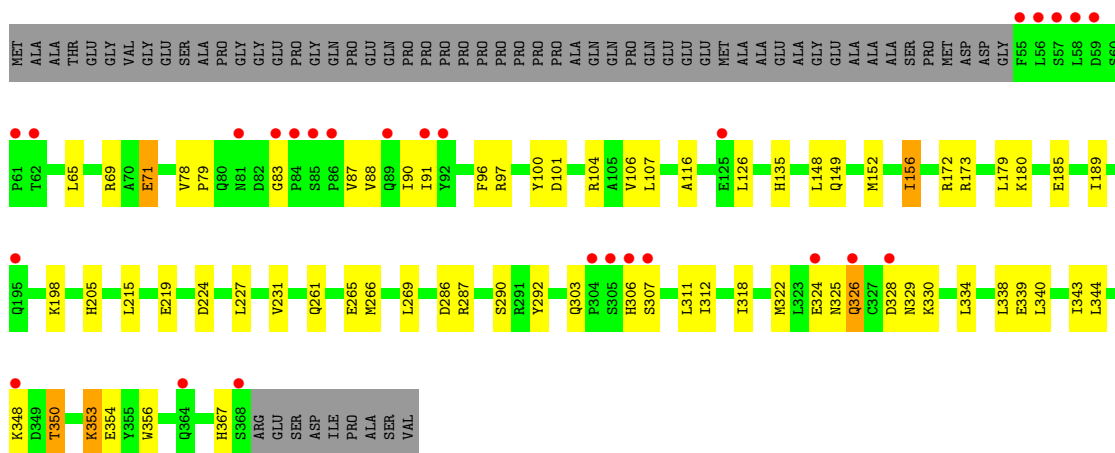


- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

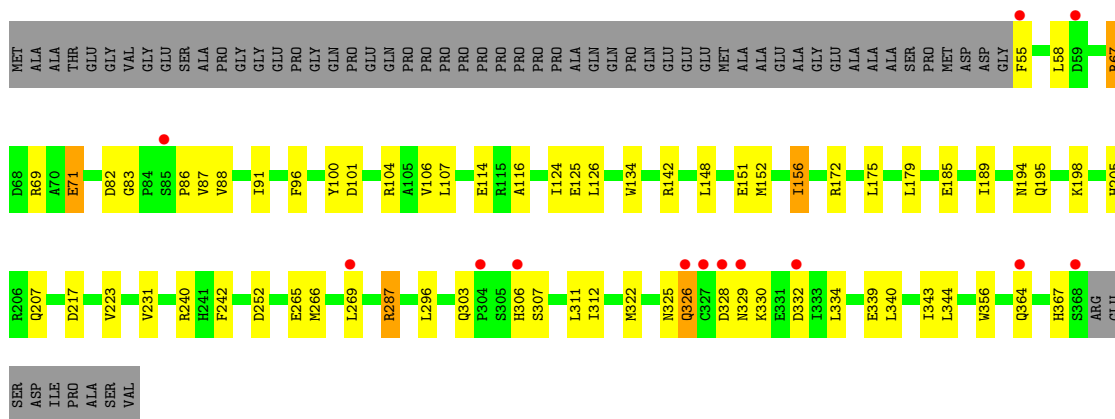




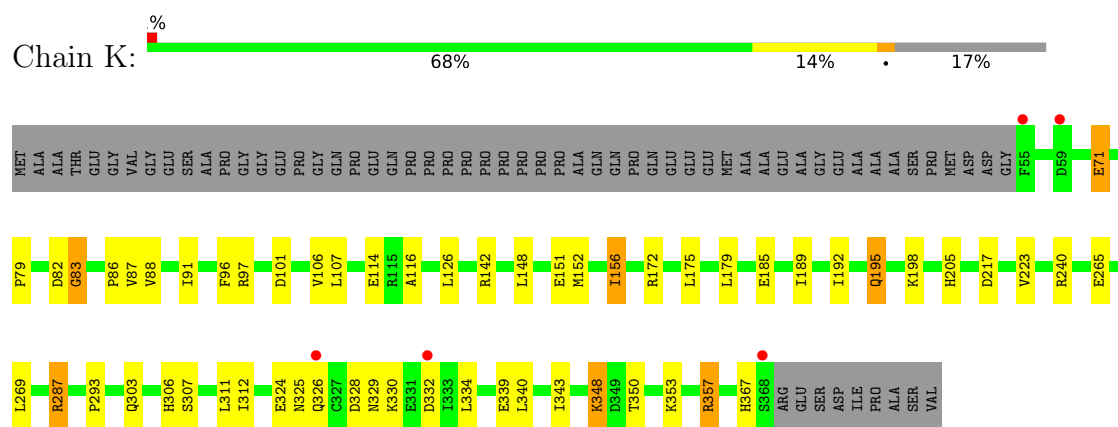
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



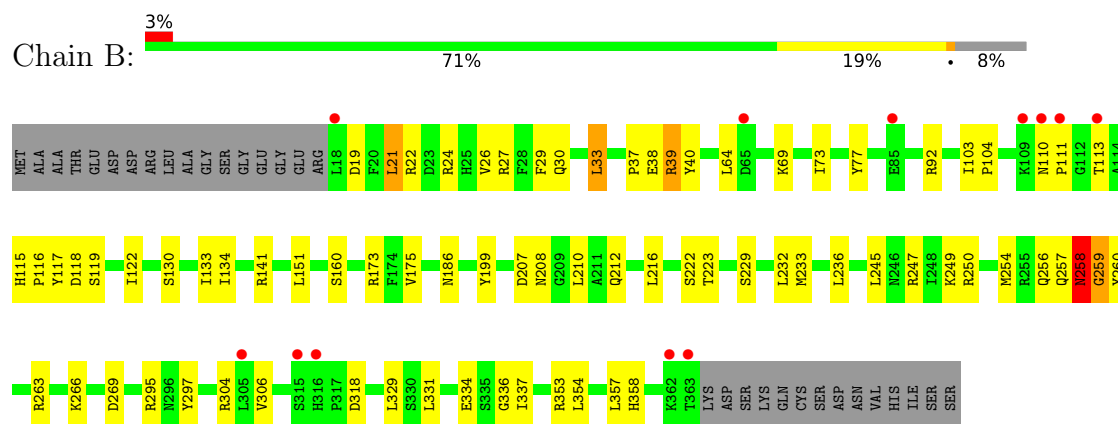
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



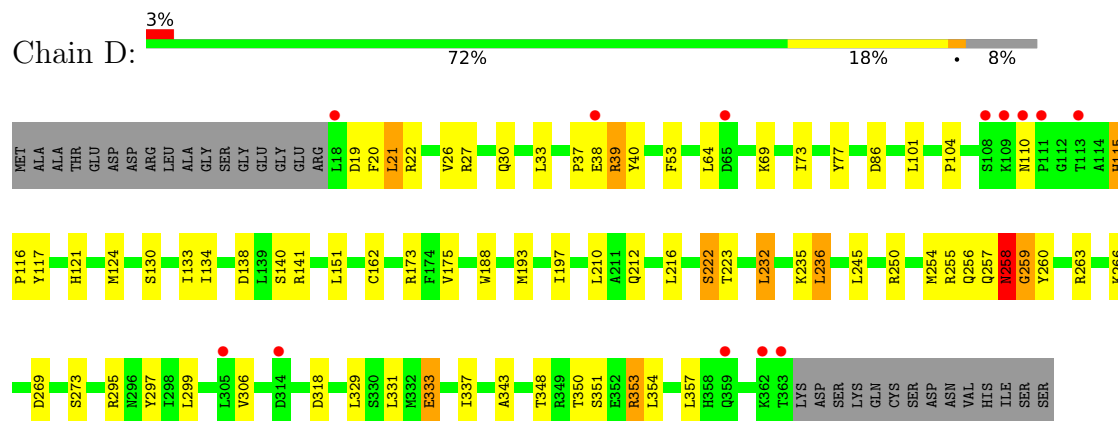
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



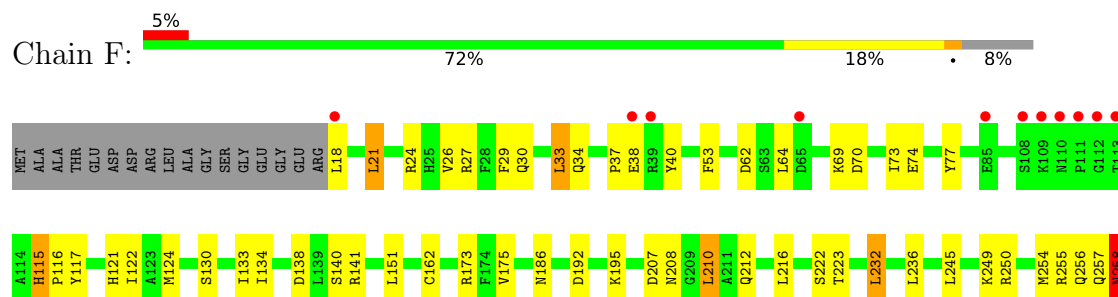
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

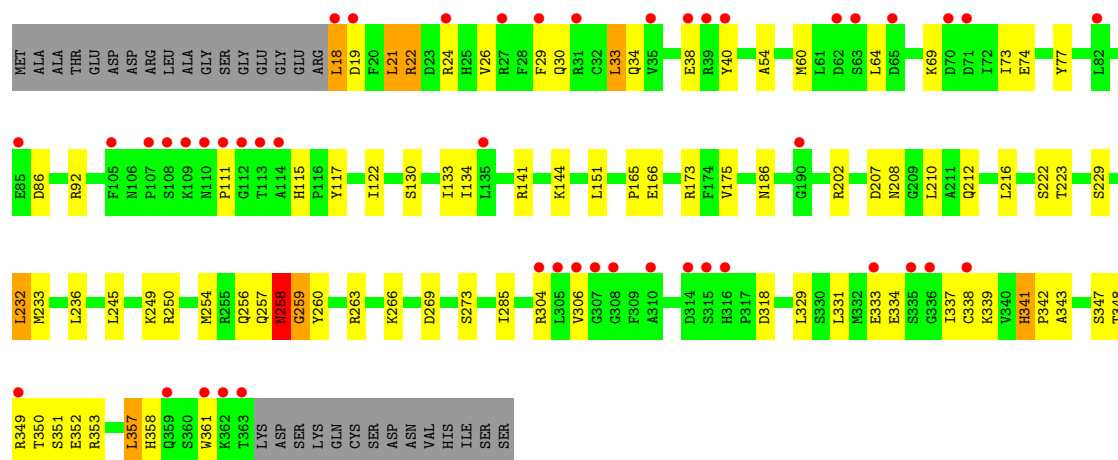


- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

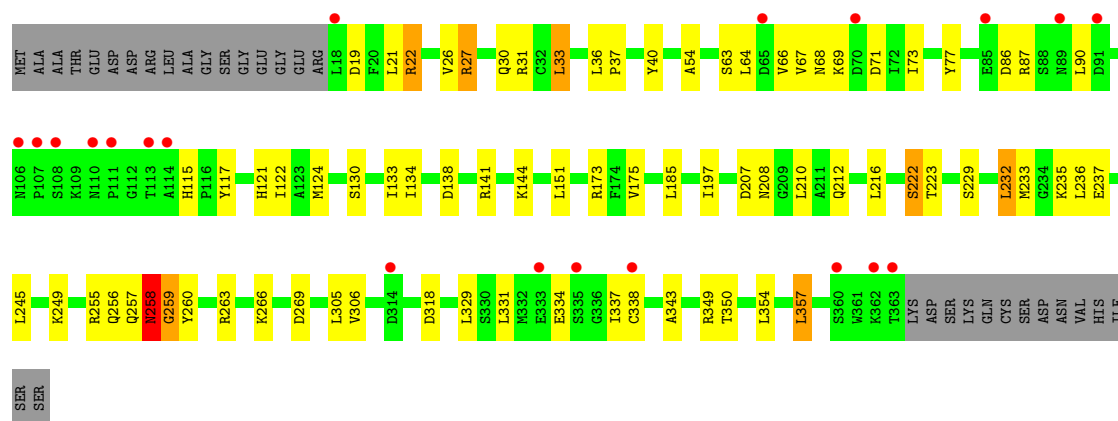




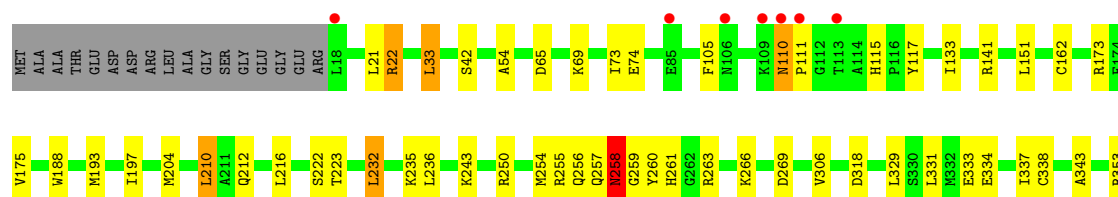
• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

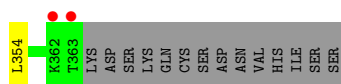


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

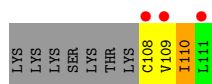


• Molecule 2: Geranylgeranyl transferase type-1 subunit beta

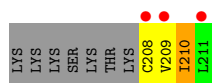




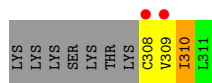
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



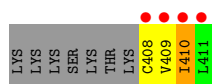
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



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



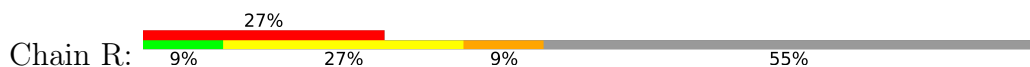
- Molecule 3: Fusion protein consisting of transforming protein p21b and Ras related protein Rap-2b



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



LYS	LYS	LYS	SER	LYS	THR	K607	C608	V609	I610	L611
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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 29.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.98-2.60) 99.7 (29.98-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.214 0.195 , 0.214	Depositor DCC
R_{free} test set	14968 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.078 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33924	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/2695	0.83	4/3668 (0.1%)
1	C	0.41	0/2709	0.84	5/3684 (0.1%)
1	E	0.41	0/2708	0.83	5/3684 (0.1%)
1	G	0.40	0/2699	0.83	6/3672 (0.2%)
1	I	0.41	0/2722	0.83	4/3700 (0.1%)
1	K	0.45	0/2737	0.84	6/3717 (0.2%)
2	B	0.40	0/2759	0.90	5/3733 (0.1%)
2	D	0.42	0/2775	0.90	9/3752 (0.2%)
2	F	0.42	0/2780	0.90	9/3758 (0.2%)
2	H	0.39	0/2756	0.90	11/3729 (0.3%)
2	J	0.41	0/2773	0.89	8/3750 (0.2%)
2	L	0.46	1/2785 (0.0%)	0.91	8/3764 (0.2%)
3	M	0.67	0/29	1.58	1/37 (2.7%)
3	N	0.63	0/29	1.54	1/37 (2.7%)
3	O	0.62	0/29	1.54	1/37 (2.7%)
3	P	0.59	0/29	1.67	1/37 (2.7%)
3	Q	0.63	0/29	1.55	1/37 (2.7%)
3	R	0.67	0/38	1.49	1/48 (2.1%)
All	All	0.42	1/33081 (0.0%)	0.87	86/44844 (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	D	0	1
2	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	204	MET	SD-CE	5.57	1.93	1.79

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	259	GLY	N-CA-C	-9.89	98.46	112.60
2	H	259	GLY	N-CA-C	-9.84	98.53	112.60
2	D	259	GLY	N-CA-C	-9.84	98.53	112.60
2	J	259	GLY	N-CA-C	-9.81	98.57	112.60
2	L	259	GLY	N-CA-C	-9.63	98.83	112.60
2	B	259	GLY	N-CA-C	-9.33	99.26	112.60
1	K	185	GLU	N-CA-C	9.08	122.09	111.02
1	I	185	GLU	N-CA-C	8.77	121.72	111.02
1	E	185	GLU	N-CA-C	8.66	121.58	111.02
1	A	185	GLU	N-CA-C	8.49	121.38	111.02
1	C	185	GLU	N-CA-C	8.48	121.36	111.02
1	G	185	GLU	N-CA-C	8.38	121.24	111.02
3	N	210	ILE	N-CA-C	7.46	120.22	112.83
3	P	410	ILE	N-CA-C	7.40	119.20	112.17
1	K	348	LYS	N-CA-C	7.34	121.48	112.23
3	M	110	ILE	N-CA-C	7.33	119.93	112.90
3	Q	510	ILE	N-CA-C	7.22	119.98	112.83
3	O	310	ILE	N-CA-C	7.12	119.87	112.83
2	J	258	ASN	N-CA-C	-7.09	95.70	110.80
3	R	610	ILE	N-CA-C	7.04	119.66	112.90
2	B	258	ASN	N-CA-C	-6.88	96.14	110.80
2	F	258	ASN	N-CA-C	-6.74	96.44	110.80
2	D	258	ASN	N-CA-C	-6.74	96.45	110.80
2	H	258	ASN	N-CA-C	-6.67	96.60	110.80
2	L	258	ASN	N-CA-C	-6.67	96.59	110.80
2	J	22	ARG	N-CA-C	6.05	118.37	111.11
2	F	257	GLN	N-CA-C	-6.02	105.96	113.55
1	I	217	ASP	N-CA-C	6.01	121.28	111.37
2	B	257	GLN	N-CA-C	-5.95	106.57	113.88
1	C	350	THR	N-CA-C	5.82	118.41	111.71
1	C	83	GLY	CA-C-N	5.82	125.51	119.05
1	C	83	GLY	C-N-CA	5.82	125.51	119.05
1	K	217	ASP	N-CA-C	5.80	120.94	111.37
2	D	257	GLN	N-CA-C	-5.75	106.30	113.55
1	E	83	GLY	CA-C-N	5.73	125.20	119.24
1	E	83	GLY	C-N-CA	5.73	125.20	119.24
2	H	257	GLN	N-CA-C	-5.67	106.41	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	217	ASP	N-CA-C	5.64	120.67	111.37
2	H	175	VAL	N-CA-C	-5.64	105.03	110.72
1	A	83	GLY	CA-C-N	5.63	125.10	119.24
1	A	83	GLY	C-N-CA	5.63	125.10	119.24
1	A	217	ASP	N-CA-C	5.58	120.58	111.37
1	K	350	THR	N-CA-C	5.58	118.13	111.71
2	J	257	GLN	N-CA-C	-5.54	106.57	113.55
2	L	257	GLN	N-CA-C	-5.52	106.60	113.55
2	D	115	HIS	CA-C-N	5.51	125.86	119.47
2	D	115	HIS	C-N-CA	5.51	125.86	119.47
2	D	353	ARG	N-CA-C	-5.44	105.35	111.28
2	L	115	HIS	CA-C-N	5.32	125.38	119.32
2	L	115	HIS	C-N-CA	5.32	125.38	119.32
2	F	175	VAL	N-CA-C	-5.31	105.35	110.72
2	H	22	ARG	N-CA-C	5.30	117.47	111.11
1	G	350	THR	N-CA-C	5.27	117.70	111.33
1	K	83	GLY	CA-C-N	5.27	124.45	118.97
1	K	83	GLY	C-N-CA	5.27	124.45	118.97
1	G	83	GLY	CA-C-N	5.24	124.87	119.05
1	G	83	GLY	C-N-CA	5.24	124.87	119.05
1	E	346	LYS	N-CA-C	5.19	118.77	112.23
2	F	115	HIS	CA-C-N	5.18	125.48	119.47
2	F	115	HIS	C-N-CA	5.18	125.48	119.47
2	H	115	HIS	CA-C-N	5.17	125.47	119.47
2	H	115	HIS	C-N-CA	5.17	125.47	119.47
2	H	122	ILE	N-CA-C	5.17	116.51	110.62
2	J	122	ILE	N-CA-C	5.15	116.49	110.62
2	L	175	VAL	N-CA-C	-5.12	105.55	110.72
1	G	292	TYR	CA-C-N	5.11	125.15	119.32
1	G	292	TYR	C-N-CA	5.11	125.15	119.32
2	B	175	VAL	N-CA-C	-5.11	105.56	110.72
2	F	273	SER	N-CA-C	-5.09	105.85	111.71
2	B	122	ILE	N-CA-C	5.09	116.42	110.62
2	H	341	HIS	CA-C-N	5.09	126.20	119.84
2	H	341	HIS	C-N-CA	5.09	126.20	119.84
2	D	273	SER	N-CA-C	-5.08	105.87	111.71
2	F	122	ILE	N-CA-C	5.07	116.40	110.62
1	C	217	ASP	N-CA-C	5.06	119.71	111.37
2	J	115	HIS	CA-C-N	5.05	125.33	119.47
2	J	115	HIS	C-N-CA	5.05	125.33	119.47
2	F	162	CYS	N-CA-C	-5.03	103.02	110.46
2	D	175	VAL	N-CA-C	-5.02	105.65	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	175	VAL	N-CA-C	-5.02	105.65	110.72
2	L	22	ARG	N-CA-C	5.01	117.13	111.11
2	H	273	SER	N-CA-C	-5.01	106.27	112.38
1	I	83	GLY	CA-C-N	5.01	124.18	118.97
1	I	83	GLY	C-N-CA	5.01	124.18	118.97
2	L	162	CYS	N-CA-C	-5.01	103.05	110.46
2	D	162	CYS	N-CA-C	-5.01	103.05	110.46

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2520	45	0
1	C	2643	0	2540	42	0
1	E	2642	0	2534	55	0
1	G	2633	0	2524	54	0
1	I	2656	0	2560	38	0
1	K	2671	0	2588	39	0
2	B	2697	0	2600	52	0
2	D	2713	0	2628	54	0
2	F	2718	0	2635	42	0
2	H	2694	0	2590	65	0
2	J	2711	0	2616	49	0
2	L	2723	0	2643	31	0
3	M	30	0	34	4	0
3	N	30	0	34	3	0
3	O	30	0	34	4	0
3	P	30	0	34	5	0
3	Q	30	0	34	3	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	1	0	0	0	0
8	P	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	3	0	0	2	0
All	All	33924	0	31591	575	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (575) 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
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.24	1.03
2:L:212:GLN:HE21	2:L:222:SER:HB3	1.21	1.02
2:J:212:GLN:NE2	2:J:222:SER:HB3	1.82	0.94
2:J:212:GLN:HE21	2:J:222:SER:HB3	1.31	0.94
2:H:18:LEU:HA	2:H:304:ARG:NH2	1.84	0.92
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.85	0.92
2:H:21:LEU:HD21	2:H:304:ARG:HG2	1.52	0.90
5:G:1405:CL:CL	8:G:1411:HOH:O	2.28	0.89
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.39	0.86
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.91	0.84
2:D:39:ARG:H	2:D:39:ARG:HD2	1.42	0.83
1:A:152:MET:O	1:A:156:ILE:HG13	1.79	0.83
2:B:173:ARG:HG2	6:B:1501:GRG:H112	1.62	0.81
2:L:212:GLN:NE2	2:L:222:SER:HB3	1.95	0.81
2:L:173:ARG:HG2	6:L:1506:GRG:H112	1.63	0.80
1:G:152:MET:O	1:G:156:ILE:HG13	1.82	0.80
2:D:37:PRO:HB2	2:D:39:ARG:CD	2.12	0.79
2:J:173:ARG:HG2	6:J:1505:GRG:H112	1.64	0.79
1:G:231:VAL:HG23	1:G:266:MET:HE3	1.65	0.78
1:K:152:MET:O	1:K:156:ILE:HG13	1.82	0.78
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.64	0.78
2:D:173:ARG:HG2	6:D:1502:GRG:H112	1.65	0.78
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.49	0.78
1:I:152:MET:O	1:I:156:ILE:HG13	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:MET:O	1:E:156:ILE:HG13	1.84	0.77
2:B:353:ARG:HD2	8:B:1566:HOH:O	1.83	0.77
2:F:173:ARG:HG2	6:F:1503:GRG:H112	1.65	0.77
1:E:214:ARG:O	1:E:214:ARG:HG3	1.85	0.76
1:C:152:MET:O	1:C:156:ILE:HG13	1.84	0.75
2:H:173:ARG:HG2	6:H:1504:GRG:H112	1.69	0.75
1:E:231:VAL:HG23	1:E:266:MET:HE3	1.68	0.75
2:H:348:THR:O	2:H:352:GLU:HG2	1.88	0.74
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.02	0.74
2:H:229:SER:O	2:H:233:MET:HG3	1.86	0.74
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.70	0.73
5:K:1408:CL:CL	8:K:1417:HOH:O	2.43	0.73
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.04	0.73
2:F:212:GLN:NE2	2:F:222:SER:HB3	2.04	0.73
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.53	0.72
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.96	0.72
2:B:24:ARG:HD3	2:B:27:ARG:HH22	1.54	0.71
2:D:37:PRO:HB2	2:D:39:ARG:HD2	1.72	0.71
1:E:296:LEU:HD22	1:E:322:MET:HE1	1.72	0.71
2:D:37:PRO:HB2	2:D:39:ARG:HD3	1.73	0.71
2:L:42:SER:HG	3:R:607:LYS:N	1.88	0.71
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.93	0.70
1:E:353:LYS:HE3	1:E:357:ARG:HH22	1.56	0.70
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.72	0.70
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.73	0.70
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.73	0.69
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.97	0.69
2:B:318:ASP:HB2	7:M:1108:GER:H71	1.75	0.68
1:E:353:LYS:HE2	1:E:357:ARG:HH12	1.58	0.68
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.75	0.68
2:H:144:LYS:HE2	8:H:1546:HOH:O	1.95	0.67
2:F:318:ASP:HB2	7:O:1308:GER:H71	1.76	0.67
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.75	0.67
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.95	0.67
1:I:91:ILE:HD12	1:I:91:ILE:O	1.94	0.67
1:E:156:ILE:CG1	1:E:172:ARG:HH12	2.01	0.67
2:H:212:GLN:NE2	2:H:222:SER:HB3	2.09	0.67
2:D:69:LYS:O	2:D:73:ILE:HG13	1.94	0.66
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.26	0.66
2:J:318:ASP:HB2	7:Q:1508:GER:H71	1.77	0.66
1:G:91:ILE:HD12	1:G:91:ILE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:338:CYS:HB3	8:L:1637:HOH:O	1.96	0.66
2:H:18:LEU:HD22	2:H:18:LEU:N	2.10	0.66
2:J:263:ARG:HG3	2:J:266:LYS:HG3	1.77	0.66
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.76	0.65
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.60	0.65
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.79	0.65
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.79	0.65
2:B:263:ARG:HG3	2:B:266:LYS:HG3	1.79	0.65
1:K:91:ILE:HD12	1:K:91:ILE:O	1.96	0.65
1:C:339:GLU:O	1:C:343:ILE:HG13	1.97	0.65
1:A:97:ARG:HG2	1:A:101:ASP:OD2	1.97	0.65
2:B:69:LYS:O	2:B:73:ILE:HG13	1.97	0.65
2:H:21:LEU:CD2	2:H:304:ARG:HG2	2.27	0.65
1:K:330:LYS:HE2	1:K:367:HIS:HB3	1.79	0.65
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.79	0.64
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.62	0.64
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.80	0.64
1:A:91:ILE:HD12	1:A:91:ILE:O	1.97	0.64
1:A:339:GLU:O	1:A:343:ILE:HG13	1.98	0.64
2:D:212:GLN:NE2	2:D:222:SER:HB3	2.12	0.64
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.12	0.64
2:D:263:ARG:HG3	2:D:266:LYS:HG3	1.80	0.64
2:D:318:ASP:HB2	7:N:1208:GER:H71	1.79	0.64
2:F:26:VAL:O	2:F:30:GLN:HG3	1.98	0.64
2:J:87:ARG:HH12	2:J:90:LEU:HD11	1.61	0.64
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.63	0.63
1:G:261:GLN:O	1:G:265:GLU:HG2	1.99	0.63
2:H:263:ARG:HG3	2:H:266:LYS:HG3	1.79	0.63
2:F:263:ARG:HG3	2:F:266:LYS:HG3	1.79	0.63
2:H:69:LYS:O	2:H:73:ILE:HG13	1.99	0.63
2:B:92:ARG:NH1	2:B:119:SER:HB3	2.13	0.63
2:F:69:LYS:O	2:F:73:ILE:HG13	1.99	0.63
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.81	0.62
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.82	0.62
2:L:263:ARG:HG3	2:L:266:LYS:HG3	1.80	0.62
1:G:100:TYR:O	1:G:104:ARG:HG3	1.98	0.62
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.34	0.62
2:H:318:ASP:HB2	7:P:1408:GER:H71	1.80	0.62
3:N:209:VAL:N	7:N:1208:GER:H11	2.14	0.62
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.00	0.62
1:G:334:LEU:HD22	1:G:367:HIS:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.00	0.61
2:H:245:LEU:O	2:H:249:LYS:HG3	2.00	0.61
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.66	0.61
1:A:328:ASP:O	1:A:329:ASN:HB2	2.00	0.61
1:E:91:ILE:O	1:E:91:ILE:HD12	2.00	0.61
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.82	0.60
1:C:91:ILE:O	1:C:91:ILE:HD12	2.01	0.60
2:H:349:ARG:O	2:H:352:GLU:HB2	2.01	0.60
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.64	0.60
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.66	0.60
1:E:198:LYS:HD3	2:F:266:LYS:HD3	1.83	0.60
2:L:210:LEU:HB2	2:L:223:THR:HA	1.83	0.60
2:H:21:LEU:HD23	2:H:24:ARG:HE	1.66	0.60
1:A:214:ARG:HG3	1:A:214:ARG:O	2.01	0.60
2:D:39:ARG:H	2:D:39:ARG:CD	2.14	0.60
3:M:109:VAL:N	7:M:1108:GER:H11	2.17	0.60
3:Q:509:VAL:N	7:Q:1508:GER:H11	2.17	0.60
2:H:210:LEU:HB2	2:H:223:THR:HA	1.83	0.59
3:O:309:VAL:N	7:O:1308:GER:H11	2.18	0.59
2:J:210:LEU:HB2	2:J:223:THR:HA	1.82	0.59
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.83	0.59
2:L:318:ASP:HB2	7:R:1608:GER:H71	1.85	0.59
2:B:212:GLN:NE2	2:B:222:SER:HB3	2.18	0.59
1:I:311:LEU:HD23	1:I:311:LEU:C	2.28	0.59
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.85	0.59
1:I:207:GLN:HG2	1:I:242:PHE:CE2	2.38	0.58
2:B:210:LEU:HB2	2:B:223:THR:HA	1.85	0.58
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.38	0.58
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.69	0.58
2:B:92:ARG:HH11	2:B:119:SER:HB3	1.67	0.58
3:P:409:VAL:N	7:P:1408:GER:H11	2.17	0.58
1:K:311:LEU:C	1:K:311:LEU:HD23	2.28	0.58
3:R:609:VAL:N	7:R:1608:GER:H11	2.19	0.58
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.85	0.58
1:I:334:LEU:HD22	1:I:367:HIS:O	2.03	0.58
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.85	0.58
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.85	0.58
1:K:293:PRO:HD3	8:K:1527:HOH:O	2.03	0.58
1:K:311:LEU:HD23	1:K:311:LEU:O	2.04	0.58
2:F:210:LEU:HB2	2:F:223:THR:HA	1.86	0.57
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.18	0.57
1:K:334:LEU:HD22	1:K:367:HIS:O	2.03	0.57
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.86	0.57
1:E:265:GLU:O	1:E:269:LEU:HD13	2.05	0.57
2:D:210:LEU:HB2	2:D:223:THR:HA	1.85	0.57
2:H:339:LYS:HG2	2:H:348:THR:CG2	2.34	0.57
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.70	0.57
2:B:26:VAL:O	2:B:30:GLN:HG3	2.03	0.57
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.86	0.57
2:L:353:ARG:HD3	2:L:353:ARG:O	2.05	0.57
2:B:353:ARG:HG2	2:B:353:ARG:HH11	1.69	0.57
2:H:339:LYS:HG2	2:H:348:THR:HG21	1.86	0.57
1:E:214:ARG:O	1:E:214:ARG:CG	2.53	0.56
3:P:409:VAL:HG23	3:P:410:ILE:HG23	1.87	0.56
1:E:318:ILE:HG22	1:E:322:MET:CE	2.33	0.56
1:E:339:GLU:O	1:E:343:ILE:HG13	2.05	0.56
2:J:27:ARG:HH12	2:J:30:GLN:NE2	2.03	0.56
1:K:192:ILE:O	1:K:195:GLN:HG3	2.05	0.56
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.87	0.56
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.87	0.56
2:H:92:ARG:HG2	2:H:165:PRO:HG3	1.88	0.55
2:J:87:ARG:NH1	2:J:90:LEU:HD11	2.21	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.41	0.55
1:I:328:ASP:O	1:I:329:ASN:HB2	2.05	0.55
3:M:109:VAL:HG23	3:M:110:ILE:HG23	1.88	0.55
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.05	0.55
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.41	0.55
1:K:198:LYS:HD3	2:L:266:LYS:HD3	1.89	0.55
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.72	0.55
1:E:261:GLN:O	1:E:265:GLU:HG2	2.06	0.55
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.71	0.55
1:C:330:LYS:HE2	1:C:367:HIS:HB3	1.87	0.55
1:A:265:GLU:O	1:A:269:LEU:HD13	2.07	0.55
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.71	0.55
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.55
3:R:609:VAL:HG23	3:R:610:ILE:HG23	1.89	0.55
1:A:71:GLU:CD	1:A:71:GLU:H	2.14	0.54
1:I:330:LYS:HE2	1:I:367:HIS:HB3	1.89	0.54
1:K:265:GLU:O	1:K:269:LEU:HD13	2.06	0.54
3:Q:509:VAL:HG23	3:Q:510:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:LEU:HD23	1:G:311:LEU:C	2.33	0.54
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.54
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.90	0.54
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.90	0.54
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.56	0.54
2:H:26:VAL:O	2:H:30:GLN:HG3	2.07	0.54
1:E:78:VAL:O	1:E:104:ARG:HD2	2.08	0.54
1:I:100:TYR:O	1:I:104:ARG:HG3	2.08	0.54
2:D:37:PRO:HB3	2:D:39:ARG:HH11	1.72	0.53
2:H:60:MET:HE1	2:H:347:SER:N	2.23	0.53
2:J:22:ARG:O	2:J:26:VAL:HG23	2.08	0.53
1:E:58:LEU:HD22	1:E:95:LYS:HD3	1.91	0.53
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.90	0.53
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.90	0.53
1:G:334:LEU:O	1:G:338:LEU:HG	2.09	0.53
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.88	0.53
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.90	0.53
2:B:39:ARG:HH11	2:B:39:ARG:CB	2.18	0.53
1:K:71:GLU:H	1:K:71:GLU:CD	2.16	0.53
1:A:334:LEU:HD22	1:A:367:HIS:O	2.07	0.53
1:C:334:LEU:HD22	1:C:367:HIS:O	2.08	0.53
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.92	0.52
2:J:212:GLN:HE21	2:J:222:SER:CB	2.12	0.52
2:F:332:MET:HB2	8:F:1537:HOH:O	2.08	0.52
1:E:92:TYR:O	1:E:97:ARG:NH2	2.42	0.52
1:I:339:GLU:O	1:I:343:ILE:HG13	2.08	0.52
1:A:78:VAL:O	1:A:104:ARG:HD2	2.08	0.52
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.74	0.52
2:F:30:GLN:O	2:F:34:GLN:HG3	2.10	0.52
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.74	0.52
3:O:309:VAL:HG23	3:O:310:ILE:HG23	1.91	0.52
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.90	0.52
2:B:245:LEU:O	2:B:249:LYS:HG3	2.10	0.52
1:I:325:ASN:O	1:I:326:GLN:C	2.52	0.52
1:G:339:GLU:O	1:G:343:ILE:HG13	2.09	0.52
1:I:198:LYS:HD3	2:J:266:LYS:HD3	1.92	0.52
1:A:325:ASN:O	1:A:326:GLN:C	2.53	0.51
2:H:202:ARG:HG3	2:H:202:ARG:NH1	2.26	0.51
2:D:26:VAL:O	2:D:30:GLN:HG3	2.10	0.51
1:G:231:VAL:CG2	1:G:266:MET:HE3	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:339:GLU:O	1:K:343:ILE:HG13	2.10	0.51
1:C:265:GLU:O	1:C:269:LEU:HD13	2.09	0.51
1:G:265:GLU:O	1:G:269:LEU:HD13	2.11	0.51
1:G:286:ASP:HB2	8:G:1440:HOH:O	2.10	0.51
1:G:325:ASN:O	1:G:326:GLN:C	2.54	0.51
2:H:318:ASP:HB2	7:P:1408:GER:C7	2.40	0.51
2:J:258:ASN:OD1	2:J:259:GLY:N	2.37	0.51
2:B:229:SER:O	2:B:233:MET:HG3	2.11	0.51
2:D:258:ASN:OD1	2:D:259:GLY:N	2.39	0.51
3:N:209:VAL:HG23	3:N:210:ILE:HG23	1.92	0.51
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.10	0.51
1:I:265:GLU:O	1:I:269:LEU:HD13	2.11	0.51
3:R:608:CYS:C	7:R:1608:GER:H11	2.36	0.51
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.10	0.50
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.11	0.50
3:R:608:CYS:HA	7:R:1608:GER:C2	2.41	0.50
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.24	0.50
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.93	0.50
1:A:311:LEU:C	1:A:311:LEU:HD23	2.36	0.50
2:J:63:SER:O	2:J:66:VAL:HG22	2.11	0.50
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.93	0.50
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.26	0.50
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.94	0.50
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.77	0.50
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.47	0.50
1:C:311:LEU:C	1:C:311:LEU:HD23	2.37	0.49
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.94	0.49
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.93	0.49
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.27	0.49
1:G:198:LYS:HD3	2:H:266:LYS:HD3	1.94	0.49
2:J:27:ARG:NH1	2:J:30:GLN:NE2	2.60	0.49
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.47	0.49
2:H:22:ARG:HH11	2:H:22:ARG:HG2	1.76	0.49
1:K:303:GLN:O	1:K:307:SER:HB2	2.12	0.49
3:O:308:CYS:C	7:O:1308:GER:H11	2.37	0.49
3:P:408:CYS:C	7:P:1408:GER:H11	2.38	0.49
2:J:144:LYS:HG2	2:J:185:LEU:HD22	1.94	0.49
1:C:303:GLN:O	1:C:307:SER:HB2	2.11	0.49
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.85	0.49
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.49
2:H:348:THR:HA	2:H:351:SER:OG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:151:GLU:HG3	1:I:175:LEU:HD11	1.94	0.49
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.43	0.49
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.48	0.49
1:C:91:ILE:HD11	2:D:38:GLU:H	1.77	0.49
1:G:303:GLN:O	1:G:307:SER:HB2	2.13	0.49
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.48	0.48
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.48	0.48
1:E:294:ASN:O	1:E:298:GLN:HG3	2.13	0.48
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.95	0.48
1:A:214:ARG:O	1:A:214:ARG:CG	2.58	0.48
2:D:348:THR:HA	2:D:351:SER:OG	2.13	0.48
2:H:19:ASP:H	2:H:304:ARG:HH21	1.61	0.48
2:H:74:GLU:CD	2:H:141:ARG:HH22	2.21	0.48
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.29	0.48
2:H:130:SER:O	2:H:134:ILE:HG13	2.13	0.48
2:B:64:LEU:HD11	2:B:134:ILE:HG22	1.96	0.48
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.95	0.48
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.49	0.48
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.96	0.48
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.29	0.48
2:B:29:PHE:O	2:B:33:LEU:HD22	2.14	0.48
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.46	0.48
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.49	0.48
2:B:258:ASN:CG	2:B:259:GLY:H	2.22	0.47
1:C:214:ARG:O	1:C:214:ARG:HG2	2.14	0.47
2:D:333:GLU:O	1:K:357:ARG:NH2	2.47	0.47
2:H:338:CYS:HB3	8:H:1551:HOH:O	2.14	0.47
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.96	0.47
1:K:223:VAL:HG11	1:K:240:ARG:HB2	1.96	0.47
3:N:208:CYS:C	7:N:1208:GER:H11	2.38	0.47
3:Q:508:CYS:C	7:Q:1508:GER:H11	2.39	0.47
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.94	0.47
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.95	0.47
2:B:269:ASP:C	2:B:269:ASP:OD1	2.58	0.47
1:C:105:ALA:O	1:C:109:ARG:HG3	2.14	0.47
1:E:325:ASN:O	1:E:326:GLN:C	2.56	0.47
2:F:130:SER:O	2:F:134:ILE:HG13	2.14	0.47
1:G:90:ILE:HD13	2:H:40:TYR:O	2.14	0.47
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.49	0.47
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.96	0.47
2:D:86:ASP:OD2	2:D:86:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:LEU:HD11	2:F:134:ILE:HG22	1.97	0.47
2:H:258:ASN:OD1	2:H:259:GLY:N	2.41	0.47
3:R:608:CYS:HB3	8:R:1002:HOH:O	2.14	0.47
1:C:106:VAL:HG11	1:C:116:ALA:HB1	1.96	0.47
1:C:325:ASN:O	1:C:326:GLN:C	2.57	0.47
1:E:97:ARG:HG2	1:E:101:ASP:OD2	2.14	0.47
1:E:334:LEU:HD22	1:E:367:HIS:O	2.14	0.47
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.50	0.47
1:G:328:ASP:O	1:G:329:ASN:HB2	2.14	0.47
1:K:325:ASN:O	1:K:326:GLN:C	2.57	0.47
1:K:353:LYS:HB2	1:K:353:LYS:HE3	1.68	0.47
2:L:333:GLU:HA	8:L:1636:HOH:O	2.15	0.47
1:A:91:ILE:HD11	2:B:38:GLU:H	1.79	0.47
2:H:29:PHE:O	2:H:33:LEU:HD22	2.14	0.47
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.80	0.47
2:J:318:ASP:HB2	7:Q:1508:GER:C7	2.45	0.47
3:M:108:CYS:C	7:M:1108:GER:H11	2.39	0.47
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.96	0.47
2:H:269:ASP:OD1	2:H:269:ASP:C	2.59	0.47
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.50	0.47
1:G:353:LYS:HG2	1:G:354:GLU:N	2.29	0.46
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.51	0.46
2:J:133:ILE:HG22	2:J:350:THR:HG23	1.97	0.46
1:K:328:ASP:O	1:K:329:ASN:HB2	2.15	0.46
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.81	0.46
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.30	0.46
1:A:104:ARG:NH2	8:A:389:HOH:O	2.49	0.46
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.98	0.46
1:G:173:ARG:HD2	8:G:1452:HOH:O	2.14	0.46
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.30	0.46
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.50	0.46
2:B:207:ASP:O	2:B:208:ASN:HB2	2.16	0.46
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.51	0.46
2:D:22:ARG:HG2	2:D:22:ARG:NH1	2.30	0.46
1:E:189:ILE:HD11	1:E:205:HIS:CD2	2.50	0.46
2:J:130:SER:O	2:J:134:ILE:HG13	2.16	0.46
2:F:38:GLU:O	2:F:38:GLU:HG2	2.16	0.46
2:H:21:LEU:CD1	2:H:21:LEU:N	2.78	0.46
1:K:106:VAL:HG11	1:K:116:ALA:HB1	1.98	0.46
2:B:130:SER:O	2:B:134:ILE:HG13	2.15	0.46
2:F:333:GLU:HA	8:F:1569:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.97	0.46
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.51	0.46
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.98	0.46
2:D:250:ARG:O	2:D:254:MET:HG2	2.16	0.46
2:L:22:ARG:HG2	2:L:22:ARG:HH11	1.81	0.46
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.97	0.46
1:C:104:ARG:HG2	2:D:101:LEU:O	2.15	0.46
2:F:62:ASP:HA	2:F:349:ARG:HH22	1.81	0.46
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.51	0.46
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.51	0.46
2:B:38:GLU:O	2:B:38:GLU:HG2	2.14	0.45
1:E:287:ARG:H	1:E:287:ARG:HG2	1.49	0.45
1:E:353:LYS:CE	1:E:357:ARG:HH22	2.28	0.45
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.52	0.45
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.97	0.45
2:H:18:LEU:HA	2:H:304:ARG:HH22	1.74	0.45
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.98	0.45
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.99	0.45
2:B:24:ARG:HD3	2:B:27:ARG:NH2	2.28	0.45
2:B:92:ARG:NH1	2:B:118:ASP:O	2.50	0.45
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.52	0.45
1:I:231:VAL:HG23	1:I:266:MET:HE3	1.99	0.45
1:E:274:GLU:HG3	1:E:310:TYR:CE2	2.52	0.45
1:G:350:THR:O	1:G:353:LYS:HB3	2.15	0.45
2:H:202:ARG:HD2	8:H:1547:HOH:O	2.16	0.45
2:J:27:ARG:HH12	2:J:30:GLN:HE22	1.63	0.45
2:J:27:ARG:HD3	8:J:1564:HOH:O	2.16	0.45
3:R:608:CYS:CB	8:R:1002:HOH:O	2.64	0.45
1:A:287:ARG:O	1:A:291:ARG:HD3	2.17	0.45
1:A:303:GLN:O	1:A:307:SER:HB2	2.16	0.45
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.51	0.45
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.17	0.45
1:E:311:LEU:C	1:E:311:LEU:HD23	2.42	0.45
2:H:207:ASP:O	2:H:208:ASN:HB2	2.17	0.45
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.52	0.45
2:B:250:ARG:O	2:B:254:MET:HG2	2.15	0.45
2:D:130:SER:O	2:D:134:ILE:HG13	2.16	0.45
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.52	0.45
1:G:290:SER:HB2	1:G:322:MET:HG2	1.99	0.45
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.52	0.45
2:D:64:LEU:HD11	2:D:134:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:N	2:H:18:LEU:CD2	2.79	0.45
1:K:151:GLU:HG3	1:K:175:LEU:HD11	1.98	0.45
2:F:269:ASP:OD1	2:F:269:ASP:C	2.60	0.45
1:G:91:ILE:HD11	2:H:38:GLU:H	1.82	0.45
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.52	0.44
1:G:71:GLU:H	1:G:71:GLU:CD	2.21	0.44
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.52	0.44
1:A:340:LEU:HD23	1:A:343:ILE:HD12	2.00	0.44
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.83	0.44
2:D:295:ARG:NH1	2:D:299:LEU:CD1	2.80	0.44
2:D:333:GLU:HA	8:D:1561:HOH:O	2.17	0.44
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.52	0.44
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.99	0.44
1:A:296:LEU:CD2	1:A:322:MET:HE1	2.47	0.44
1:E:100:TYR:O	1:E:104:ARG:HG3	2.18	0.44
2:F:245:LEU:O	2:F:249:LYS:HG3	2.17	0.44
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.52	0.44
2:F:192:ASP:OD1	2:F:195:LYS:HG3	2.17	0.44
1:I:303:GLN:O	1:I:307:SER:HB2	2.17	0.44
2:J:207:ASP:O	2:J:208:ASN:HB2	2.17	0.44
1:I:287:ARG:H	1:I:287:ARG:HG2	1.56	0.44
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.77	0.44
2:B:160:SER:HB3	2:B:199:TYR:CE1	2.53	0.44
1:G:215:LEU:HA	8:G:1449:HOH:O	2.17	0.44
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.98	0.44
1:K:97:ARG:HG2	1:K:101:ASP:OD2	2.18	0.44
2:B:21:LEU:CD1	2:B:21:LEU:N	2.81	0.44
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.53	0.44
2:D:38:GLU:O	2:D:38:GLU:HG2	2.17	0.44
1:E:223:VAL:HG11	1:E:240:ARG:HB2	2.00	0.44
1:I:58:LEU:HD12	1:I:125:GLU:OE2	2.18	0.44
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.44
1:A:296:LEU:HD22	1:A:322:MET:HE1	2.00	0.44
2:F:27:ARG:HA	2:F:30:GLN:HE21	1.83	0.44
2:F:353:ARG:NE	8:F:1557:HOH:O	2.49	0.44
2:H:40:TYR:CE2	7:P:1408:GER:H101	2.52	0.44
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.53	0.43
2:F:250:ARG:O	2:F:254:MET:HG2	2.17	0.43
2:J:69:LYS:O	2:J:73:ILE:HG13	2.17	0.43
2:B:295:ARG:HD3	8:B:1549:HOH:O	2.18	0.43
2:D:104:PRO:HG2	8:D:1593:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.54	0.43
1:I:296:LEU:CD2	1:I:322:MET:HE1	2.48	0.43
1:A:92:TYR:O	1:A:97:ARG:NH2	2.50	0.43
2:D:258:ASN:CG	2:D:259:GLY:H	2.24	0.43
1:E:121:ARG:NH1	1:E:121:ARG:HG3	2.33	0.43
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.18	0.43
1:K:156:ILE:HD12	8:K:1585:HOH:O	2.18	0.43
2:L:250:ARG:O	2:L:254:MET:HG2	2.19	0.43
1:E:303:GLN:O	1:E:307:SER:HB2	2.17	0.43
2:F:70:ASP:O	2:F:74:GLU:HG2	2.19	0.43
1:G:65:LEU:O	1:G:69:ARG:HG3	2.19	0.43
1:K:348:LYS:HD2	8:K:1541:HOH:O	2.18	0.43
1:A:303:GLN:N	1:A:304:PRO:CD	2.82	0.43
2:H:352:GLU:OE2	2:H:352:GLU:HA	2.19	0.43
2:B:258:ASN:OD1	2:B:259:GLY:N	2.47	0.43
2:D:115:HIS:ND1	2:D:116:PRO:HD2	2.33	0.43
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.53	0.43
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.53	0.43
1:E:296:LEU:HD22	1:E:322:MET:CE	2.46	0.43
2:F:258:ASN:CG	2:F:259:GLY:H	2.26	0.43
2:B:103:ILE:HG23	2:B:104:PRO:HD2	2.00	0.43
2:H:133:ILE:HG22	2:H:350:THR:HG23	2.00	0.43
1:K:287:ARG:H	1:K:287:ARG:HG2	1.56	0.43
2:L:110:ASN:CB	2:L:111:PRO:HD2	2.49	0.43
1:C:287:ARG:H	1:C:287:ARG:HG2	1.63	0.43
6:L:1506:GRG:HC62	6:L:1506:GRG:H101	1.88	0.43
2:D:269:ASP:OD1	2:D:269:ASP:C	2.62	0.42
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.34	0.42
2:F:207:ASP:O	2:F:208:ASN:HB2	2.18	0.42
2:H:341:HIS:HA	2:H:342:PRO:HD2	1.84	0.42
1:I:223:VAL:HG11	1:I:240:ARG:HB2	2.01	0.42
2:J:19:ASP:OD2	2:J:19:ASP:N	2.52	0.42
2:B:318:ASP:HB2	7:M:1108:GER:C7	2.47	0.42
2:F:192:ASP:CG	2:F:195:LYS:HG3	2.43	0.42
2:F:318:ASP:HB2	7:O:1308:GER:C7	2.47	0.42
1:K:329:ASN:HB3	1:K:332:ASP:HB3	2.01	0.42
2:B:19:ASP:OD2	2:B:19:ASP:N	2.51	0.42
8:H:1560:HOH:O	3:P:409:VAL:HG21	2.19	0.42
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.54	0.42
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.54	0.42
2:D:19:ASP:OD2	2:D:19:ASP:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312:ILE:O	1:E:316:VAL:HG23	2.20	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.91	0.42
2:J:121:HIS:HB3	2:J:124:MET:HG2	2.02	0.42
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.84	0.42
1:E:303:GLN:N	1:E:304:PRO:CD	2.82	0.42
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.02	0.42
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.46	0.42
7:O:1308:GER:H112	7:O:1308:GER:H91	1.87	0.42
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.86	0.42
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.49	0.42
2:H:250:ARG:O	2:H:254:MET:HG2	2.20	0.42
2:J:237:GLU:HG2	8:J:1534:HOH:O	2.20	0.42
2:J:30:GLN:HE21	2:J:30:GLN:HB3	1.63	0.42
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.54	0.42
2:D:19:ASP:O	2:D:21:LEU:HD13	2.20	0.42
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.02	0.42
6:D:1502:GRG:H101	6:D:1502:GRG:HC62	1.92	0.42
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.55	0.42
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.55	0.42
1:E:338:LEU:HD11	1:E:364:GLN:HG3	2.01	0.42
2:J:269:ASP:C	2:J:269:ASP:OD1	2.62	0.42
2:L:193:MET:HE3	2:L:193:MET:HB2	1.92	0.42
2:D:236:LEU:HD22	2:D:245:LEU:HD21	2.02	0.41
2:J:229:SER:O	2:J:233:MET:HG3	2.20	0.41
1:A:285:GLN:HE21	2:B:247:ARG:NH1	2.18	0.41
2:B:334:GLU:HB3	2:B:337:ILE:HD12	2.02	0.41
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.54	0.41
6:F:1503:GRG:HC62	6:F:1503:GRG:H101	1.90	0.41
1:G:135:HIS:CD2	2:H:166:GLU:HG2	2.55	0.41
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.51	0.41
3:P:408:CYS:HA	7:P:1408:GER:C2	2.50	0.41
1:A:198:LYS:CD	2:B:266:LYS:HD3	2.51	0.41
1:C:296:LEU:HD22	1:C:322:MET:HE1	2.01	0.41
1:A:251:SER:HA	1:A:287:ARG:HH22	1.85	0.41
1:C:318:ILE:HG22	1:C:322:MET:HE3	2.02	0.41
2:F:29:PHE:O	2:F:33:LEU:HD22	2.20	0.41
2:J:33:LEU:HD22	2:J:54:ALA:HB1	2.02	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.55	0.41
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.28	0.41
2:D:188:TRP:CE3	2:D:193:MET:HE2	2.56	0.41
2:F:207:ASP:OD2	2:F:207:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:VAL:O	1:G:104:ARG:HD2	2.21	0.41
1:G:149:GLN:HG3	8:G:1443:HOH:O	2.19	0.41
1:G:318:ILE:HG22	1:G:322:MET:CE	2.51	0.41
2:H:353:ARG:O	2:H:357:LEU:HB2	2.20	0.41
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.55	0.41
2:L:243:LYS:HB2	2:L:243:LYS:HE3	1.91	0.41
3:O:308:CYS:HA	7:O:1308:GER:C2	2.50	0.41
1:C:244:ILE:HD11	1:C:259:GLU:OE1	2.21	0.41
2:H:258:ASN:CG	2:H:259:GLY:H	2.28	0.41
2:J:64:LEU:O	2:J:67:VAL:HG22	2.19	0.41
2:J:68:ASN:CG	2:J:71:ASP:OD2	2.64	0.41
2:B:110:ASN:CB	2:B:111:PRO:HD2	2.50	0.41
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.56	0.41
1:I:67:ARG:HD2	8:I:462:HOH:O	2.20	0.41
2:L:69:LYS:O	2:L:73:ILE:HG13	2.21	0.41
7:N:1208:GER:H112	7:N:1208:GER:H91	1.89	0.41
1:A:294:ASN:O	1:A:298:GLN:HG3	2.20	0.41
1:C:124:ILE:HD13	1:C:134:TRP:CH2	2.56	0.41
2:D:53:PHE:HE1	7:N:1208:GER:H42	1.86	0.41
2:J:245:LEU:O	2:J:249:LYS:HG3	2.21	0.41
7:R:1608:GER:H112	7:R:1608:GER:H91	1.87	0.41
2:B:208:ASN:CG	2:B:247:ARG:HB3	2.46	0.41
1:E:328:ASP:O	1:E:329:ASN:HB2	2.21	0.41
2:H:86:ASP:OD2	2:H:86:ASP:N	2.54	0.41
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.91	0.41
1:A:71:GLU:O	1:A:115:ARG:NH1	2.54	0.40
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.50	0.40
1:E:231:VAL:CG2	1:E:266:MET:HE3	2.45	0.40
2:F:18:LEU:HD12	2:F:304:ARG:NH1	2.36	0.40
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.20	0.40
1:I:82:ASP:HB2	1:I:86:PRO:HB3	2.02	0.40
1:I:124:ILE:HD13	1:I:134:TRP:CH2	2.56	0.40
1:I:252:ASP:OD2	1:I:252:ASP:C	2.64	0.40
2:L:188:TRP:CE3	2:L:193:MET:HE2	2.56	0.40
2:L:269:ASP:C	2:L:269:ASP:OD1	2.63	0.40
3:M:108:CYS:HA	7:M:1108:GER:C2	2.51	0.40
1:A:334:LEU:O	1:A:338:LEU:HG	2.22	0.40
1:C:78:VAL:O	1:C:104:ARG:HD2	2.21	0.40
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.94	0.40
1:C:251:SER:HA	1:C:287:ARG:HH12	1.87	0.40
2:D:101:LEU:HD23	2:D:101:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:LYS:HE3	1:E:357:ARG:NH2	2.29	0.40
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.53	0.40
3:R:608:CYS:HA	7:R:1608:GER:H21	2.02	0.40
2:D:318:ASP:HB2	7:N:1208:GER:C7	2.47	0.40
2:F:53:PHE:HE1	7:O:1308:GER:H42	1.86	0.40
2:H:33:LEU:HD22	2:H:54:ALA:HB1	2.03	0.40
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.02	0.40
2:J:86:ASP:OD2	2:J:86:ASP:N	2.54	0.40
1:C:184:GLN:HB2	8:C:1404:HOH:O	2.21	0.40
1:C:296:LEU:CD2	1:C:322:MET:HE1	2.51	0.40
1:G:97:ARG:NH1	1:G:97:ARG:CB	2.85	0.40
1:G:219:GLU:HA	1:G:219:GLU:OE1	2.21	0.40
2:L:33:LEU:HD22	2:L:54:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	21	42
1	C	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	36	58
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	36	58
1	G	312/377 (83%)	294 (94%)	16 (5%)	2 (1%)	21	42
1	I	312/377 (83%)	293 (94%)	17 (5%)	2 (1%)	21	42
1	K	312/377 (83%)	294 (94%)	17 (5%)	1 (0%)	36	58
2	B	344/377 (91%)	334 (97%)	9 (3%)	1 (0%)	36	58
2	D	344/377 (91%)	333 (97%)	9 (3%)	2 (1%)	21	42
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	36	58
2	H	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	36	58
2	L	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	36	58
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%)	24	46

All (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
2	F	258	ASN
2	H	258	ASN
1	I	326	GLN
2	J	258	ASN
2	L	258	ASN
1	E	326	GLN
1	G	306	HIS
2	H	333	GLU
1	I	306	HIS
1	K	306	HIS
2	D	333	GLU
1	A	306	HIS
2	H	111	PRO

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	76
1	C	283/338 (84%)	273 (96%)	10 (4%)	32	59
1	E	284/338 (84%)	276 (97%)	8 (3%)	38	66
1	G	281/338 (83%)	275 (98%)	6 (2%)	47	73
1	I	287/338 (85%)	277 (96%)	10 (4%)	32	59
1	K	291/338 (86%)	283 (97%)	8 (3%)	39	67
2	B	289/326 (89%)	276 (96%)	13 (4%)	24	50
2	D	293/326 (90%)	279 (95%)	14 (5%)	23	47
2	F	294/326 (90%)	281 (96%)	13 (4%)	25	50
2	H	288/326 (88%)	277 (96%)	11 (4%)	29	56
2	J	292/326 (90%)	278 (95%)	14 (5%)	23	47
2	L	296/326 (91%)	283 (96%)	13 (4%)	25	50
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%)	3358 (96%)	125 (4%)	31	58

All (125) 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	232	LEU

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Mol	Chain	Res	Type
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	76	ASP
1	C	114	GLU
1	C	156	ILE
1	C	182	PRO
1	C	217	ASP
1	C	287	ARG
1	C	324	GLU
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	306	VAL
2	D	329	LEU
2	D	331	LEU
1	E	55	PHE
1	E	71	GLU
1	E	156	ILE
1	E	214	ARG
1	E	257	GLU
1	E	287	ARG
1	E	324	GLU
1	E	364	GLN
2	F	21	LEU
2	F	24	ARG
2	F	33	LEU
2	F	151	LEU

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Mol	Chain	Res	Type
2	F	210	LEU
2	F	216	LEU
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	156	ILE
1	G	224	ASP
1	G	287	ARG
1	G	324	GLU
1	G	353	LYS
2	H	18	LEU
2	H	21	LEU
2	H	33	LEU
2	H	151	LEU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	357	LEU
1	I	55	PHE
1	I	67	ARG
1	I	71	GLU
1	I	114	GLU
1	I	142	ARG
1	I	156	ILE
1	I	194	ASN
1	I	195	GLN
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

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Mol	Chain	Res	Type
2	J	222	SER
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	357	LEU
1	K	71	GLU
1	K	114	GLU
1	K	142	ARG
1	K	156	ILE
1	K	195	GLN
1	K	287	ARG
1	K	324	GLU
1	K	357	ARG
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	110	ASN
2	L	151	LEU
2	L	210	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	258	ASN
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 (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	89	GLN
1	A	135	HIS
1	A	184	GLN
1	A	272	HIS
1	A	285	GLN
1	A	325	ASN
1	A	329	ASN
1	A	335	ASN

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Mol	Chain	Res	Type
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	218	ASN
1	C	272	HIS
1	C	285	GLN
1	C	298	GLN
1	C	303	GLN
1	C	364	GLN
2	D	30	GLN
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	184	GLN
1	E	194	ASN
1	E	272	HIS
1	E	298	GLN
1	E	335	ASN
2	F	30	GLN
2	F	212	GLN
2	F	246	ASN
1	G	80	GLN
1	G	81	ASN
1	G	89	GLN
1	G	135	HIS
1	G	149	GLN
1	G	162	GLN
1	G	184	GLN
1	G	194	ASN
1	G	297	ASN
1	G	303	GLN
1	G	325	ASN
2	H	257	GLN
1	I	89	GLN
1	I	108	GLN

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Mol	Chain	Res	Type
1	I	135	HIS
1	I	195	GLN
1	I	285	GLN
1	I	364	GLN
2	J	30	GLN
2	J	208	ASN
2	J	212	GLN
2	J	246	ASN
1	K	81	ASN
1	K	89	GLN
1	K	149	GLN
1	K	285	GLN
1	K	298	GLN
1	K	325	ASN
1	K	367	HIS
2	L	110	ASN
2	L	208	ASN
2	L	212	GLN
2	L	257	GLN
2	L	345	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GRG	L	1506	-	27,28,28	0.80	0	33,37,37	0.93	1 (3%)
6	GRG	J	1505	-	27,28,28	0.77	0	33,37,37	0.89	1 (3%)
6	GRG	D	1502	-	27,28,28	0.82	0	33,37,37	0.89	1 (3%)
7	GER	P	1408	3	19,19,19	0.93	0	21,22,22	0.61	0
7	GER	N	1208	3	19,19,19	0.92	0	21,22,22	0.63	0
7	GER	Q	1508	3	19,19,19	0.89	0	21,22,22	0.63	0
6	GRG	B	1501	-	27,28,28	0.78	0	33,37,37	0.89	1 (3%)
7	GER	O	1308	3	19,19,19	0.94	1 (5%)	21,22,22	0.63	0
7	GER	R	1608	3	19,19,19	0.91	0	21,22,22	0.65	0
6	GRG	F	1503	-	27,28,28	0.81	0	33,37,37	0.90	1 (3%)
6	GRG	H	1504	-	27,28,28	0.77	0	33,37,37	0.90	1 (3%)
7	GER	M	1108	3	19,19,19	0.93	0	21,22,22	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GRG	L	1506	-	-	8/31/31/31	-
6	GRG	J	1505	-	-	9/31/31/31	-
6	GRG	D	1502	-	-	8/31/31/31	-
7	GER	P	1408	3	-	10/20/20/20	-
7	GER	N	1208	3	-	10/20/20/20	-
7	GER	Q	1508	3	-	9/20/20/20	-
6	GRG	B	1501	-	-	7/31/31/31	-
7	GER	O	1308	3	-	9/20/20/20	-
7	GER	R	1608	3	-	10/20/20/20	-
6	GRG	F	1503	-	-	7/31/31/31	-
6	GRG	H	1504	-	-	8/31/31/31	-
7	GER	M	1108	3	-	9/20/20/20	-

All (1) bond length outliers are listed below:

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

All (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
6	F	1503	GRG	O1B-PB-O3A	2.40	112.70	104.64

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1501	GRG	PA-O3A-PB-O1B
6	D	1502	GRG	PA-O3A-PB-O1B
6	F	1503	GRG	PA-O3A-PB-O1B
6	H	1504	GRG	PA-O3A-PB-O1B
6	J	1505	GRG	PA-O3A-PB-O1B
6	L	1506	GRG	PA-O3A-PB-O1B
7	M	1108	GER	C4-C3-C5-C6
7	M	1108	GER	C11-C10-C8-C9
7	N	1208	GER	C11-C10-C8-C9
7	O	1308	GER	C4-C3-C5-C6
7	O	1308	GER	C11-C10-C8-C9
7	P	1408	GER	C11-C10-C8-C9
7	Q	1508	GER	C4-C3-C5-C6
7	Q	1508	GER	C11-C10-C8-C9
7	R	1608	GER	C11-C10-C8-C9
7	M	1108	GER	C2-C3-C5-C6
7	M	1108	GER	C11-C10-C8-C7
7	N	1208	GER	C11-C10-C8-C7
7	O	1308	GER	C11-C10-C8-C7
7	P	1408	GER	C11-C10-C8-C7
7	Q	1508	GER	C2-C3-C5-C6
7	Q	1508	GER	C11-C10-C8-C7
7	R	1608	GER	C11-C10-C8-C7
7	N	1208	GER	C4-C3-C5-C6
7	P	1408	GER	C4-C3-C5-C6
7	R	1608	GER	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	O	1308	GER	C2-C3-C5-C6
7	P	1408	GER	C2-C3-C5-C6
7	M	1108	GER	C13-C15-C16-C17
7	O	1308	GER	C13-C15-C16-C17
7	R	1608	GER	C2-C3-C5-C6
7	N	1208	GER	C2-C3-C5-C6
7	P	1408	GER	C12-C13-C15-C16
7	R	1608	GER	C12-C13-C15-C16
7	Q	1508	GER	C14-C13-C15-C16
7	Q	1508	GER	C12-C13-C15-C16
7	P	1408	GER	C14-C13-C15-C16
7	R	1608	GER	C14-C13-C15-C16
7	M	1108	GER	C12-C13-C15-C16
7	N	1208	GER	C12-C13-C15-C16
7	O	1308	GER	C12-C13-C15-C16
7	M	1108	GER	C14-C13-C15-C16
7	N	1208	GER	C14-C13-C15-C16
7	N	1208	GER	C13-C15-C16-C17
7	O	1308	GER	C14-C13-C15-C16
7	P	1408	GER	C13-C15-C16-C17
7	Q	1508	GER	C13-C15-C16-C17
7	R	1608	GER	C13-C15-C16-C17
6	F	1503	GRG	C14-C13-C15-C16
6	J	1505	GRG	C14-C13-C15-C16
6	D	1502	GRG	C10-C8-C9-C11
6	H	1504	GRG	C10-C8-C9-C11
6	L	1506	GRG	C10-C8-C9-C11
6	B	1501	GRG	C14-C13-C15-C16
6	B	1501	GRG	C10-C8-C9-C11
6	D	1502	GRG	C14-C13-C15-C16
6	D	1502	GRG	C4-C3-C5-C6
6	L	1506	GRG	C14-C13-C15-C16
6	B	1501	GRG	C4-C3-C5-C6
6	F	1503	GRG	C10-C8-C9-C11
6	H	1504	GRG	C14-C13-C15-C16
6	J	1505	GRG	C10-C8-C9-C11
6	J	1505	GRG	C4-C3-C5-C6
6	H	1504	GRG	C4-C3-C5-C6
6	L	1506	GRG	C4-C3-C5-C6
6	B	1501	GRG	C12-C13-C15-C16
6	H	1504	GRG	C12-C13-C15-C16
6	J	1505	GRG	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
6	L	1506	GRG	PA-O3A-PB-O3B
6	D	1502	GRG	C12-C13-C15-C16
6	B	1501	GRG	PA-O3A-PB-O2B
6	D	1502	GRG	PA-O3A-PB-O2B
6	F	1503	GRG	PA-O3A-PB-O2B
6	H	1504	GRG	PA-O3A-PB-O2B
6	J	1505	GRG	PA-O3A-PB-O2B
6	L	1506	GRG	PA-O3A-PB-O2B
6	F	1503	GRG	C4-C3-C5-C6
6	L	1506	GRG	C12-C13-C15-C16
6	J	1505	GRG	C9-C11-C12-C13
6	L	1506	GRG	C9-C11-C12-C13
7	M	1108	GER	C10-C11-C12-C13
7	N	1208	GER	C10-C11-C12-C13
7	N	1208	GER	C15-C16-C17-C18
7	O	1308	GER	C10-C11-C12-C13
7	P	1408	GER	C10-C11-C12-C13
7	P	1408	GER	C15-C16-C17-C18
7	Q	1508	GER	C10-C11-C12-C13
7	Q	1508	GER	C15-C16-C17-C18
7	R	1608	GER	C10-C11-C12-C13
7	R	1608	GER	C15-C16-C17-C18
6	F	1503	GRG	C9-C11-C12-C13
6	H	1504	GRG	C9-C11-C12-C13
7	M	1108	GER	C15-C16-C17-C18
7	N	1208	GER	C5-C6-C7-C8
7	O	1308	GER	C15-C16-C17-C18
6	F	1503	GRG	C12-C13-C15-C16
6	J	1505	GRG	C12-C13-C15-C16
6	B	1501	GRG	C9-C11-C12-C13
6	D	1502	GRG	C9-C11-C12-C13
7	P	1408	GER	C5-C6-C7-C8
6	D	1502	GRG	C15-C16-C17-C18
6	H	1504	GRG	C15-C16-C17-C18
6	J	1505	GRG	C15-C16-C17-C18
7	R	1608	GER	C5-C6-C7-C8

There are no ring outliers.

12 monomers are involved in 43 short contacts:

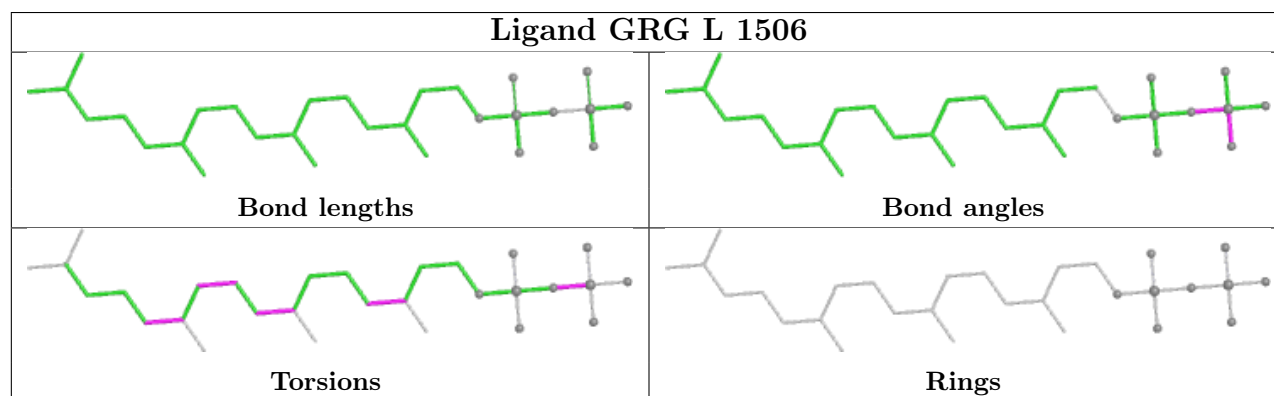
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1506	GRG	2	0

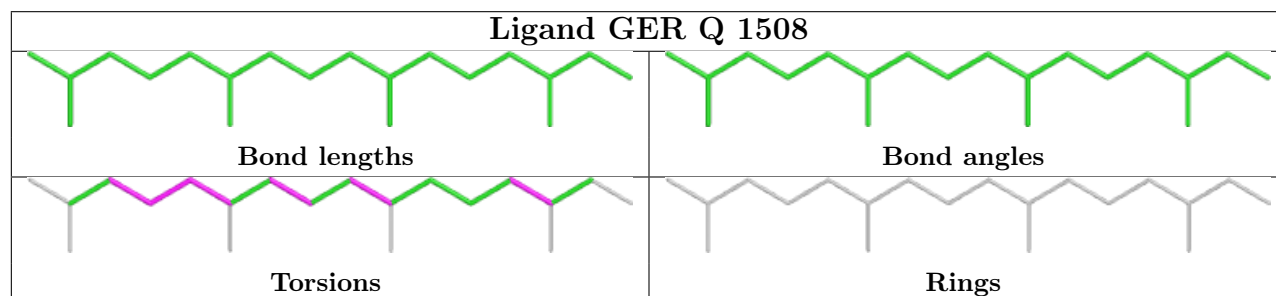
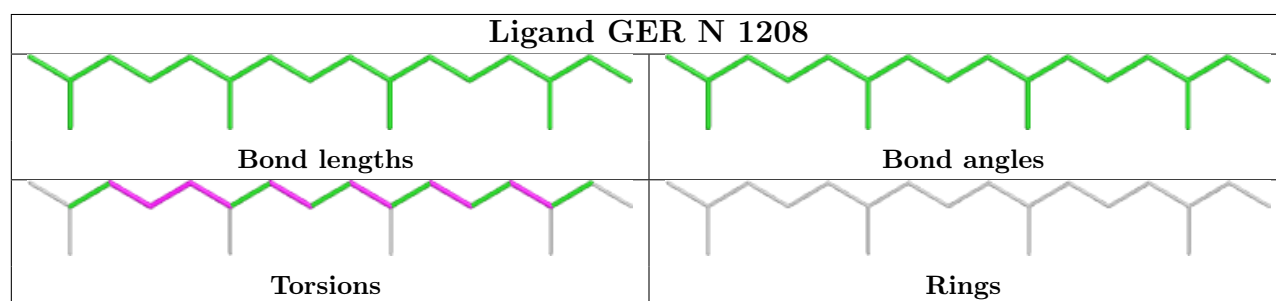
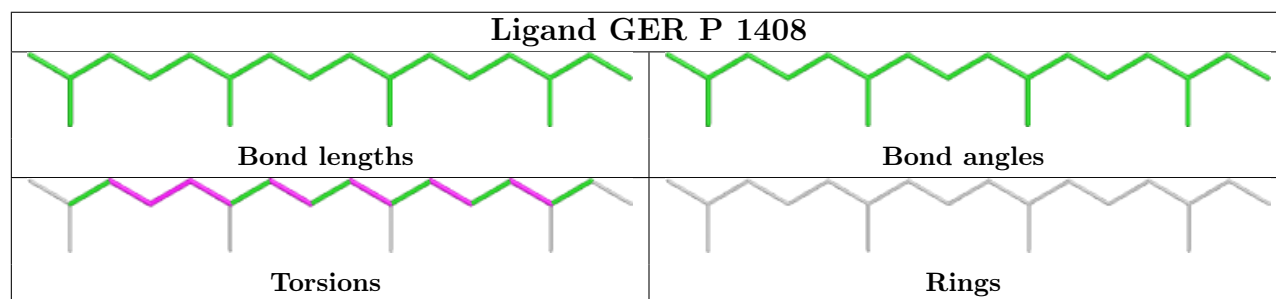
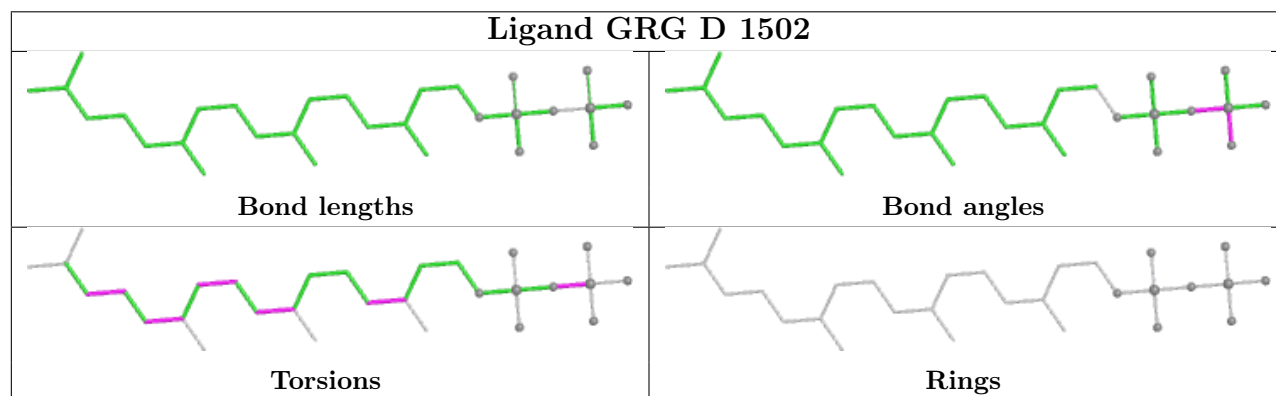
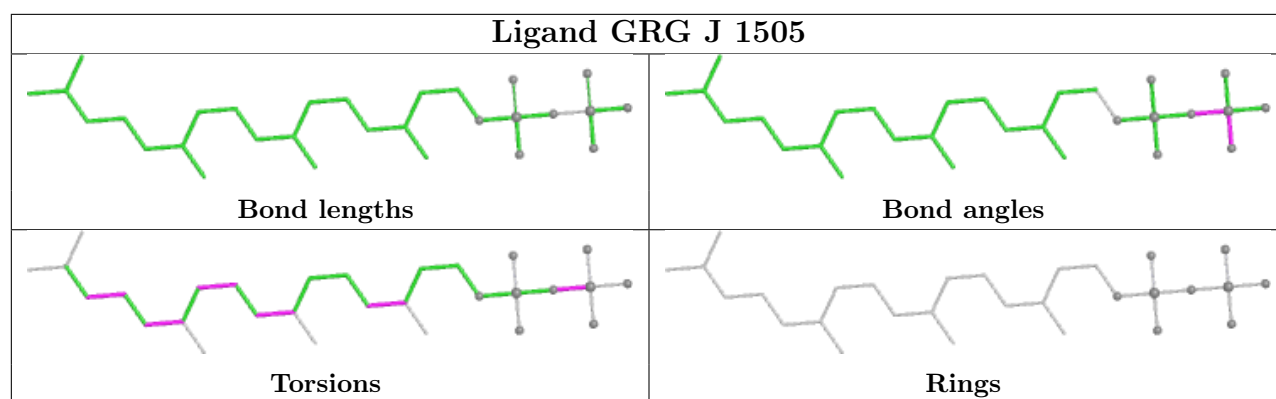
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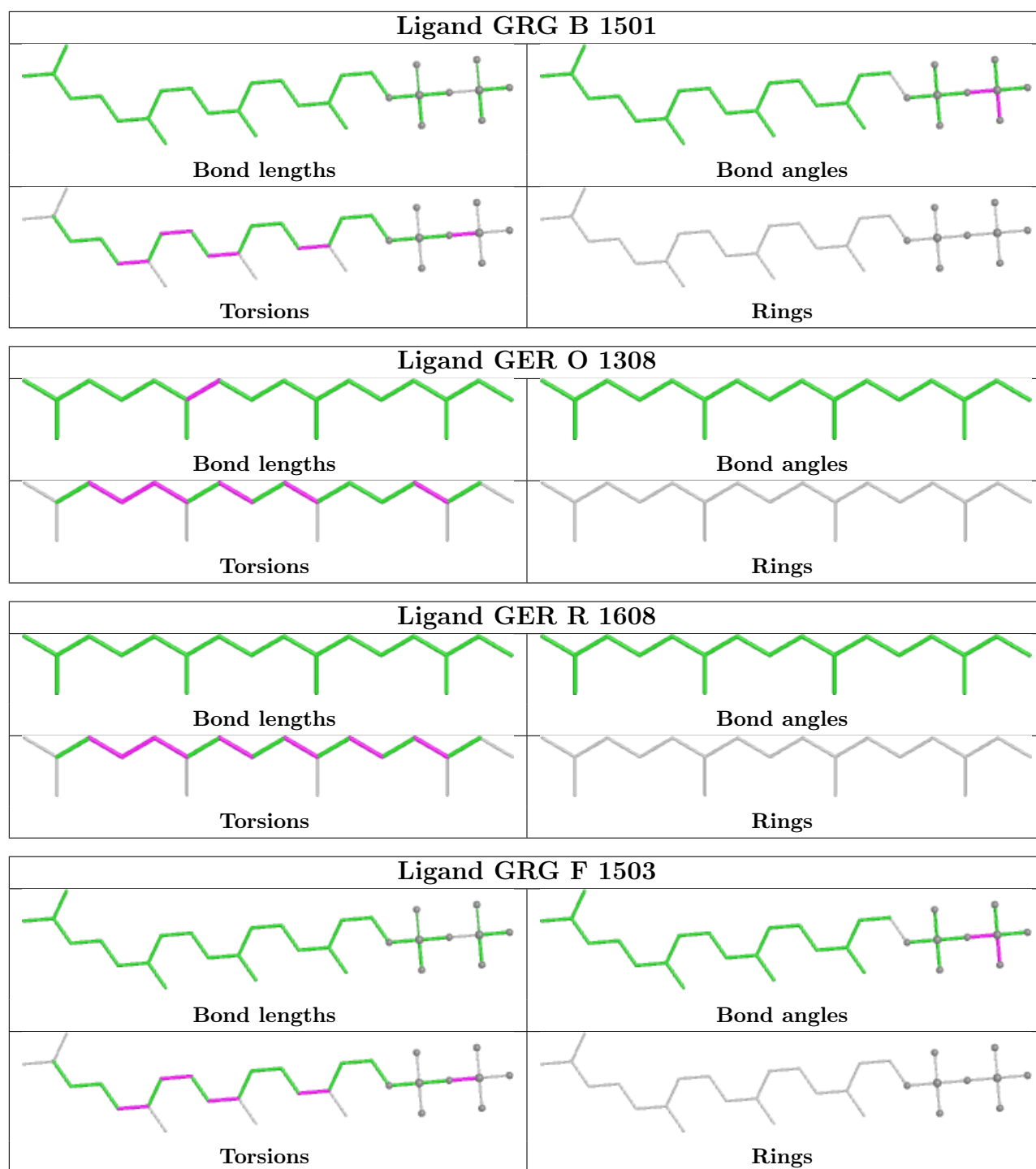
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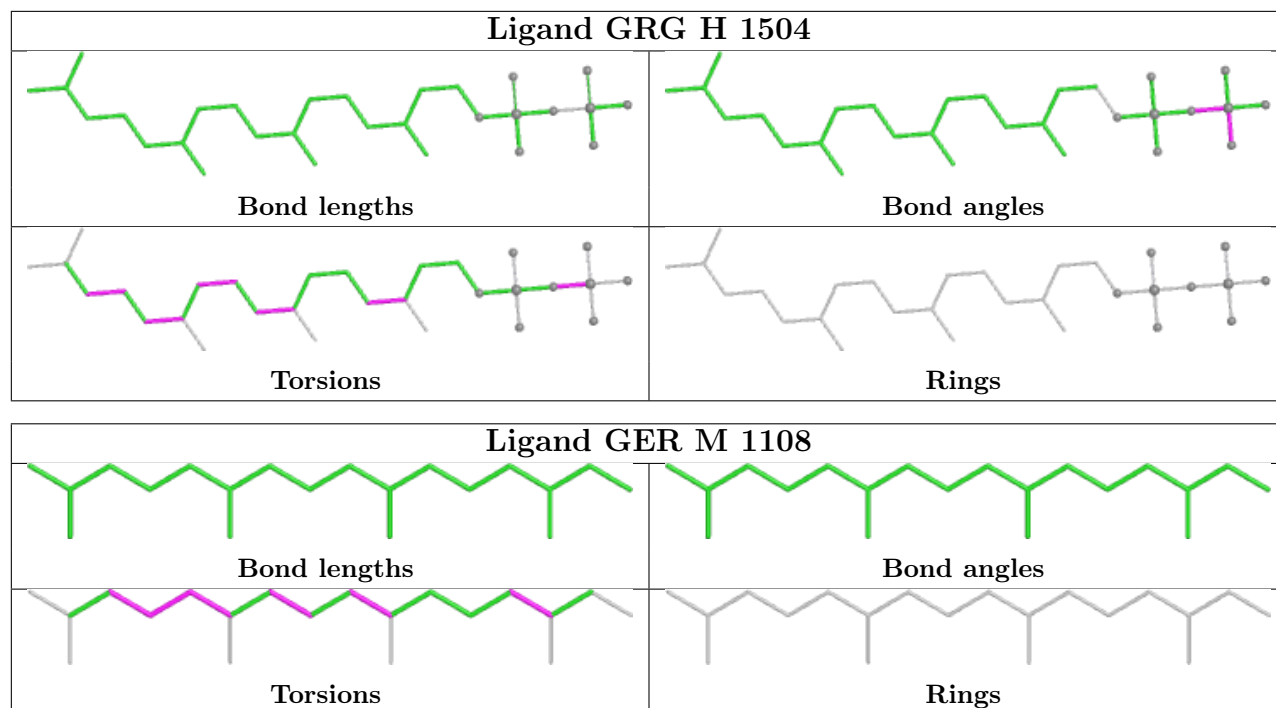
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	1505	GRG	1	0
6	D	1502	GRG	2	0
7	P	1408	GER	6	0
7	N	1208	GER	6	0
7	Q	1508	GER	4	0
6	B	1501	GRG	1	0
7	O	1308	GER	7	0
7	R	1608	GER	6	0
6	F	1503	GRG	2	0
6	H	1504	GRG	1	0
7	M	1108	GER	5	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	314/377 (83%)	0.36	15 (4%)	35 30	35, 57, 91, 109	0
1	C	314/377 (83%)	0.34	17 (5%)	31 26	33, 54, 82, 99	0
1	E	314/377 (83%)	0.49	14 (4%)	38 32	33, 58, 86, 104	0
1	G	314/377 (83%)	0.56	27 (8%)	16 12	36, 58, 88, 102	0
1	I	314/377 (83%)	0.27	13 (4%)	41 36	29, 53, 84, 95	0
1	K	314/377 (83%)	-0.16	5 (1%)	70 66	23, 43, 67, 82	0
2	B	346/377 (91%)	0.07	12 (3%)	47 41	36, 51, 77, 102	0
2	D	346/377 (91%)	-0.06	13 (3%)	44 38	31, 47, 74, 94	0
2	F	346/377 (91%)	-0.02	17 (4%)	35 29	32, 47, 75, 100	0
2	H	346/377 (91%)	0.86	46 (13%)	7 5	37, 65, 95, 113	0
2	J	346/377 (91%)	0.16	20 (5%)	29 23	30, 50, 78, 104	0
2	L	346/377 (91%)	-0.27	9 (2%)	57 51	26, 41, 64, 95	0
3	M	4/11 (36%)	5.48	3 (75%)	0 0	45, 50, 55, 62	4 (100%)
3	N	4/11 (36%)	4.86	3 (75%)	0 0	47, 50, 55, 61	4 (100%)
3	O	4/11 (36%)	5.19	2 (50%)	0 0	43, 48, 53, 60	4 (100%)
3	P	4/11 (36%)	5.18	4 (100%)	0 0	43, 46, 50, 56	4 (100%)
3	Q	4/11 (36%)	3.54	2 (50%)	0 0	49, 54, 61, 69	4 (100%)
3	R	5/11 (45%)	3.63	3 (60%)	0 0	50, 54, 72, 73	5 (100%)
All	All	3985/4590 (86%)	0.24	225 (5%)	30 24	23, 52, 83, 113	25 (0%)

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	308	CYS	10.3
3	M	108	CYS	9.6
3	N	208	CYS	9.1

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Mol	Chain	Res	Type	RSRZ
3	P	408	CYS	9.1
1	G	55	PHE	8.0
3	M	109	VAL	8.0
3	Q	508	CYS	7.5
1	C	55	PHE	7.3
3	O	309	VAL	6.9
2	F	18	LEU	6.6
3	P	409	VAL	6.5
3	N	209	VAL	6.1
2	H	18	LEU	6.1
1	I	55	PHE	5.9
1	E	55	PHE	5.8
3	R	607	LYS	5.6
2	B	18	LEU	5.5
2	F	113	THR	5.1
2	L	363	THR	4.9
2	H	113	THR	4.9
3	R	608	CYS	4.9
2	J	110	ASN	4.9
1	A	368	SER	4.8
2	J	18	LEU	4.8
1	E	332	ASP	4.7
2	B	110	ASN	4.7
2	H	111	PRO	4.6
2	F	110	ASN	4.6
3	R	609	VAL	4.5
1	K	55	PHE	4.5
2	J	363	THR	4.5
1	A	328	ASP	4.5
2	J	108	SER	4.4
2	L	111	PRO	4.4
2	H	363	THR	4.4
2	J	111	PRO	4.3
2	H	85	GLU	4.3
1	G	368	SER	4.3
2	B	111	PRO	4.2
2	B	362	LYS	4.2
1	G	326	GLN	4.2
1	E	368	SER	4.2
3	Q	509	VAL	4.2
2	F	363	THR	4.2
1	I	368	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	111	PRO	3.9
1	C	368	SER	3.9
2	H	362	LYS	3.9
2	H	65	ASP	3.9
2	D	113	THR	3.8
2	J	85	GLU	3.8
2	H	304	ARG	3.8
2	D	314	ASP	3.8
2	B	363	THR	3.8
1	A	55	PHE	3.7
2	D	18	LEU	3.6
2	D	363	THR	3.6
2	H	108	SER	3.6
2	H	110	ASN	3.6
1	G	57	SER	3.6
2	L	113	THR	3.5
2	B	113	THR	3.5
2	L	18	LEU	3.5
2	H	305	LEU	3.5
2	F	111	PRO	3.4
2	F	85	GLU	3.4
2	J	113	THR	3.3
1	C	306	HIS	3.2
2	J	360	SER	3.2
2	H	316	HIS	3.2
1	G	59	ASP	3.2
2	H	336	GLY	3.1
2	L	362	LYS	3.1
2	H	335	SER	3.1
1	G	58	LEU	3.1
3	P	411	LEU	3.0
1	A	327	CYS	3.0
1	G	56	LEU	3.0
1	K	59	ASP	3.0
2	J	362	LYS	3.0
2	F	316	HIS	3.0
1	G	92	TYR	3.0
2	J	91	ASP	3.0
1	A	364	GLN	2.9
1	E	306	HIS	2.9
1	G	364	GLN	2.9
1	K	332	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLU	2.9
2	H	314	ASP	2.9
2	D	109	LYS	2.9
1	G	195	GLN	2.8
3	N	211	LEU	2.8
1	G	305	SER	2.8
2	L	110	ASN	2.8
1	C	328	ASP	2.8
2	F	112	GLY	2.8
2	H	70	ASP	2.8
2	B	65	ASP	2.8
2	F	314	ASP	2.8
2	F	359	GLN	2.7
2	J	106	ASN	2.7
1	E	331	GLU	2.7
1	G	328	ASP	2.7
1	C	304	PRO	2.7
2	F	109	LYS	2.7
1	A	331	GLU	2.7
2	H	114	ALA	2.7
3	M	111	LEU	2.7
1	C	81	ASN	2.7
1	C	331	GLU	2.7
1	G	61	PRO	2.7
1	K	368	SER	2.7
2	J	338	CYS	2.6
2	H	39	ARG	2.6
1	A	288	GLY	2.6
1	G	125	GLU	2.6
2	B	316	HIS	2.6
2	F	362	LYS	2.6
1	G	304	PRO	2.6
2	H	71	ASP	2.6
2	H	333	GLU	2.6
2	H	308	GLY	2.6
1	A	326	GLN	2.6
1	I	85	SER	2.5
2	H	109	LYS	2.5
2	H	35	VAL	2.5
2	B	305	LEU	2.5
1	C	225	GLN	2.5
2	L	85	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	338	CYS	2.5
2	D	305	LEU	2.5
1	A	59	ASP	2.5
1	G	306	HIS	2.5
2	H	135	LEU	2.4
1	E	94	GLU	2.4
1	G	83	GLY	2.4
2	H	27	ARG	2.4
2	J	89	ASN	2.4
1	C	305	SER	2.4
1	G	85	SER	2.4
2	F	39	ARG	2.4
1	G	62	THR	2.4
1	I	329	ASN	2.4
2	D	110	ASN	2.4
2	F	108	SER	2.4
2	F	38	GLU	2.4
2	L	109	LYS	2.4
1	G	307	SER	2.4
1	E	224	ASP	2.4
2	H	361	TRP	2.4
1	I	327	CYS	2.4
1	G	86	PRO	2.4
2	L	106	ASN	2.3
1	C	217	ASP	2.3
1	I	59	ASP	2.3
1	I	332	ASP	2.3
2	H	107	PRO	2.3
2	H	190	GLY	2.3
2	H	349	ARG	2.3
2	H	306	VAL	2.3
2	D	65	ASP	2.3
2	H	19	ASP	2.3
1	E	326	GLN	2.3
1	K	326	GLN	2.3
1	E	294	ASN	2.3
1	E	288	GLY	2.3
1	A	330	LYS	2.3
1	C	326	GLN	2.3
1	I	364	GLN	2.3
2	H	307	GLY	2.3
1	I	269	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	310	ALA	2.2
2	J	114	ALA	2.2
2	H	38	GLU	2.2
1	G	81	ASN	2.2
2	B	315	SER	2.2
2	D	108	SER	2.2
2	H	82	LEU	2.2
1	G	348	LYS	2.2
1	C	265	GLU	2.2
1	I	326	GLN	2.2
2	D	359	GLN	2.2
2	F	315	SER	2.2
2	H	112	GLY	2.2
2	B	109	LYS	2.2
2	H	105	PHE	2.2
1	A	217	ASP	2.2
1	A	366	LYS	2.2
2	H	63	SER	2.2
2	J	314	ASP	2.2
1	E	268	LYS	2.2
1	C	57	SER	2.2
1	G	91	ILE	2.2
1	I	328	ASP	2.1
1	G	324	GLU	2.1
2	J	333	GLU	2.1
1	G	84	PRO	2.1
1	C	329	ASN	2.1
1	A	224	ASP	2.1
1	A	301	ASP	2.1
1	E	59	ASP	2.1
1	E	328	ASP	2.1
3	P	410	ILE	2.1
1	C	251	SER	2.1
2	H	29	PHE	2.1
2	H	315	SER	2.1
1	C	347	GLU	2.1
1	A	142	ARG	2.1
2	H	24	ARG	2.1
2	H	359	GLN	2.1
2	H	62	ASP	2.1
2	J	70	ASP	2.1
2	H	31	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	304	PRO	2.1
2	J	107	PRO	2.1
1	G	89	GLN	2.1
2	F	65	ASP	2.0
2	J	65	ASP	2.0
1	C	307	SER	2.0
2	D	362	LYS	2.0
1	I	306	HIS	2.0
1	E	191	ASP	2.0
2	D	38	GLU	2.0
2	J	335	SER	2.0
2	H	40	TYR	2.0

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 oligosaccharides 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.

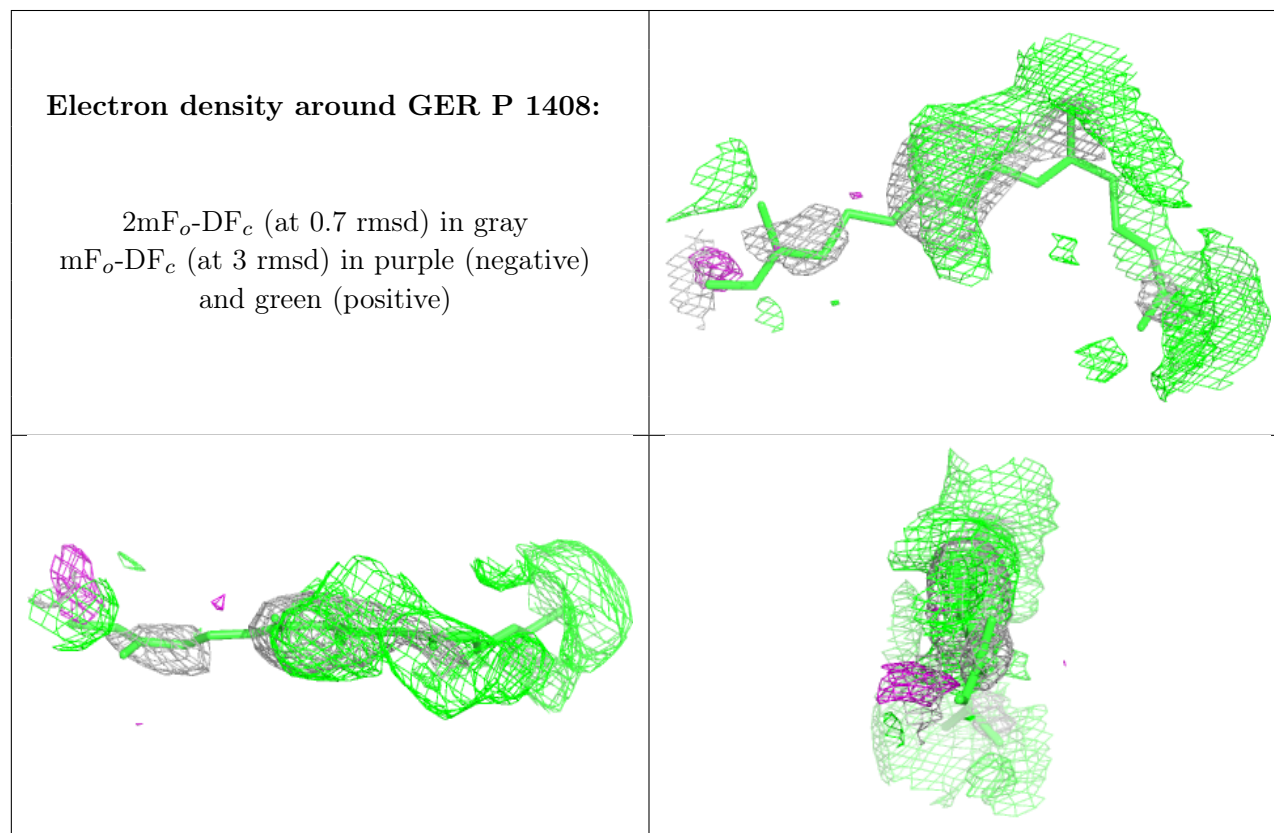
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GER	P	1408	20/20	0.73	0.51	72,78,81,82	20
7	GER	O	1308	20/20	0.76	0.47	71,78,83,83	20
7	GER	M	1108	20/20	0.76	0.49	69,76,83,84	20
7	GER	N	1208	20/20	0.77	0.44	67,76,84,84	20
7	GER	Q	1508	20/20	0.87	0.32	69,76,84,84	20
7	GER	R	1608	20/20	0.87	0.31	64,72,82,83	20
6	GRG	H	1504	29/29	0.93	0.16	61,65,75,77	0
6	GRG	B	1501	29/29	0.95	0.14	56,60,69,71	0
6	GRG	L	1506	29/29	0.95	0.12	40,45,53,58	0
6	GRG	D	1502	29/29	0.95	0.13	49,56,65,66	0
6	GRG	F	1503	29/29	0.95	0.13	50,58,70,71	0

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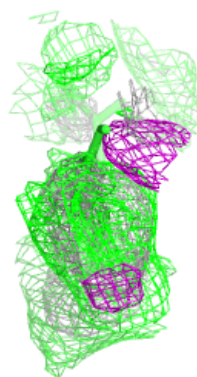
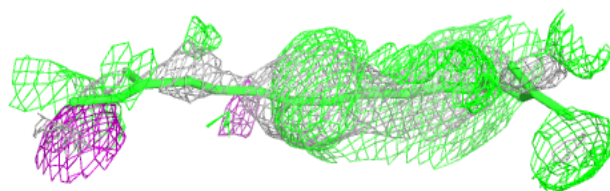
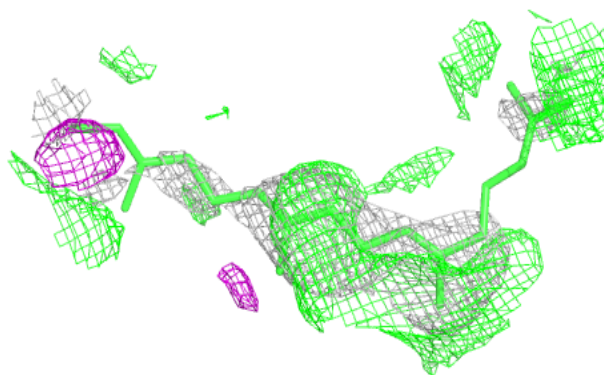
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GRG	J	1505	29/29	0.96	0.12	43,48,56,58	0
5	CL	H	1406	1/1	0.96	0.07	60,60,60,60	0
5	CL	J	1407	1/1	0.96	0.08	61,61,61,61	0
5	CL	C	1402	1/1	0.96	0.26	59,59,59,59	0
5	CL	B	1401	1/1	0.97	0.10	61,61,61,61	0
5	CL	G	1405	1/1	0.98	0.19	53,53,53,53	0
5	CL	D	1403	1/1	0.98	0.04	43,43,43,43	0
5	CL	F	1404	1/1	0.98	0.06	47,47,47,47	0
4	ZN	H	378	1/1	0.99	0.03	60,60,60,60	0
5	CL	K	1408	1/1	0.99	0.11	57,57,57,57	0
5	CL	L	1409	1/1	0.99	0.04	45,45,45,45	0
4	ZN	F	378	1/1	1.00	0.03	47,47,47,47	0
4	ZN	B	378	1/1	1.00	0.02	47,47,47,47	0
4	ZN	J	378	1/1	1.00	0.02	42,42,42,42	0
4	ZN	L	378	1/1	1.00	0.01	34,34,34,34	0
4	ZN	D	378	1/1	1.00	0.01	45,45,45,45	0

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

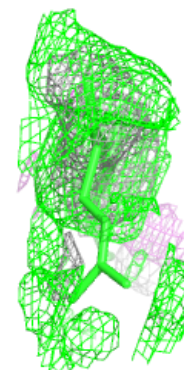
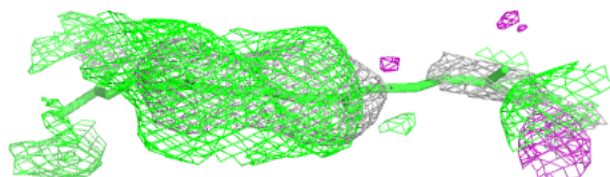
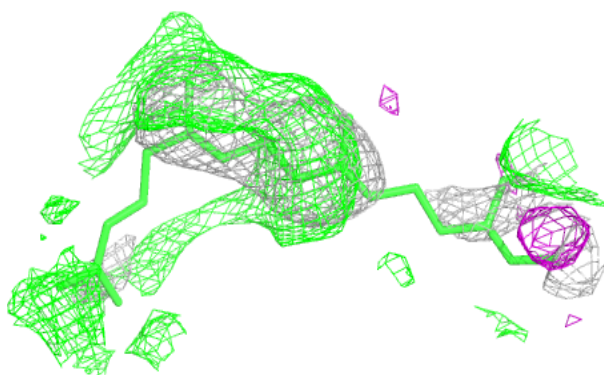


Electron density around GER O 1308:

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

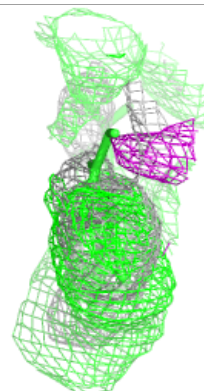
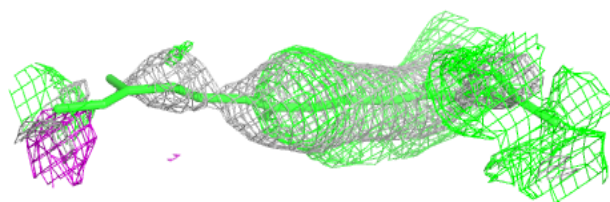
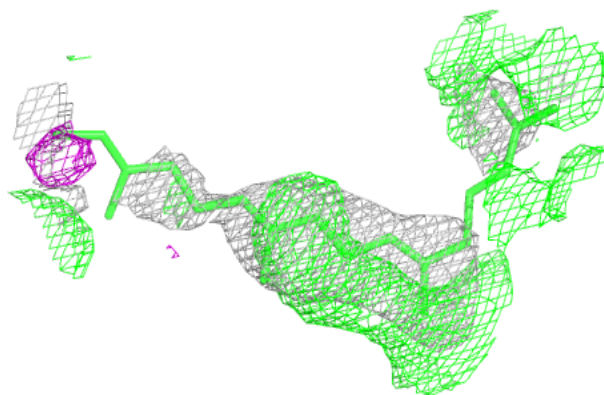
**Electron density around GER M 1108:**

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

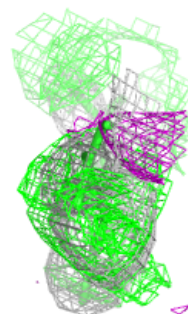
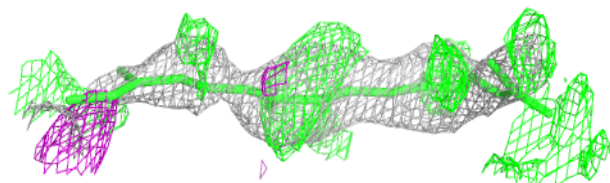
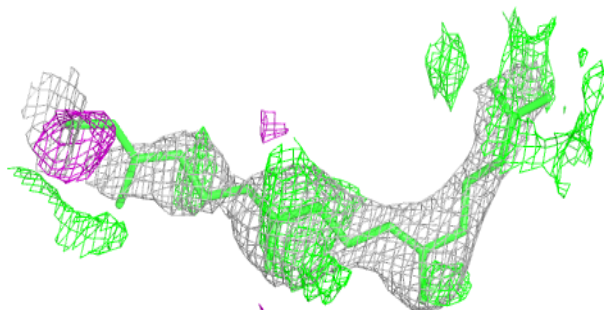


Electron density around GER N 1208:

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

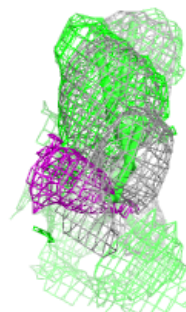
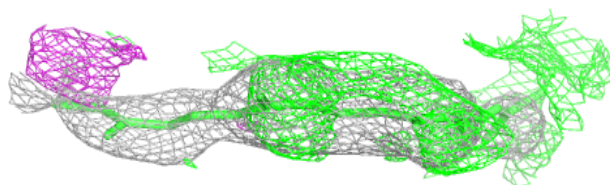
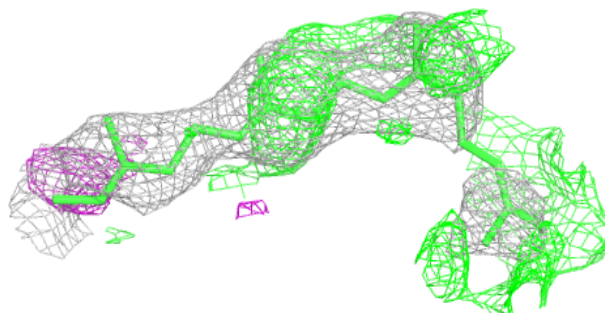
**Electron density around GER Q 1508:**

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

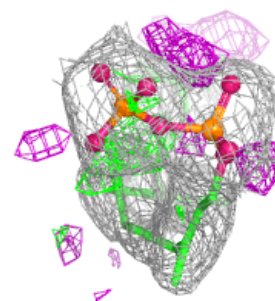
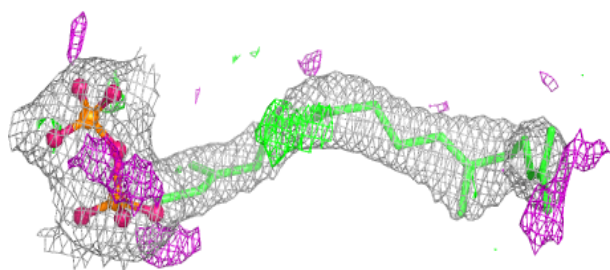
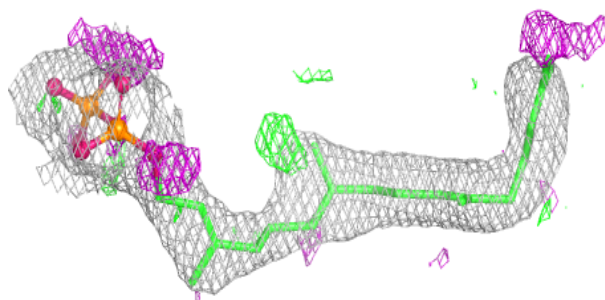


Electron density around GER R 1608:

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

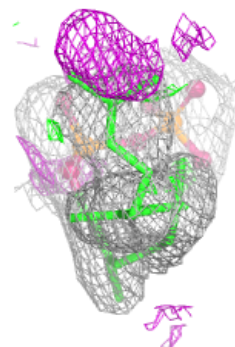
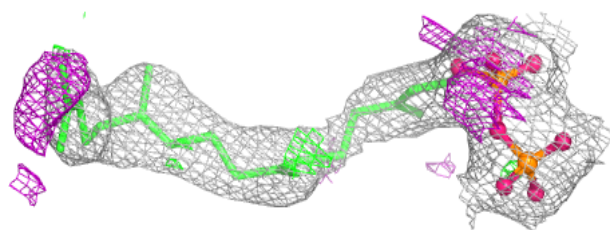
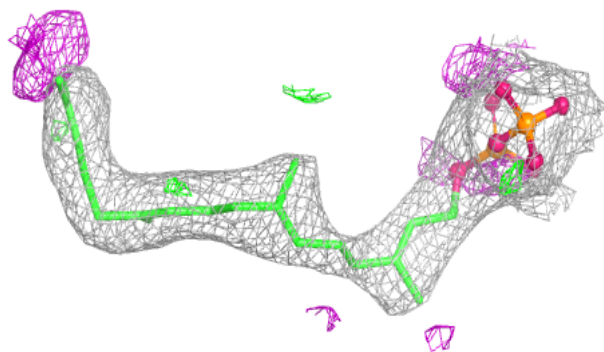
**Electron density around GRG H 1504:**

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

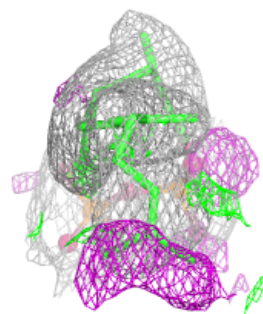
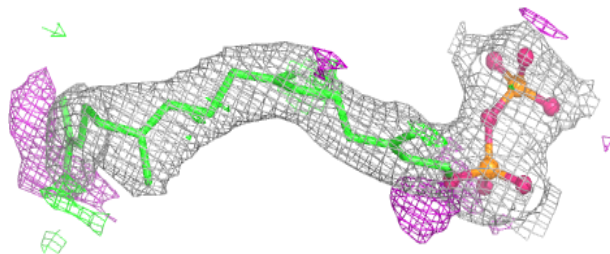
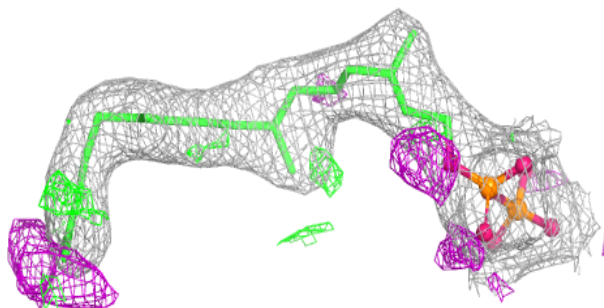


Electron density around GRG B 1501:

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

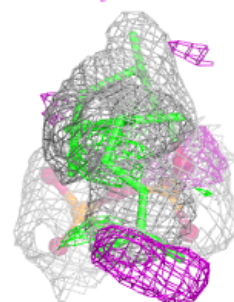
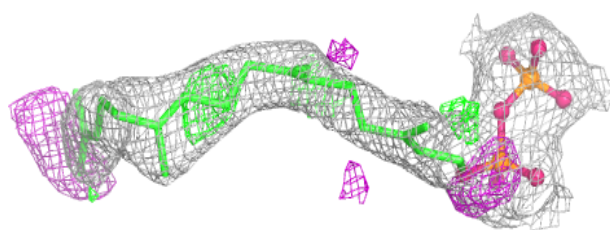
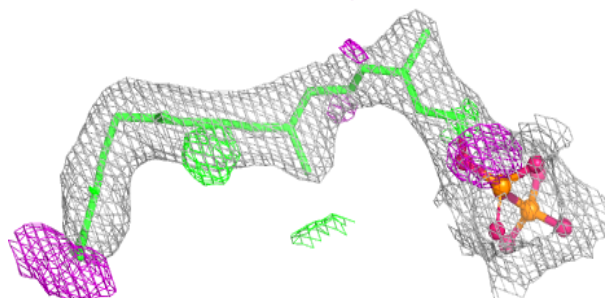
**Electron density around GRG L 1506:**

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

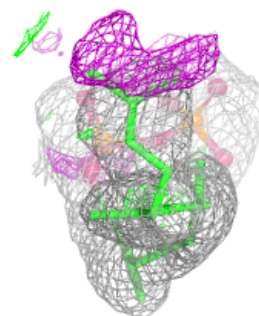
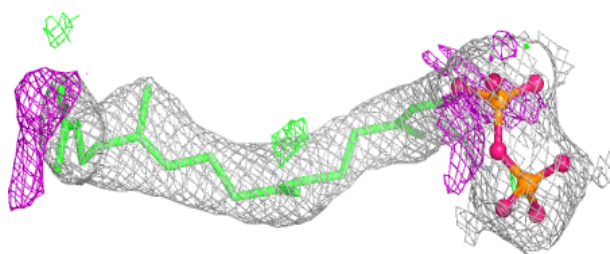
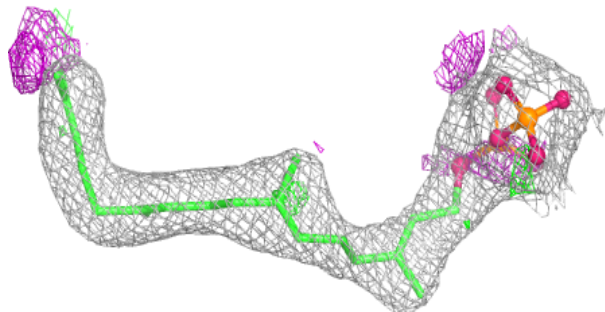


Electron density around GRG D 1502:

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

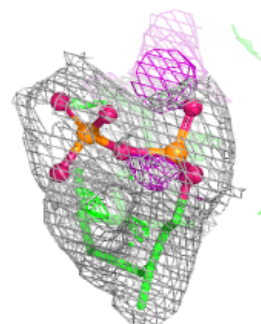
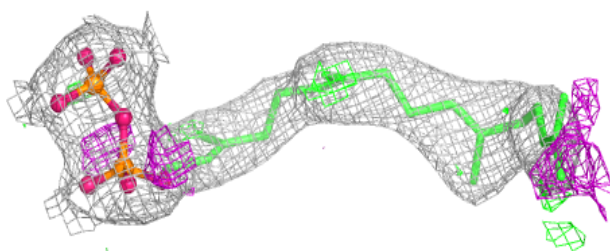
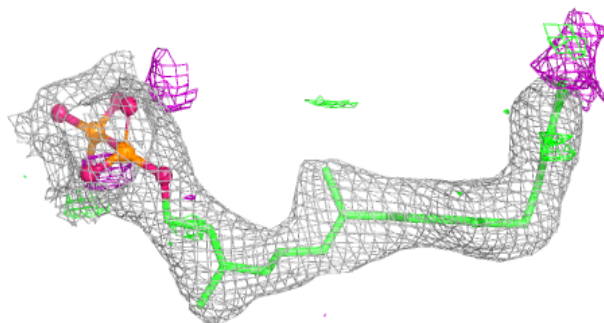
**Electron density around GRG F 1503:**

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



Electron density around GRG J 1505:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.