



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 10:52 pm BST

PDB ID : 1TNZ  
Title : Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a RRCVLL Peptide Derived from Cdc42 splice isoform-2  
Authors : Reid, T.S.; Terry, K.L.; Casey, P.J.; Beese, L.S.  
Deposited on : 2004-06-11  
Resolution : 2.90 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](mailto: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.

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

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

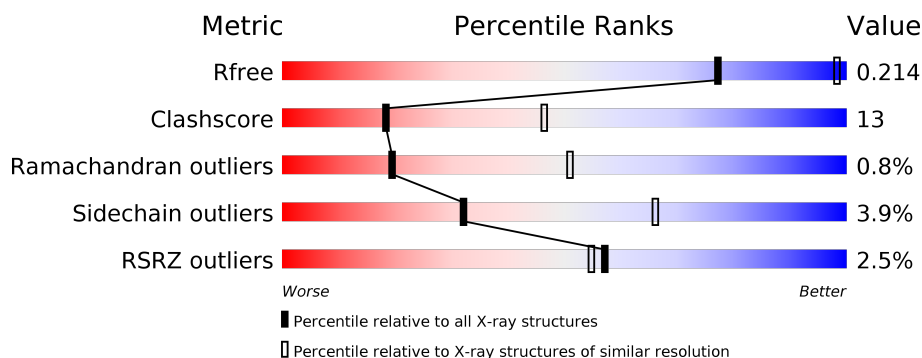
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>58%</div> <div>24%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	377	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>22%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	377	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>21%</div> <div>•</div> <div>17%</div> </div> </div>
1	G	377	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>22%</div> <div>•</div> <div>17%</div> </div> </div>
1	I	377	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>•</div> <div>17%</div> </div> </div>
1	K	377	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>21%</div> <div>•</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	B	377	<p>2% 64% 25% 8%</p>
2	D	377	<p>2% 67% 21% 8%</p>
2	F	377	<p>1% 67% 23% 8%</p>
2	H	377	<p>3% 60% 30% 8%</p>
2	J	377	<p>2% 64% 25% 8%</p>
2	L	377	<p>1% 68% 22% 8%</p>
3	M	6	<p>67% 17% 17%</p>
3	N	6	<p>67% 17% 17%</p>
3	O	6	<p>50% 33% 17%</p>
3	P	6	<p>83% 17%</p>
3	Q	6	<p>67% 17% 17%</p>
3	R	6	<p>67% 17% 17%</p>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32873 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 geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2636	1682	463	486	5			
1	C	314	Total	C	N	O	S	0	0	0
			2655	1695	465	490	5			
1	E	314	Total	C	N	O	S	0	0	0
			2664	1698	466	495	5			
1	G	314	Total	C	N	O	S	0	0	0
			2651	1694	465	487	5			
1	I	314	Total	C	N	O	S	0	0	0
			2648	1691	461	491	5			
1	K	314	Total	C	N	O	S	0	0	0
			2675	1705	468	497	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2703	1709	468	502	24			
2	D	346	Total	C	N	O	S	0	0	0
			2706	1713	467	502	24			
2	F	346	Total	C	N	O	S	0	0	0
			2717	1716	473	504	24			
2	H	346	Total	C	N	O	S	0	0	0
			2694	1705	464	501	24			
2	J	346	Total	C	N	O	S	0	0	0
			2708	1711	471	502	24			
2	L	346	Total	C	N	O	S	0	0	0
			2719	1718	473	504	24			

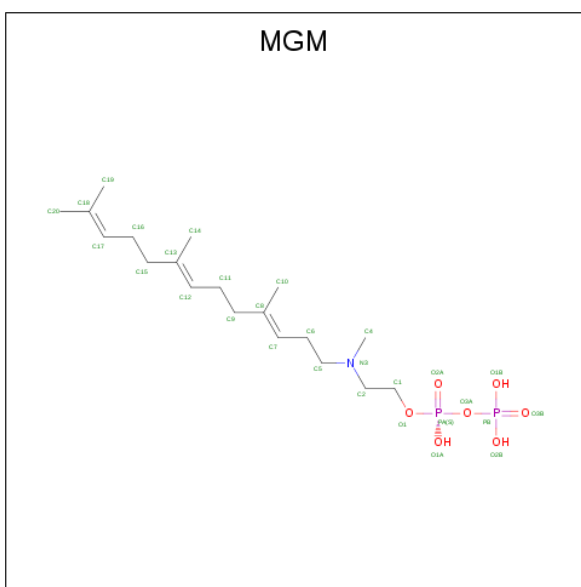
- Molecule 3 is a protein called Cell division control protein 42 homolog (Cdc42).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	S	2	0	0
			41	26	8	6	1			
3	N	5	Total	C	N	O	S	2	0	0
			41	26	8	6	1			
3	O	5	Total	C	N	O	S	2	0	0
			41	26	8	6	1			
3	P	5	Total	C	N	O	S	2	0	0
			41	26	8	6	1			
3	Q	5	Total	C	N	O	S	2	0	0
			41	26	8	6	1			
3	R	5	Total	C	N	O	S	2	0	0
			41	26	8	6	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (three-letter code: MGM) (formula: C<sub>19</sub>H<sub>37</sub>NO<sub>7</sub>P<sub>2</sub>).

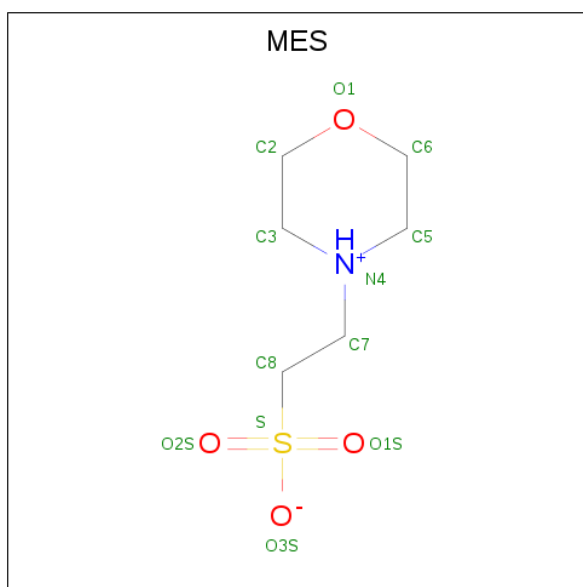


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	D	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	F	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	H	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	J	1	Total 29	C 19	N 1	O 7	P 2	0	0
5	L	1	Total 29	C 19	N 1	O 7	P 2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Cl 1 1	0	0
6	D	1	Total Cl 1 1	0	0
6	F	1	Total Cl 1 1	0	0

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	11	Total	O	0	0
			11	11		
8	C	16	Total	O	0	0
			16	16		
8	D	12	Total	O	0	0
			12	12		
8	E	14	Total	O	0	0
			14	14		
8	F	26	Total	O	0	0
			26	26		
8	G	18	Total	O	0	0
			18	18		
8	H	10	Total	O	0	0
			10	10		
8	I	14	Total	O	0	0
			14	14		
8	J	18	Total	O	0	0
			18	18		
8	K	55	Total	O	0	0
			55	55		

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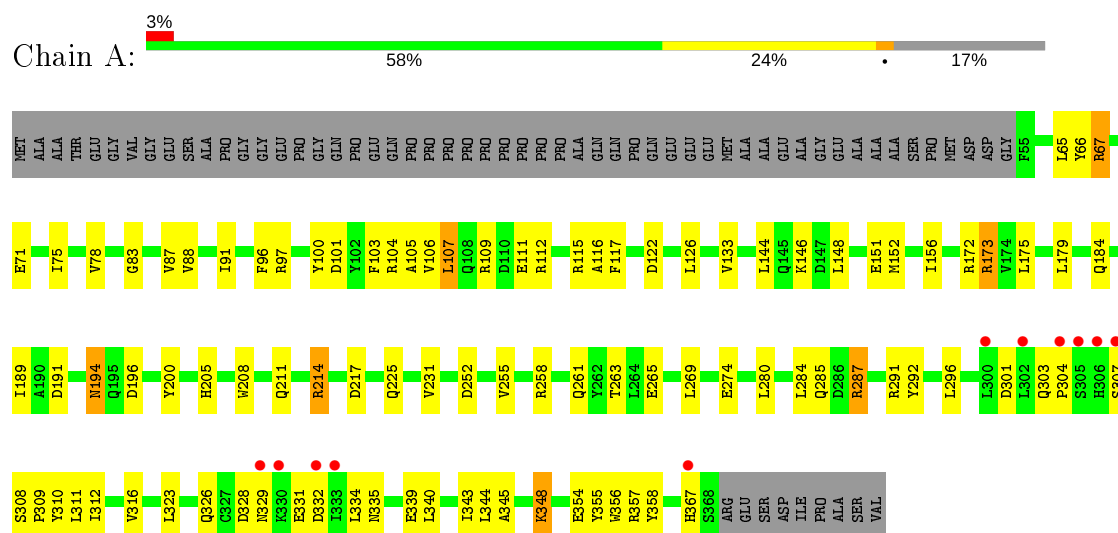
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	37	Total 37	O 37	0	0
8	M	2	Total 2	O 2	0	0
8	N	2	Total 2	O 2	0	0
8	Q	1	Total 1	O 1	0	0
8	R	1	Total 1	O 1	0	0

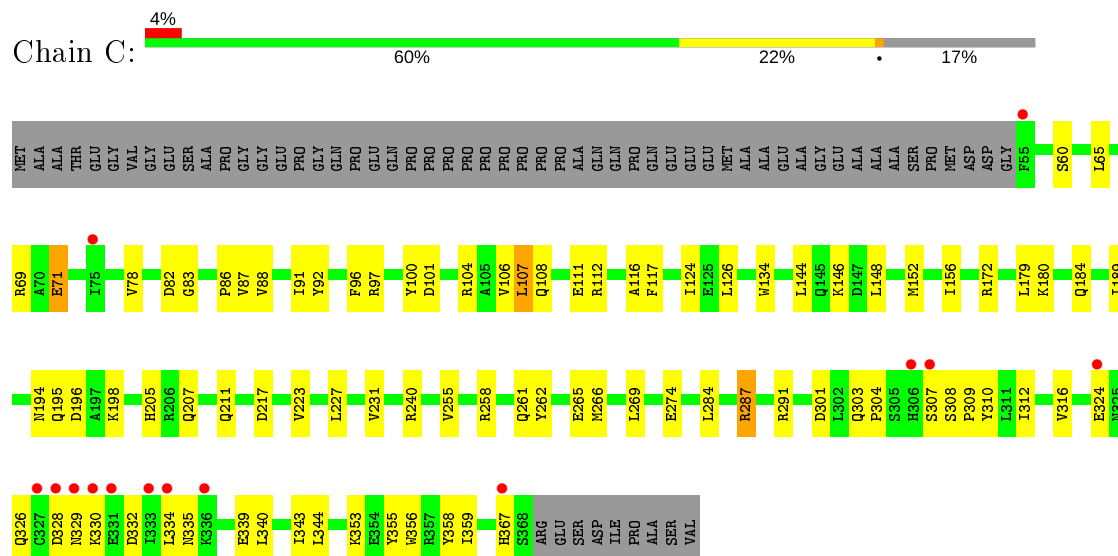
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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: geranylgeranyltransferase type I alpha subunit

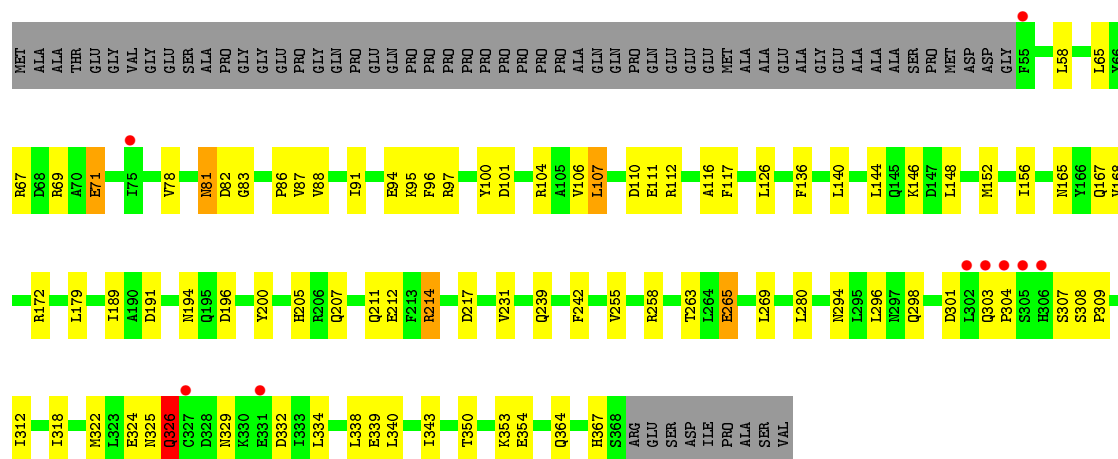


- Molecule 1: geranylgeranyltransferase type I alpha subunit

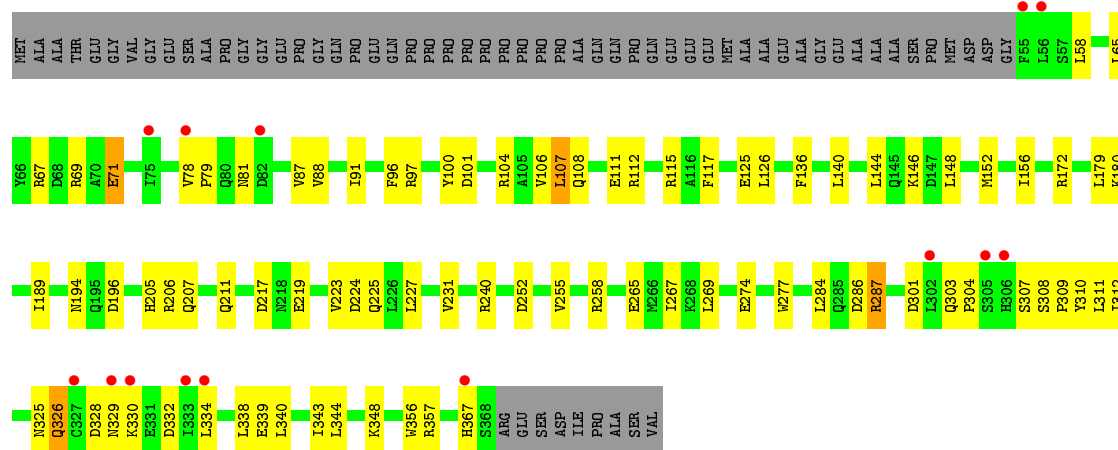


- Molecule 1: geranylgeranyltransferase type I alpha subunit

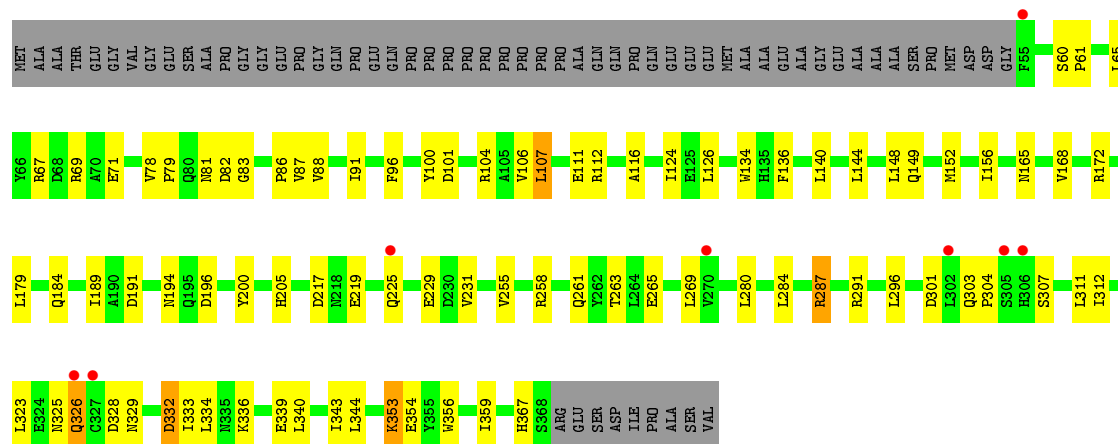




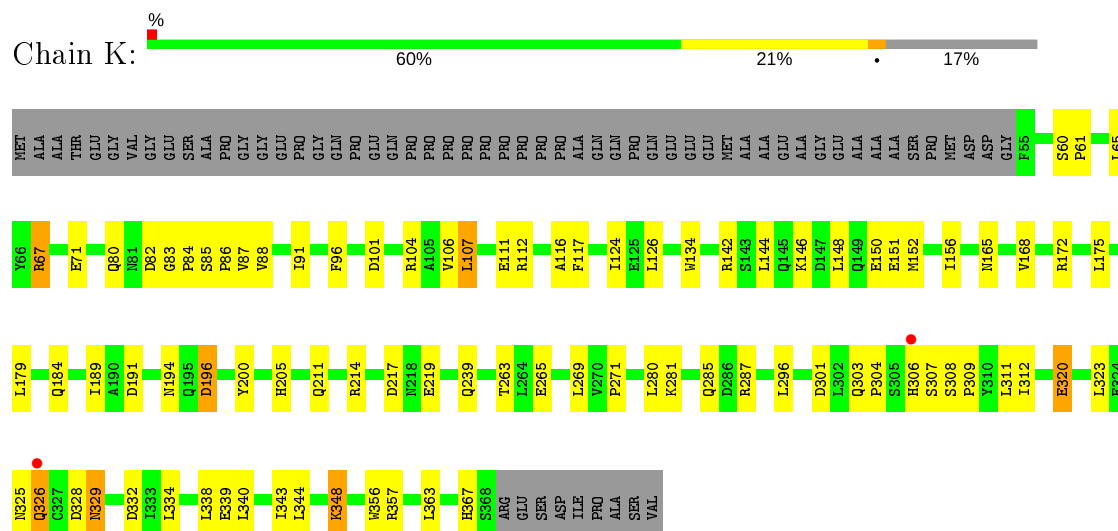
- Molecule 1: geranylgeranyltransferase type I alpha subunit



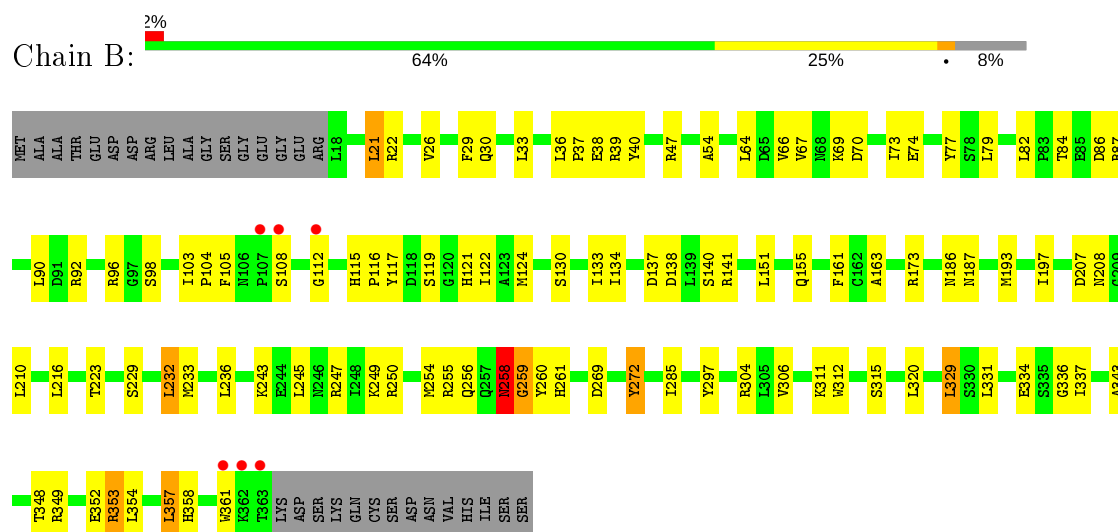
- Molecule 1: geranylgeranyltransferase type I alpha subunit



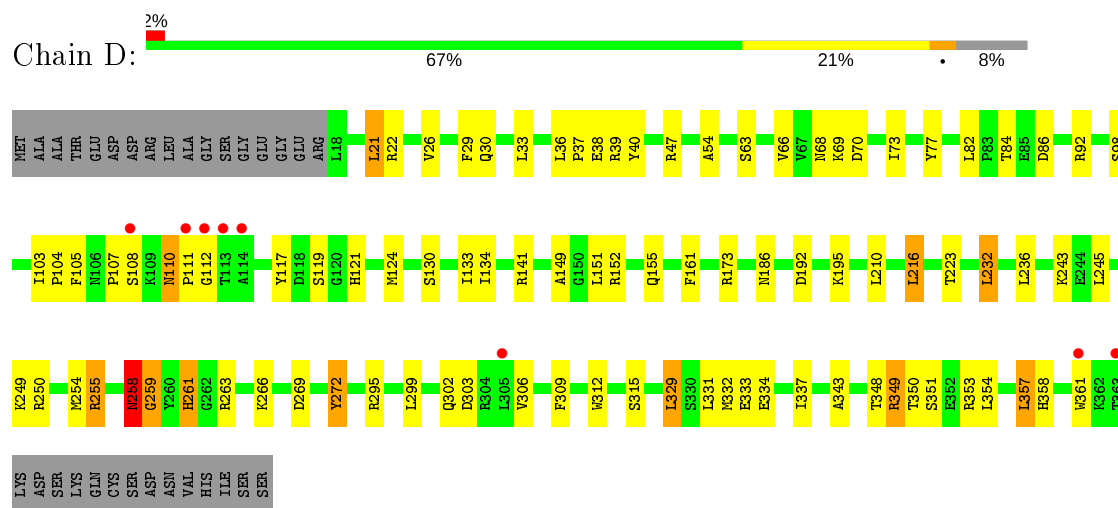
- Molecule 1: geranylgeranyltransferase type I alpha subunit



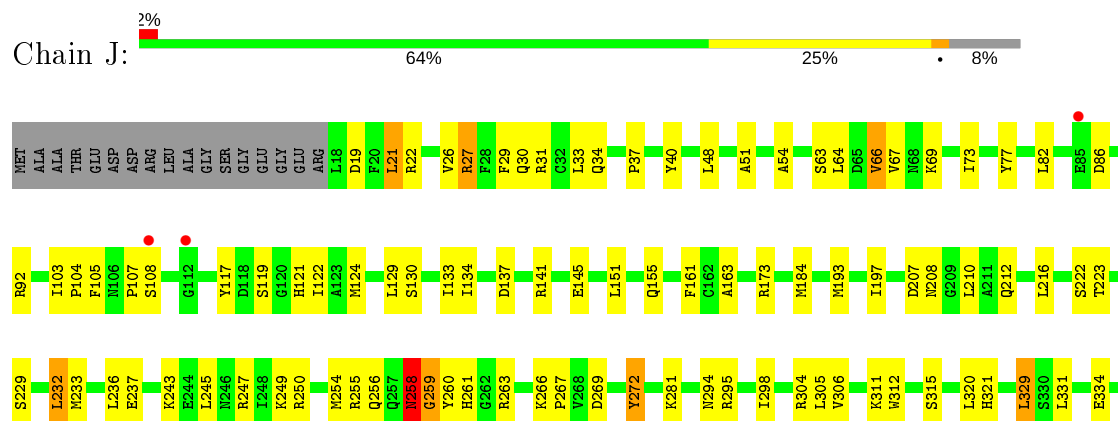
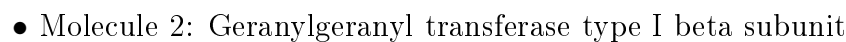
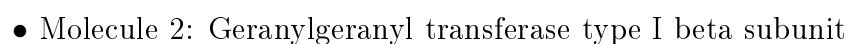
- Molecule 2: Geranylgeranyl transferase type I beta subunit

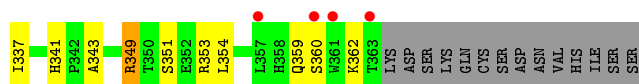


- Molecule 2: Geranylgeranyl transferase type I beta subunit

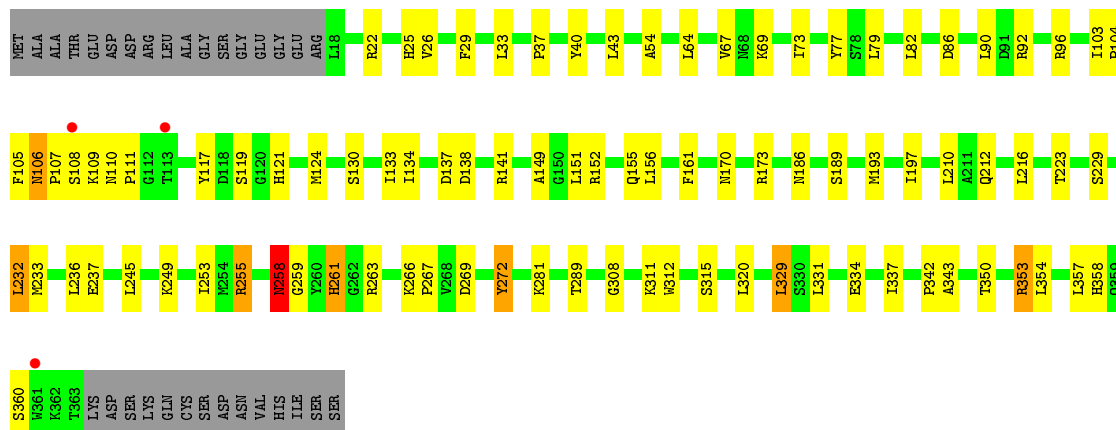


- Molecule 2: Geranylgeranyl transferase type I beta subunit





- Molecule 2: Geranylgeranyl transferase type I beta subunit



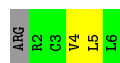
- Molecule 3: Cell division control protein 42 homolog (Cdc42)



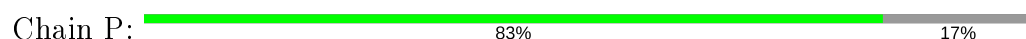
- Molecule 3: Cell division control protein 42 homolog (Cdc42)



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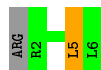


- Molecule 3: Cell division control protein 42 homolog (Cdc42)



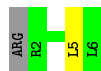
- Molecule 3: Cell division control protein 42 homolog (Cdc42)

Chain Q:  67% 17% 17%



- Molecule 3: Cell division control protein 42 homolog (Cdc42)

Chain R:  67% 17% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	271.26Å 266.92Å 185.75Å 90.00° 131.91° 90.00°	Depositor
Resolution (Å)	29.96 – 2.90 48.18 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.4 (29.96-2.90) 91.0 (48.18-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.34 (at 2.91Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.218 0.196 , 0.214	Depositor DCC
$R_{free}$ test set	10064 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.089 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, MGM, MES, CL

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	0.35	0/2702	0.53	0/3677
1	C	0.38	0/2721	0.54	0/3698
1	E	0.37	0/2730	0.55	0/3710
1	G	0.37	0/2717	0.54	0/3692
1	I	0.38	0/2714	0.54	0/3690
1	K	0.41	0/2741	0.56	0/3722
2	B	0.38	0/2765	0.60	2/3741 (0.1%)
2	D	0.40	0/2768	0.60	2/3743 (0.1%)
2	F	0.40	0/2779	0.62	2/3757 (0.1%)
2	H	0.39	0/2755	0.60	2/3727 (0.1%)
2	J	0.38	0/2769	0.61	2/3744 (0.1%)
2	L	0.41	0/2781	0.63	2/3759 (0.1%)
3	M	0.47	0/40	0.65	0/51
3	N	0.38	0/40	0.63	0/51
3	O	0.53	0/40	0.58	0/51
3	P	0.43	0/40	0.71	0/51
3	Q	0.55	0/40	0.76	0/51
3	R	0.47	0/40	0.69	0/51
All	All	0.39	0/33182	0.58	12/44966 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	D	0	1
2	F	0	2
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	8

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-6.08	97.91	113.10
2	D	259	GLY	N-CA-C	-5.77	98.67	113.10
2	L	259	GLY	N-CA-C	-5.71	98.82	113.10
2	F	259	GLY	N-CA-C	-5.68	98.90	113.10
2	H	259	GLY	N-CA-C	-5.68	98.90	113.10
2	D	258	ASN	N-CA-C	-5.67	95.69	111.00
2	B	259	GLY	N-CA-C	-5.66	98.96	113.10
2	J	258	ASN	N-CA-C	-5.49	96.18	111.00
2	L	258	ASN	N-CA-C	-5.43	96.35	111.00
2	H	258	ASN	N-CA-C	-5.41	96.40	111.00
2	F	258	ASN	N-CA-C	-5.39	96.45	111.00
2	B	258	ASN	N-CA-C	-5.33	96.60	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	TYR	Sidechain
2	B	297	TYR	Sidechain
2	D	272	TYR	Sidechain
2	F	272	TYR	Sidechain
2	F	297	TYR	Sidechain
2	H	272	TYR	Sidechain
2	J	272	TYR	Sidechain
2	L	272	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	2636	0	2526	79	0
1	C	2655	0	2562	70	0
1	E	2664	0	2570	74	0
1	G	2651	0	2563	71	0
1	I	2648	0	2547	64	0
1	K	2675	0	2594	66	0
2	B	2703	0	2606	80	0
2	D	2706	0	2616	77	0
2	F	2717	0	2635	64	0
2	H	2694	0	2589	98	0
2	J	2708	0	2613	78	0
2	L	2719	0	2639	65	0
3	M	41	0	47	1	0
3	N	41	0	47	1	0
3	O	41	0	47	2	0
3	P	41	0	47	0	0
3	Q	41	0	47	5	0
3	R	41	0	47	1	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	29	0	34	2	0
5	D	29	0	34	2	0
5	F	29	0	34	4	0
5	H	29	0	34	2	0
5	J	29	0	34	3	0
5	L	29	0	34	3	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	F	12	0	13	0	0
8	A	19	0	0	0	0
8	B	11	0	0	0	0
8	C	16	0	0	0	0
8	D	12	0	0	0	0
8	E	14	0	0	0	0
8	F	26	0	0	0	0
8	G	18	0	0	1	0
8	H	10	0	0	0	0
8	I	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	18	0	0	1	0
8	K	55	0	0	1	0
8	L	37	0	0	0	0
8	M	2	0	0	0	0
8	N	2	0	0	0	0
8	Q	1	0	0	0	0
8	R	1	0	0	0	0
All	All	32873	0	31559	850	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 13.

All (850) 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:A:156:ILE:HG12	1:A:172:ARG:HH12	1.05	1.13
1:G:255:VAL:HG13	1:G:258:ARG:HH12	1.11	1.11
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.01	1.10
1:K:156:ILE:HG12	1:K:172:ARG:HH12	1.01	1.07
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.18	1.05
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.24	0.97
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.36	0.90
1:E:255:VAL:HG13	1:E:258:ARG:NH2	1.86	0.89
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.87	0.89
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.87	0.88
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.56	0.87
1:A:255:VAL:HG13	1:A:258:ARG:HH12	1.41	0.86
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.56	0.86
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.37	0.86
2:J:258:ASN:ND2	2:J:259:GLY:H	1.76	0.83
2:F:241:SER:OG	2:F:244:GLU:HG3	1.78	0.82
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.93	0.81
1:G:255:VAL:HG13	1:G:258:ARG:NH1	1.95	0.80
1:E:81:ASN:HD22	1:E:81:ASN:N	1.79	0.79
1:E:255:VAL:CG1	1:E:258:ARG:HH21	1.91	0.79
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.63	0.78
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.65	0.78
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.66	0.77
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.66	0.77
2:L:106:ASN:HD21	2:L:109:LYS:H	1.32	0.77
1:G:303:GLN:HB3	1:G:304:PRO:HD3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:229:SER:O	2:H:233:MET:HG3	1.84	0.77
2:H:69:LYS:O	2:H:73:ILE:HG13	1.84	0.77
1:E:340:LEU:HD23	1:E:343:ILE:HD12	1.66	0.77
1:I:156:ILE:CG1	1:I:172:ARG:HH12	1.97	0.76
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.67	0.76
1:K:91:ILE:O	1:K:91:ILE:HD12	1.85	0.76
1:A:348:LYS:HA	1:A:348:LYS:NZ	2.00	0.76
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.51	0.76
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.67	0.75
1:I:91:ILE:O	1:I:91:ILE:HD12	1.86	0.75
1:E:156:ILE:HG12	1:E:172:ARG:NH1	2.00	0.75
1:C:329:ASN:HB3	1:C:332:ASP:HB3	1.67	0.75
2:H:296:ASN:C	2:H:296:ASN:HD22	1.88	0.75
2:D:37:PRO:HB2	2:D:39:ARG:HG2	1.69	0.74
1:E:81:ASN:HD22	1:E:81:ASN:H	1.32	0.74
1:K:156:ILE:HD11	1:K:184:GLN:HE21	1.53	0.73
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.69	0.73
2:H:21:LEU:HD11	2:H:304:ARG:NH2	2.02	0.73
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.92	0.73
1:E:301:ASP:O	1:E:304:PRO:HD2	1.89	0.73
1:I:156:ILE:HG12	1:I:172:ARG:NH1	2.01	0.73
1:G:91:ILE:HD12	1:G:91:ILE:O	1.87	0.73
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.24	0.73
1:A:152:MET:O	1:A:156:ILE:HG13	1.89	0.72
1:A:339:GLU:O	1:A:343:ILE:HG13	1.88	0.72
1:A:91:ILE:O	1:A:91:ILE:HD12	1.89	0.72
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.53	0.72
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.69	0.72
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.24	0.72
1:I:340:LEU:HD23	1:I:343:ILE:HD12	1.72	0.72
2:F:110:ASN:HB3	2:F:111:PRO:HD2	1.71	0.72
1:E:339:GLU:O	1:E:343:ILE:HG13	1.90	0.72
1:G:340:LEU:HD23	1:G:343:ILE:HD12	1.72	0.72
1:I:303:GLN:HB3	1:I:304:PRO:HD3	1.72	0.72
1:E:214:ARG:O	1:E:214:ARG:HG3	1.91	0.71
1:E:91:ILE:HD12	1:E:91:ILE:O	1.89	0.71
2:L:266:LYS:HG3	2:L:267:PRO:HD2	1.73	0.71
2:L:353:ARG:NH1	2:L:357:LEU:HG	2.04	0.71
2:F:69:LYS:O	2:F:73:ILE:HG13	1.89	0.71
1:K:152:MET:O	1:K:156:ILE:HG13	1.89	0.71
1:K:65:LEU:HD12	1:K:67:ARG:NH1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.72	0.69
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.74	0.69
1:C:91:ILE:HD12	1:C:91:ILE:O	1.91	0.69
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.73	0.69
1:C:97:ARG:HG2	1:C:101:ASP:OD2	1.92	0.69
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.27	0.69
1:E:152:MET:O	1:E:156:ILE:HG13	1.93	0.69
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.74	0.68
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.74	0.68
1:G:152:MET:O	1:G:156:ILE:HG13	1.92	0.68
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.58	0.68
2:J:359:GLN:HA	2:J:359:GLN:NE2	2.09	0.68
1:C:303:GLN:O	1:C:307:SER:HB2	1.94	0.68
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.75	0.68
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.75	0.68
1:C:339:GLU:O	1:C:343:ILE:HG13	1.92	0.68
2:H:193:MET:HG3	2:H:233:MET:CE	2.24	0.67
2:D:349:ARG:HH11	2:D:349:ARG:CB	2.06	0.67
1:K:156:ILE:HD11	1:K:184:GLN:NE2	2.09	0.67
1:I:301:ASP:O	1:I:304:PRO:HD2	1.93	0.67
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.76	0.67
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.29	0.67
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.76	0.67
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.77	0.67
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.30	0.67
1:C:156:ILE:CG1	1:C:172:ARG:HH12	2.08	0.67
1:I:152:MET:O	1:I:156:ILE:HG13	1.94	0.67
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.74	0.67
2:H:186:ASN:HB2	2:H:358:HIS:NE2	2.10	0.67
2:D:69:LYS:O	2:D:73:ILE:HG13	1.95	0.67
2:J:359:GLN:HA	2:J:359:GLN:HE21	1.60	0.67
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.30	0.66
2:B:26:VAL:O	2:B:30:GLN:HG3	1.95	0.66
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.77	0.66
1:I:81:ASN:HD21	2:J:105:PHE:H	1.41	0.66
1:G:97:ARG:HG2	1:G:101:ASP:OD2	1.94	0.66
1:A:65:LEU:HD12	1:A:67:ARG:NH1	2.11	0.66
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.78	0.66
1:C:152:MET:O	1:C:156:ILE:HG13	1.95	0.66
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.78	0.66
2:D:349:ARG:HH11	2:D:349:ARG:HB2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:252:ASP:OD2	1:G:255:VAL:HG23	1.96	0.66
2:B:69:LYS:O	2:B:73:ILE:HG13	1.96	0.66
1:A:303:GLN:O	1:A:307:SER:HB2	1.95	0.66
2:B:245:LEU:O	2:B:249:LYS:HG3	1.96	0.66
2:J:320:LEU:CD1	3:Q:5:LEU:HD11	2.26	0.66
1:G:339:GLU:O	1:G:343:ILE:HG13	1.96	0.65
2:L:106:ASN:ND2	2:L:109:LYS:H	1.94	0.65
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.78	0.65
1:G:69:ARG:HB3	1:G:71:GLU:OE1	1.96	0.65
1:E:329:ASN:HB3	1:E:332:ASP:HB3	1.78	0.65
1:I:353:LYS:HG2	1:I:354:GLU:N	2.10	0.65
1:I:339:GLU:O	1:I:343:ILE:HG13	1.97	0.64
2:L:105:PHE:CE2	2:L:107:PRO:HD3	2.31	0.64
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.80	0.64
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.62	0.64
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.62	0.64
1:I:332:ASP:O	1:I:336:LYS:HG3	1.98	0.64
1:C:353:LYS:HE3	1:K:339:GLU:HG3	1.79	0.64
1:A:301:ASP:O	1:A:304:PRO:HD2	1.97	0.64
2:F:269:ASP:HB3	2:F:272:TYR:HD2	1.61	0.64
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.62	0.63
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.80	0.63
1:K:320:GLU:HG2	1:K:363:LEU:HD21	1.79	0.63
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.79	0.63
1:A:287:ARG:HG3	1:A:292:TYR:OH	1.99	0.63
1:A:214:ARG:HG3	1:A:214:ARG:O	1.97	0.63
2:H:130:SER:O	2:H:134:ILE:HG13	1.99	0.63
1:C:301:ASP:O	1:C:304:PRO:HD2	1.98	0.63
2:J:258:ASN:ND2	2:J:259:GLY:N	2.47	0.63
1:G:97:ARG:HH11	1:G:97:ARG:HB3	1.63	0.63
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.81	0.63
1:A:173:ARG:HD2	1:A:208:TRP:CE2	2.34	0.62
3:Q:5:LEU:HD12	3:Q:5:LEU:H	1.63	0.62
1:A:348:LYS:HA	1:A:348:LYS:HZ2	1.63	0.62
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.13	0.62
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.80	0.62
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.34	0.62
2:L:212:GLN:NE2	2:L:212:GLN:HA	2.13	0.62
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.35	0.62
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.64	0.62
1:A:328:ASP:O	1:A:329:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:N	2:H:18:LEU:HD22	2.15	0.62
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.82	0.62
2:D:357:LEU:HD22	2:D:361:TRP:CZ2	2.35	0.61
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.35	0.61
1:A:265:GLU:O	1:A:269:LEU:HD13	1.99	0.61
2:B:269:ASP:HB3	2:B:272:TYR:HD2	1.65	0.61
1:E:78:VAL:O	1:E:104:ARG:HD2	1.99	0.61
2:F:130:SER:O	2:F:134:ILE:HG13	2.00	0.61
2:L:22:ARG:O	2:L:26:VAL:HG23	2.00	0.61
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.36	0.61
1:A:173:ARG:HD2	1:A:208:TRP:CD2	2.35	0.61
1:I:100:TYR:O	1:I:104:ARG:HG3	2.00	0.61
1:K:265:GLU:O	1:K:269:LEU:HD13	2.01	0.61
1:G:81:ASN:HD21	2:H:105:PHE:H	1.47	0.61
2:J:27:ARG:HH12	2:J:30:GLN:NE2	1.98	0.61
1:G:303:GLN:O	1:G:307:SER:HB2	2.01	0.61
1:G:357:ARG:HG3	1:G:357:ARG:HH11	1.66	0.61
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.83	0.60
1:K:301:ASP:O	1:K:304:PRO:HD2	2.00	0.60
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.81	0.60
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.66	0.60
2:H:77:TYR:CE1	2:H:141:ARG:HB2	2.36	0.60
1:K:329:ASN:HB3	1:K:332:ASP:HB3	1.82	0.60
2:J:320:LEU:HD12	3:Q:5:LEU:HD11	1.84	0.60
2:J:22:ARG:O	2:J:26:VAL:HG23	2.01	0.60
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.17	0.60
2:B:87:ARG:HH12	2:B:90:LEU:HD11	1.66	0.60
1:E:326:GLN:CA	1:E:326:GLN:HE21	2.15	0.60
2:L:212:GLN:HE21	2:L:212:GLN:HA	1.67	0.60
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.84	0.60
1:G:301:ASP:O	1:G:304:PRO:HD2	2.02	0.59
1:E:265:GLU:O	1:E:269:LEU:HD13	2.01	0.59
1:I:265:GLU:O	1:I:269:LEU:HD13	2.02	0.59
2:J:212:GLN:NE2	2:J:222:SER:HB3	2.17	0.59
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.32	0.59
2:H:184:MET:HA	2:H:354:LEU:HD21	1.85	0.59
1:C:88:VAL:CG1	2:D:36:LEU:HD11	2.32	0.59
1:A:303:GLN:HB3	1:A:304:PRO:HD3	1.85	0.59
1:I:323:LEU:HB3	1:I:367:HIS:CD2	2.38	0.59
2:D:105:PHE:CE2	2:D:107:PRO:HD3	2.37	0.58
2:D:30:GLN:OE1	2:D:66:VAL:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:MET:HG3	2:H:233:MET:HE1	1.84	0.58
2:H:348:THR:O	2:H:352:GLU:HG2	2.03	0.58
2:D:186:ASN:HB2	2:D:358:HIS:CE1	2.39	0.58
1:E:303:GLN:O	1:E:307:SER:HB2	2.02	0.58
2:L:229:SER:O	2:L:233:MET:HG3	2.03	0.58
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.85	0.58
1:G:78:VAL:HG21	1:G:108:GLN:NE2	2.18	0.58
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.03	0.58
2:J:269:ASP:HB3	2:J:272:TYR:HD2	1.69	0.58
2:D:110:ASN:HB3	2:D:111:PRO:HD2	1.86	0.58
1:G:334:LEU:HD22	1:G:367:HIS:O	2.03	0.58
1:K:320:GLU:CG	1:K:363:LEU:HD21	2.32	0.58
2:L:79:LEU:O	2:L:96:ARG:HG3	2.03	0.58
2:L:77:TYR:CE1	2:L:141:ARG:HB2	2.39	0.58
1:A:78:VAL:O	1:A:104:ARG:HD2	2.04	0.57
2:D:245:LEU:O	2:D:249:LYS:HG3	2.04	0.57
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.39	0.57
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.39	0.57
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.39	0.57
1:A:348:LYS:HA	1:A:348:LYS:HZ3	1.69	0.57
2:H:269:ASP:HB3	2:H:272:TYR:HD2	1.70	0.57
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.35	0.57
2:J:349:ARG:HH11	2:J:349:ARG:HB3	1.68	0.57
1:G:100:TYR:O	1:G:104:ARG:HG3	2.05	0.56
2:J:320:LEU:HD11	3:Q:5:LEU:HD21	1.87	0.56
1:A:156:ILE:CG1	1:A:172:ARG:HH12	1.98	0.56
1:C:78:VAL:HG21	1:C:108:GLN:NE2	2.19	0.56
1:C:255:VAL:HG13	1:C:258:ARG:NH2	2.19	0.56
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.86	0.56
2:D:121:HIS:HB3	2:D:124:MET:HG2	1.88	0.56
2:D:348:THR:HA	2:D:351:SER:OG	2.06	0.56
1:C:265:GLU:O	1:C:269:LEU:HD13	2.05	0.56
1:E:81:ASN:N	1:E:81:ASN:ND2	2.52	0.56
2:H:296:ASN:ND2	2:H:296:ASN:C	2.59	0.56
2:H:22:ARG:O	2:H:26:VAL:HG23	2.05	0.56
2:J:351:SER:O	2:J:354:LEU:HB3	2.06	0.56
2:J:121:HIS:HB3	2:J:124:MET:HG2	1.88	0.56
2:L:269:ASP:HB3	2:L:272:TYR:HD2	1.71	0.56
1:C:340:LEU:HD23	1:C:343:ILE:HD12	1.87	0.55
1:G:265:GLU:O	1:G:269:LEU:HD13	2.06	0.55
2:L:263:ARG:NH2	2:L:266:LYS:HE3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ALA:HA	2:D:152:ARG:NH2	2.21	0.55
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.41	0.55
1:C:328:ASP:O	1:C:329:ASN:HB2	2.07	0.55
2:F:245:LEU:O	2:F:249:LYS:HG3	2.05	0.55
2:H:77:TYR:HE2	2:H:137:ASP:OD2	1.90	0.55
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.41	0.55
1:I:334:LEU:HD22	1:I:367:HIS:O	2.07	0.55
2:L:29:PHE:O	2:L:33:LEU:HD22	2.06	0.55
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.87	0.55
1:K:191:ASP:O	1:K:194:ASN:HB2	2.07	0.55
1:K:340:LEU:HD23	1:K:343:ILE:HD12	1.88	0.55
2:F:208:ASN:ND2	2:F:247:ARG:HB3	2.21	0.55
1:G:88:VAL:CG1	2:H:36:LEU:HD11	2.35	0.55
2:H:210:LEU:HB2	2:H:223:THR:HA	1.89	0.55
2:L:210:LEU:HB2	2:L:223:THR:HA	1.89	0.55
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.41	0.55
1:A:312:ILE:O	1:A:316:VAL:HG23	2.06	0.55
2:B:130:SER:O	2:B:134:ILE:HG13	2.06	0.55
2:D:333:GLU:O	1:K:357:ARG:NH2	2.39	0.55
2:D:77:TYR:CE1	2:D:141:ARG:HB2	2.43	0.54
2:B:33:LEU:CD2	2:B:54:ALA:HB1	2.37	0.54
1:G:97:ARG:NH1	1:G:97:ARG:CB	2.71	0.54
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.89	0.54
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.37	0.54
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.42	0.54
2:B:258:ASN:OD1	2:B:259:GLY:N	2.39	0.54
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.88	0.54
2:F:121:HIS:HB3	2:F:124:MET:HG2	1.89	0.54
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.90	0.54
2:F:210:LEU:HB2	2:F:223:THR:HA	1.89	0.54
2:H:21:LEU:HD23	2:H:24:ARG:HD2	1.89	0.54
2:H:245:LEU:O	2:H:249:LYS:HG3	2.07	0.54
2:H:47:ARG:HH11	2:H:98:SER:HB2	1.72	0.54
2:J:245:LEU:O	2:J:249:LYS:HG3	2.08	0.54
2:B:210:LEU:HB2	2:B:223:THR:HA	1.88	0.54
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.54
2:J:64:LEU:O	2:J:67:VAL:HG22	2.08	0.54
1:K:334:LEU:O	1:K:338:LEU:HG	2.07	0.54
2:D:269:ASP:HB3	2:D:272:TYR:HD2	1.72	0.54
2:D:334:GLU:HB3	2:D:337:ILE:HD12	1.89	0.54
2:J:210:LEU:HB2	2:J:223:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.72	0.54
2:L:40:TYR:HB3	2:L:43:LEU:HD12	1.90	0.54
1:A:66:TYR:OH	1:A:122:ASP:OD1	2.23	0.53
2:B:39:ARG:HG2	2:B:40:TYR:CE1	2.44	0.53
1:E:65:LEU:HD12	1:E:67:ARG:HE	1.74	0.53
1:G:286:ASP:HB2	8:G:392:HOH:O	2.07	0.53
2:J:69:LYS:O	2:J:73:ILE:HG13	2.07	0.53
1:A:191:ASP:O	1:A:194:ASN:HB2	2.08	0.53
1:C:106:VAL:HG13	1:C:111:GLU:HB3	1.91	0.53
2:F:30:GLN:O	2:F:34:GLN:HG3	2.08	0.53
2:J:21:LEU:HD11	2:J:304:ARG:NH2	2.23	0.53
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.44	0.53
2:B:258:ASN:CG	2:B:259:GLY:H	2.10	0.53
1:C:112:ARG:O	1:C:144:LEU:HD21	2.09	0.53
1:G:106:VAL:HG13	1:G:111:GLU:HB3	1.90	0.53
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.43	0.53
1:K:271:PRO:HG3	1:K:306:HIS:HD2	1.74	0.53
1:A:344:LEU:HA	1:A:348:LYS:HB2	1.91	0.53
2:J:130:SER:O	2:J:134:ILE:HG13	2.09	0.53
2:B:232:LEU:HD13	2:B:343:ALA:HB1	1.91	0.53
2:D:29:PHE:O	2:D:33:LEU:HD22	2.08	0.53
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.43	0.53
1:A:214:ARG:CG	1:A:214:ARG:O	2.57	0.53
2:B:22:ARG:O	2:B:26:VAL:HG23	2.07	0.53
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.90	0.53
2:D:210:LEU:HB2	2:D:223:THR:HA	1.90	0.52
2:D:354:LEU:HD11	2:D:358:HIS:HE2	1.75	0.52
2:F:320:LEU:HD11	3:O:5:LEU:HD11	1.90	0.52
1:I:106:VAL:HG13	1:I:111:GLU:HB3	1.90	0.52
2:D:22:ARG:O	2:D:26:VAL:HG23	2.09	0.52
1:G:274:GLU:HG3	1:G:310:TYR:CE2	2.44	0.52
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.73	0.52
2:F:311:LYS:HE2	2:F:312:TRP:CE2	2.44	0.52
1:G:112:ARG:O	1:G:144:LEU:HD21	2.09	0.52
1:I:112:ARG:O	1:I:144:LEU:HD21	2.09	0.52
1:A:91:ILE:HD11	2:B:38:GLU:H	1.75	0.52
2:H:21:LEU:CD1	2:H:21:LEU:N	2.72	0.52
1:I:328:ASP:O	1:I:329:ASN:HB2	2.09	0.52
2:F:263:ARG:HB2	2:F:266:LYS:HG3	1.91	0.52
1:K:339:GLU:O	1:K:343:ILE:HG13	2.09	0.52
1:E:214:ARG:O	1:E:214:ARG:CG	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:GLY:HA3	2:F:105:PHE:CD1	2.45	0.52
2:H:29:PHE:CD2	2:H:54:ALA:HA	2.45	0.52
1:A:252:ASP:OD2	1:A:255:VAL:HG23	2.10	0.52
2:D:37:PRO:HB2	2:D:39:ARG:CG	2.38	0.52
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.44	0.52
1:K:200:TYR:HB3	5:L:379:MGM:HC12	1.91	0.52
1:A:261:GLN:O	1:A:265:GLU:HG2	2.09	0.52
2:B:121:HIS:HB3	2:B:124:MET:HG2	1.92	0.52
2:F:269:ASP:HB3	2:F:272:TYR:CD2	2.43	0.52
2:F:133:ILE:CD1	2:F:354:LEU:HD13	2.40	0.52
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.75	0.52
2:H:29:PHE:O	2:H:33:LEU:HD22	2.10	0.52
1:A:106:VAL:HG13	1:A:111:GLU:HB3	1.91	0.52
2:B:186:ASN:HB2	2:B:358:HIS:NE2	2.25	0.52
2:F:339:LYS:NZ	2:F:339:LYS:HB3	2.25	0.52
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.45	0.51
2:J:229:SER:O	2:J:233:MET:HG3	2.09	0.51
2:L:106:ASN:ND2	2:L:106:ASN:C	2.62	0.51
2:J:267:PRO:HG2	8:J:391:HOH:O	2.10	0.51
2:L:106:ASN:C	2:L:106:ASN:HD22	2.13	0.51
1:C:312:ILE:CG2	1:C:340:LEU:HD22	2.39	0.51
1:C:355:TYR:O	1:C:358:TYR:HB3	2.09	0.51
2:F:138:ASP:OD1	2:F:140:SER:HB3	2.11	0.51
1:G:58:LEU:HB2	1:G:125:GLU:OE2	2.11	0.51
1:A:287:ARG:O	1:A:291:ARG:HD3	2.11	0.51
2:F:92:ARG:HB3	2:F:119:SER:CB	2.40	0.51
2:L:311:LYS:HE2	2:L:312:TRP:CE2	2.46	0.51
2:L:138:ASP:HA	2:L:357:LEU:HD11	1.92	0.51
2:B:269:ASP:OD2	2:B:311:LYS:HE3	2.11	0.51
2:L:130:SER:O	2:L:134:ILE:HG13	2.10	0.51
1:G:97:ARG:HH11	1:G:97:ARG:CB	2.23	0.51
2:F:105:PHE:CE2	2:F:107:PRO:HD3	2.46	0.51
2:F:138:ASP:HA	2:F:357:LEU:HD11	1.92	0.51
2:H:103:ILE:HG23	2:H:104:PRO:HD2	1.93	0.51
1:I:200:TYR:HB3	5:J:379:MGM:HC12	1.92	0.51
2:B:334:GLU:HB3	2:B:337:ILE:HD12	1.92	0.50
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.93	0.50
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.46	0.50
1:A:285:GLN:NE2	2:B:247:ARG:NH1	2.59	0.50
2:D:353:ARG:HH12	2:D:357:LEU:HG	1.75	0.50
1:E:326:GLN:H	1:E:326:GLN:HE21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:GLN:HE21	1:E:326:GLN:N	2.09	0.50
2:F:250:ARG:O	2:F:254:MET:HG2	2.11	0.50
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.93	0.50
1:I:81:ASN:ND2	2:J:105:PHE:H	2.09	0.50
2:J:155:GLN:HB2	2:J:161:PHE:CE2	2.46	0.50
2:J:92:ARG:HB3	2:J:119:SER:HB3	1.92	0.50
2:L:312:TRP:O	2:L:315:SER:HB3	2.11	0.50
2:B:269:ASP:HB3	2:B:272:TYR:CD2	2.46	0.50
2:D:155:GLN:HB2	2:D:161:PHE:CE2	2.45	0.50
2:F:352:GLU:HG2	2:F:355:ARG:HH12	1.76	0.50
1:I:78:VAL:O	1:I:104:ARG:HD2	2.11	0.50
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.46	0.50
1:K:106:VAL:HG13	1:K:111:GLU:HB3	1.93	0.50
2:B:155:GLN:HB2	2:B:161:PHE:CE2	2.46	0.50
2:B:193:MET:O	2:B:197:ILE:HG13	2.11	0.50
2:B:348:THR:O	2:B:352:GLU:HG3	2.12	0.50
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.46	0.50
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.46	0.50
1:C:198:LYS:HD3	2:D:266:LYS:HD3	1.93	0.50
1:E:106:VAL:HG13	1:E:111:GLU:HB3	1.93	0.50
1:K:281:LYS:O	1:K:285:GLN:HB3	2.12	0.50
1:A:105:ALA:O	1:A:109:ARG:HG3	2.12	0.50
2:F:103:ILE:HG23	2:F:104:PRO:HD2	1.94	0.50
1:G:156:ILE:CG1	1:G:172:ARG:HH12	2.14	0.50
1:G:330:LYS:HE2	1:G:367:HIS:HB3	1.94	0.50
1:I:333:ILE:HD13	1:I:336:LYS:HD3	1.94	0.50
2:L:155:GLN:HB2	2:L:161:PHE:CE2	2.47	0.50
1:C:100:TYR:O	1:C:104:ARG:HG3	2.11	0.50
1:C:344:LEU:HD13	1:C:356:TRP:CE2	2.46	0.50
2:D:173:ARG:HG2	5:D:380:MGM:H112	1.93	0.50
1:I:325:ASN:O	1:I:326:GLN:C	2.50	0.50
2:J:33:LEU:CD2	2:J:54:ALA:HB1	2.42	0.50
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.94	0.50
2:B:349:ARG:HH11	2:B:349:ARG:HG2	1.77	0.50
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.77	0.50
2:L:121:HIS:HB3	2:L:124:MET:HG2	1.94	0.50
1:K:303:GLN:HB3	1:K:304:PRO:CD	2.40	0.49
2:L:133:ILE:HG22	2:L:350:THR:HG23	1.94	0.49
2:B:122:ILE:HG22	2:B:163:ALA:HA	1.94	0.49
2:B:33:LEU:HD21	2:B:54:ALA:HB1	1.94	0.49
2:B:39:ARG:HG2	2:B:40:TYR:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:GLY:HA3	2:J:105:PHE:CD1	2.47	0.49
2:H:256:GLN:HE22	2:H:290:ASN:HB3	1.76	0.49
2:J:63:SER:O	2:J:66:VAL:HG22	2.12	0.49
2:F:122:ILE:HG22	2:F:163:ALA:HA	1.94	0.49
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.48	0.49
1:I:303:GLN:O	1:I:307:SER:HB2	2.12	0.49
2:J:173:ARG:HG2	5:J:379:MGM:H112	1.94	0.49
1:K:196:ASP:HB3	8:K:431:HOH:O	2.12	0.49
1:G:284:LEU:O	1:G:287:ARG:HG2	2.13	0.49
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.78	0.49
2:J:129:LEU:HB2	2:J:184:MET:CE	2.42	0.49
2:H:349:ARG:O	2:H:352:GLU:HB2	2.12	0.49
2:H:33:LEU:HD22	2:H:54:ALA:HB1	1.94	0.49
2:D:250:ARG:O	2:D:254:MET:HG2	2.13	0.49
2:D:33:LEU:CD2	2:D:54:ALA:HB1	2.43	0.49
1:E:191:ASP:O	1:E:194:ASN:HB2	2.13	0.49
1:E:200:TYR:HB3	5:F:381:MGM:HC12	1.95	0.49
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.95	0.49
2:F:155:GLN:HB2	2:F:161:PHE:CE2	2.48	0.49
2:H:64:LEU:O	2:H:67:VAL:HG22	2.13	0.49
1:K:323:LEU:HB3	1:K:367:HIS:CD2	2.47	0.49
1:C:312:ILE:O	1:C:316:VAL:HG23	2.13	0.49
2:D:303:ASP:OD1	2:D:306:VAL:HG13	2.13	0.49
1:E:308:SER:HB2	1:E:309:PRO:HD2	1.95	0.49
2:F:92:ARG:HB3	2:F:119:SER:HB3	1.95	0.49
1:I:225:GLN:NE2	1:I:229:GLU:OE2	2.46	0.49
2:L:320:LEU:HD11	3:R:5:LEU:HD11	1.94	0.49
2:D:92:ARG:HD2	2:D:119:SER:HB3	1.95	0.48
2:D:354:LEU:HD11	2:D:358:HIS:NE2	2.28	0.48
2:H:312:TRP:HB3	2:H:313:PRO:HD2	1.95	0.48
1:I:82:ASP:HB2	1:I:86:PRO:HB3	1.95	0.48
2:J:122:ILE:HG22	2:J:163:ALA:HA	1.94	0.48
2:J:92:ARG:HB3	2:J:119:SER:CB	2.43	0.48
1:K:112:ARG:O	1:K:144:LEU:HD21	2.13	0.48
1:A:100:TYR:C	1:A:104:ARG:NH1	2.67	0.48
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.48	0.48
2:D:255:ARG:HD3	2:D:261:HIS:CD2	2.48	0.48
1:E:296:LEU:O	1:E:296:LEU:HD12	2.13	0.48
2:J:173:ARG:HB3	5:J:379:MGM:H143	1.94	0.48
1:C:308:SER:HB2	1:C:309:PRO:HD2	1.94	0.48
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.78	0.48
1:A:284:LEU:O	1:A:287:ARG:HG2	2.13	0.48
2:F:29:PHE:O	2:F:33:LEU:HD22	2.14	0.48
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.78	0.48
1:I:291:ARG:HH11	1:I:291:ARG:CB	2.27	0.48
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.48	0.48
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.21	0.48
2:B:84:THR:HG22	2:B:112:GLY:O	2.14	0.48
2:H:105:PHE:CE2	2:H:107:PRO:HG3	2.48	0.48
2:H:250:ARG:O	2:H:254:MET:HG2	2.14	0.48
2:J:258:ASN:CG	2:J:259:GLY:H	2.17	0.48
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.28	0.48
2:B:21:LEU:CD1	2:B:21:LEU:N	2.76	0.48
2:B:250:ARG:O	2:B:254:MET:HG2	2.13	0.48
1:E:167:GLN:CD	1:E:167:GLN:H	2.17	0.48
1:G:308:SER:HB2	1:G:309:PRO:HD2	1.96	0.48
1:A:345:ALA:HB1	1:A:357:ARG:NH1	2.29	0.48
2:B:82:LEU:HD11	2:B:108:SER:HA	1.95	0.48
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.29	0.48
2:H:169:GLU:OE1	2:H:169:GLU:N	2.41	0.48
2:H:186:ASN:HB2	2:H:358:HIS:CD2	2.49	0.48
2:J:312:TRP:O	2:J:315:SER:HB3	2.13	0.48
1:K:303:GLN:O	1:K:307:SER:HB2	2.13	0.48
2:L:212:GLN:HE21	2:L:212:GLN:CA	2.21	0.48
1:A:334:LEU:HD22	1:A:367:HIS:O	2.13	0.48
1:C:189:ILE:HD11	1:C:205:HIS:CD2	2.43	0.48
1:C:97:ARG:HB3	1:C:97:ARG:HH11	1.79	0.48
1:E:101:ASP:HA	1:E:104:ARG:HH11	1.79	0.48
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.43	0.48
1:C:101:ASP:HA	1:C:104:ARG:HH11	1.77	0.48
2:D:82:LEU:HD11	2:D:108:SER:HA	1.96	0.48
1:E:112:ARG:O	1:E:144:LEU:HD21	2.14	0.48
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.16	0.48
2:L:245:LEU:O	2:L:249:LYS:HG3	2.13	0.48
1:E:312:ILE:CG2	1:E:340:LEU:HD22	2.41	0.47
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.49	0.47
2:B:87:ARG:NH1	2:B:90:LEU:HD11	2.29	0.47
2:J:311:LYS:HB3	2:J:321:HIS:NE2	2.30	0.47
1:A:112:ARG:O	1:A:144:LEU:HD21	2.15	0.47
2:B:29:PHE:O	2:B:33:LEU:HD22	2.14	0.47
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:191:ASP:O	1:I:194:ASN:HB2	2.13	0.47
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.49	0.47
2:B:312:TRP:O	2:B:315:SER:HB3	2.15	0.47
2:D:130:SER:O	2:D:134:ILE:HG13	2.14	0.47
2:H:121:HIS:HB3	2:H:124:MET:HG2	1.96	0.47
2:D:92:ARG:HB3	2:D:119:SER:HB3	1.96	0.47
2:D:192:ASP:OD1	2:D:195:LYS:HG3	2.14	0.47
1:K:308:SER:HB2	1:K:309:PRO:HD2	1.97	0.47
2:L:92:ARG:HB3	2:L:119:SER:CB	2.45	0.47
2:B:73:ILE:HD13	2:B:137:ASP:HB2	1.96	0.47
2:B:22:ARG:HH11	2:B:22:ARG:HG2	1.80	0.47
2:D:302:GLN:HB2	2:D:309:PHE:CE2	2.49	0.47
1:A:83:GLY:HA3	2:B:105:PHE:CD1	2.49	0.47
2:B:29:PHE:O	2:B:33:LEU:CD2	2.62	0.47
1:C:91:ILE:HD11	2:D:38:GLU:H	1.80	0.47
1:E:100:TYR:O	1:E:104:ARG:HG3	2.14	0.47
1:K:311:LEU:HD23	1:K:311:LEU:C	2.35	0.47
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.49	0.47
2:B:92:ARG:HB3	2:B:119:SER:HB3	1.97	0.47
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.95	0.47
1:E:326:GLN:CA	1:E:326:GLN:NE2	2.77	0.47
1:I:60:SER:OG	1:I:61:PRO:HD2	2.15	0.47
2:B:92:ARG:HB3	2:B:119:SER:CB	2.45	0.47
1:G:357:ARG:HG3	1:G:357:ARG:NH1	2.29	0.47
1:C:308:SER:O	1:C:312:ILE:HG12	2.15	0.47
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.50	0.47
1:A:311:LEU:HD23	1:A:311:LEU:O	2.15	0.47
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.97	0.47
2:L:37:PRO:HG2	2:L:40:TYR:CE1	2.49	0.46
1:I:149:GLN:NE2	1:I:179:LEU:HD13	2.30	0.46
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.47	0.46
2:J:21:LEU:HD11	2:J:304:ARG:HH22	1.79	0.46
2:H:137:ASP:OD1	2:H:139:LEU:N	2.39	0.46
1:C:88:VAL:HG12	2:D:36:LEU:HD11	1.97	0.46
2:D:92:ARG:HB3	2:D:119:SER:CB	2.45	0.46
1:E:334:LEU:HD22	1:E:367:HIS:O	2.14	0.46
3:Q:5:LEU:HD12	3:Q:5:LEU:N	2.29	0.46
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.96	0.46
2:J:29:PHE:O	2:J:33:LEU:HD22	2.14	0.46
2:J:82:LEU:HD11	2:J:108:SER:HA	1.98	0.46
2:J:193:MET:O	2:J:197:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LEU:HB2	1:C:146:LYS:HD3	1.98	0.46
2:F:173:ARG:HG2	5:F:381:MGM:H112	1.98	0.46
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.98	0.46
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.98	0.46
1:I:65:LEU:O	1:I:69:ARG:HG3	2.16	0.46
2:L:86:ASP:OD1	2:L:86:ASP:N	2.44	0.46
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.51	0.46
1:A:255:VAL:HG13	1:A:258:ARG:NH1	2.19	0.46
2:B:173:ARG:HG2	5:B:379:MGM:H112	1.97	0.46
1:C:303:GLN:HB3	1:C:304:PRO:HD3	1.98	0.46
1:E:91:ILE:HD11	2:F:38:GLU:H	1.79	0.46
2:H:62:ASP:OD1	2:H:349:ARG:NH2	2.49	0.46
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.49	0.46
2:D:349:ARG:CB	2:D:349:ARG:NH1	2.77	0.46
2:H:73:ILE:HD13	2:H:137:ASP:HB2	1.98	0.46
1:I:100:TYR:C	1:I:104:ARG:NH1	2.70	0.46
1:I:291:ARG:NH1	1:I:291:ARG:HB3	2.31	0.46
1:I:291:ARG:HB2	1:I:291:ARG:HH11	1.80	0.46
1:K:239:GLN:OE1	1:K:239:GLN:HA	2.16	0.46
1:A:91:ILE:HD12	2:B:38:GLU:HB2	1.98	0.46
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.16	0.46
2:D:33:LEU:HD22	2:D:54:ALA:HB1	1.97	0.46
1:I:255:VAL:HG13	1:I:258:ARG:NH2	2.31	0.46
2:L:69:LYS:O	2:L:73:ILE:HG13	2.16	0.46
2:B:70:ASP:O	2:B:74:GLU:HG2	2.15	0.45
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.16	0.45
2:H:105:PHE:CE2	2:H:107:PRO:CG	2.99	0.45
1:I:148:LEU:CB	1:I:179:LEU:HD21	2.44	0.45
2:J:21:LEU:N	2:J:21:LEU:CD1	2.79	0.45
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.51	0.45
2:H:173:ARG:HG2	5:H:380:MGM:H112	1.98	0.45
1:A:323:LEU:HB3	1:A:367:HIS:CD2	2.51	0.45
2:J:86:ASP:N	2:J:86:ASP:OD2	2.48	0.45
5:F:381:MGM:HC43	3:O:4:VAL:O	2.17	0.45
2:J:263:ARG:HB2	2:J:266:LYS:HG3	1.97	0.45
2:D:258:ASN:CG	2:D:259:GLY:H	2.18	0.45
2:H:84:THR:HG22	2:H:112:GLY:O	2.16	0.45
1:I:106:VAL:HG11	1:I:116:ALA:CB	2.47	0.45
1:I:284:LEU:O	1:I:287:ARG:HG2	2.17	0.45
1:I:291:ARG:NH1	1:I:291:ARG:CB	2.80	0.45
2:J:311:LYS:HE2	2:J:312:TRP:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:HIS:ND1	2:L:308:GLY:N	2.61	0.45
2:L:64:LEU:HD23	2:L:64:LEU:HA	1.81	0.45
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.30	0.45
1:G:79:PRO:HA	1:G:101:ASP:OD1	2.17	0.45
1:K:344:LEU:HD13	1:K:356:TRP:CE2	2.52	0.45
1:A:296:LEU:HD12	1:A:296:LEU:O	2.17	0.45
1:C:97:ARG:NH1	1:C:97:ARG:HB3	2.31	0.45
2:H:258:ASN:OD1	2:H:259:GLY:N	2.45	0.45
2:H:26:VAL:O	2:H:30:GLN:HG3	2.16	0.45
2:H:344:LEU:HB3	2:H:346:VAL:HG22	1.99	0.45
1:I:96:PHE:CE1	1:I:126:LEU:HB3	2.51	0.45
2:L:173:ARG:HG2	5:L:379:MGM:H112	1.98	0.45
2:B:207:ASP:O	2:B:208:ASN:HB2	2.17	0.45
1:C:148:LEU:CB	1:C:179:LEU:HD21	2.45	0.45
1:C:88:VAL:HG13	2:D:36:LEU:HD11	1.97	0.45
2:F:64:LEU:O	2:F:67:VAL:HG22	2.16	0.45
2:H:312:TRP:O	2:H:315:SER:HB3	2.17	0.45
1:K:348:LYS:HD2	1:K:348:LYS:N	2.32	0.45
2:L:92:ARG:HB3	2:L:119:SER:HB3	1.98	0.45
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.82	0.45
1:G:136:PHE:CE2	1:G:140:LEU:HD11	2.52	0.45
2:H:282:LEU:HD21	2:H:343:ALA:HB2	1.99	0.45
1:G:91:ILE:HD11	2:H:38:GLU:H	1.82	0.45
2:J:295:ARG:HH11	2:J:295:ARG:HG2	1.82	0.45
2:J:304:ARG:HG2	2:J:304:ARG:HH11	1.82	0.45
1:K:219:GLU:HA	1:K:219:GLU:OE1	2.17	0.45
1:A:355:TYR:O	1:A:358:TYR:HB3	2.17	0.45
2:B:353:ARG:HG2	2:B:353:ARG:HH11	1.81	0.45
2:F:73:ILE:HD13	2:F:137:ASP:HB2	1.98	0.45
1:G:325:ASN:O	1:G:326:GLN:C	2.55	0.45
1:G:328:ASP:O	1:G:329:ASN:HB2	2.17	0.45
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.26	0.44
1:C:334:LEU:HD22	1:C:367:HIS:O	2.17	0.44
1:G:65:LEU:O	1:G:69:ARG:HG3	2.18	0.44
2:L:33:LEU:CD2	2:L:54:ALA:HB1	2.48	0.44
1:C:223:VAL:HG11	1:C:240:ARG:HB2	1.98	0.44
2:F:82:LEU:HD11	2:F:108:SER:HA	1.98	0.44
2:H:253:ILE:HD12	2:H:289:THR:HG22	1.99	0.44
1:G:88:VAL:HG13	2:H:36:LEU:HD11	1.99	0.44
2:H:82:LEU:HD11	2:H:108:SER:HA	1.98	0.44
2:L:82:LEU:HD11	2:L:108:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ASP:OD2	1:E:112:ARG:NE	2.40	0.44
1:E:91:ILE:HD12	2:F:38:GLU:HB2	1.99	0.44
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.53	0.44
1:G:65:LEU:HD12	1:G:67:ARG:CZ	2.47	0.44
2:H:269:ASP:OD2	2:H:311:LYS:HE3	2.18	0.44
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.81	0.44
1:C:83:GLY:HA3	2:D:105:PHE:CD1	2.52	0.44
1:E:263:THR:HG21	1:E:280:LEU:HB2	2.00	0.44
1:E:294:ASN:HB3	1:E:298:GLN:HE21	1.82	0.44
1:K:312:ILE:HB	1:K:344:LEU:HD21	1.98	0.44
2:L:106:ASN:HD21	2:L:109:LYS:N	2.07	0.44
2:D:22:ARG:HH11	2:D:22:ARG:HG2	1.82	0.44
1:E:148:LEU:CB	1:E:179:LEU:HD21	2.46	0.44
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.52	0.44
2:F:258:ASN:CG	2:F:259:GLY:H	2.20	0.44
2:L:253:ILE:HD12	2:L:289:THR:HG22	2.00	0.44
2:L:64:LEU:O	2:L:67:VAL:HG22	2.17	0.44
2:F:173:ARG:HB3	5:F:381:MGM:H143	1.98	0.44
2:F:202:ARG:HH11	2:F:202:ARG:HG2	1.82	0.44
1:I:136:PHE:CE2	1:I:140:LEU:HD11	2.53	0.44
1:I:311:LEU:C	1:I:311:LEU:HD23	2.37	0.44
2:J:295:ARG:HG2	2:J:295:ARG:NH1	2.33	0.44
1:A:75:ILE:CG1	1:A:115:ARG:NH2	2.81	0.44
1:E:165:ASN:O	1:E:168:VAL:HG22	2.18	0.44
1:K:325:ASN:O	1:K:326:GLN:C	2.56	0.44
2:D:312:TRP:O	2:D:315:SER:HB3	2.18	0.44
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.33	0.44
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.52	0.44
2:H:357:LEU:HG	2:H:361:TRP:CZ2	2.53	0.44
1:A:311:LEU:HD23	1:A:311:LEU:C	2.39	0.43
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.32	0.43
2:B:37:PRO:O	2:B:39:ARG:N	2.51	0.43
1:E:353:LYS:NZ	1:E:354:GLU:OE2	2.51	0.43
1:E:67:ARG:NH2	1:E:94:GLU:OE1	2.51	0.43
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.18	0.43
2:H:18:LEU:CD2	2:H:18:LEU:N	2.81	0.43
2:J:48:LEU:O	2:J:51:ALA:HB3	2.18	0.43
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.53	0.43
2:L:281:LYS:HG2	2:L:342:PRO:HG2	1.99	0.43
2:F:30:GLN:OE1	2:F:66:VAL:HB	2.18	0.43
2:J:19:ASP:OD2	2:J:19:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LEU:CB	1:G:179:LEU:HD21	2.46	0.43
2:H:202:ARG:NH1	2:H:202:ARG:HG3	2.30	0.43
2:J:73:ILE:HD13	2:J:137:ASP:HB2	2.01	0.43
1:A:328:ASP:O	1:A:329:ASN:CB	2.66	0.43
1:C:359:ILE:HD13	1:C:359:ILE:HA	1.86	0.43
2:D:22:ARG:HG2	2:D:22:ARG:NH1	2.33	0.43
2:F:24:ARG:HB2	2:F:24:ARG:HH11	1.83	0.43
2:H:269:ASP:HB3	2:H:272:TYR:CD2	2.52	0.43
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.53	0.43
1:A:200:TYR:HB3	5:B:379:MGM:HC12	2.01	0.43
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.43
2:B:243:LYS:O	2:B:247:ARG:HG3	2.18	0.43
1:C:287:ARG:O	1:C:291:ARG:HD3	2.19	0.43
1:E:231:VAL:HG22	1:E:231:VAL:O	2.18	0.43
1:E:83:GLY:HA3	2:F:105:PHE:CE1	2.54	0.43
2:H:138:ASP:OD1	2:H:140:SER:HB3	2.18	0.43
1:K:148:LEU:CB	1:K:179:LEU:HD21	2.48	0.43
2:B:79:LEU:O	2:B:96:ARG:HG3	2.19	0.43
1:C:335:ASN:O	1:C:339:GLU:HB2	2.19	0.43
2:F:207:ASP:O	2:F:208:ASN:HB2	2.18	0.43
1:K:65:LEU:HD12	1:K:67:ARG:HH12	1.80	0.43
1:K:124:ILE:HD13	1:K:134:TRP:CH2	2.54	0.43
1:K:84:PRO:HG2	1:K:85:SER:H	1.84	0.43
2:L:149:ALA:HA	2:L:152:ARG:NH2	2.33	0.43
2:B:229:SER:O	2:B:233:MET:HG3	2.17	0.43
2:H:37:PRO:HD2	2:H:40:TYR:CE1	2.53	0.43
2:H:90:LEU:HD23	2:H:90:LEU:HA	1.86	0.43
1:K:296:LEU:HD12	1:K:296:LEU:O	2.18	0.43
2:B:103:ILE:HG23	2:B:104:PRO:HD2	2.00	0.43
2:B:64:LEU:O	2:B:67:VAL:HG22	2.18	0.43
1:C:124:ILE:HD13	1:C:134:TRP:CH2	2.54	0.43
2:F:37:PRO:C	2:F:39:ARG:H	2.22	0.43
2:H:212:GLN:NE2	2:H:222:SER:HB3	2.34	0.43
2:J:311:LYS:HE2	2:J:312:TRP:CZ2	2.53	0.43
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.45	0.43
1:A:151:GLU:HG3	1:A:175:LEU:HD11	2.01	0.42
1:E:58:LEU:HD22	1:E:95:LYS:CD	2.49	0.42
2:D:86:ASP:OD2	2:D:86:ASP:N	2.51	0.42
2:F:294:ASN:O	2:F:298:ILE:HG13	2.18	0.42
2:F:312:TRP:O	2:F:315:SER:HB3	2.19	0.42
2:H:255:ARG:HA	2:H:255:ARG:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:214:ARG:HG2	1:K:214:ARG:O	2.19	0.42
1:A:106:VAL:HG11	1:A:116:ALA:CB	2.50	0.42
1:A:231:VAL:O	1:A:231:VAL:HG22	2.19	0.42
2:D:47:ARG:NH1	2:D:98:SER:HB2	2.34	0.42
1:E:65:LEU:HD12	1:E:67:ARG:NE	2.35	0.42
2:F:144:LYS:HD3	2:F:185:LEU:HD22	2.02	0.42
2:L:193:MET:O	2:L:197:ILE:HG13	2.19	0.42
1:A:83:GLY:HA3	2:B:105:PHE:CE1	2.54	0.42
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.01	0.42
1:E:239:GLN:OE1	1:E:239:GLN:HA	2.18	0.42
2:F:33:LEU:CD2	2:F:54:ALA:HB1	2.49	0.42
2:H:156:LEU:HD12	2:H:170:ASN:ND2	2.34	0.42
1:K:151:GLU:HG3	1:K:175:LEU:HD11	2.00	0.42
1:K:200:TYR:CB	5:L:379:MGM:HC12	2.49	0.42
1:A:263:THR:HG21	1:A:280:LEU:HB2	2.01	0.42
2:B:22:ARG:NH1	2:B:22:ARG:HG2	2.35	0.42
1:C:231:VAL:HG22	1:C:231:VAL:O	2.19	0.42
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.53	0.42
2:H:65:ASP:C	2:H:67:VAL:H	2.22	0.42
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.55	0.42
2:J:269:ASP:HB3	2:J:272:TYR:CD2	2.51	0.42
5:D:380:MGM:H111	3:N:5:LEU:HD22	2.01	0.42
1:C:97:ARG:NH1	1:C:97:ARG:CB	2.83	0.42
2:D:121:HIS:HB3	2:D:124:MET:CG	2.48	0.42
2:F:311:LYS:HE2	2:F:312:TRP:CZ2	2.54	0.42
2:H:21:LEU:HD11	2:H:304:ARG:HH22	1.84	0.42
5:H:380:MGM:O1	5:H:380:MGM:HC41	2.20	0.42
1:I:219:GLU:HA	1:I:219:GLU:OE1	2.20	0.42
2:J:243:LYS:O	2:J:247:ARG:HG3	2.18	0.42
2:L:37:PRO:HG2	2:L:40:TYR:CD1	2.54	0.42
2:L:90:LEU:HA	2:L:90:LEU:HD23	1.87	0.42
2:D:332:MET:O	2:D:333:GLU:HB2	2.20	0.42
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.54	0.42
2:B:258:ASN:CG	2:B:259:GLY:N	2.73	0.42
1:C:106:VAL:HG11	1:C:116:ALA:CB	2.50	0.42
2:D:258:ASN:OD1	2:D:259:GLY:N	2.45	0.42
1:E:325:ASN:O	1:E:326:GLN:C	2.57	0.42
1:E:334:LEU:O	1:E:338:LEU:HG	2.20	0.42
1:G:206:ARG:NE	1:G:219:GLU:OE2	2.44	0.42
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.01	0.42
2:J:250:ARG:O	2:J:254:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:304:ARG:HG2	2:J:304:ARG:NH1	2.35	0.42
1:K:328:ASP:O	1:K:329:ASN:HB2	2.20	0.42
1:A:88:VAL:CG1	2:B:36:LEU:HD11	2.50	0.42
2:H:20:PHE:CE2	2:H:337:ILE:HD11	2.55	0.42
1:E:318:ILE:HG22	1:E:322:MET:CE	2.49	0.42
2:F:339:LYS:NZ	2:F:339:LYS:CB	2.83	0.42
2:F:339:LYS:O	2:F:348:THR:HG23	2.20	0.42
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.82	0.42
2:H:22:ARG:NH2	2:H:61:LEU:O	2.42	0.42
2:B:21:LEU:HD11	2:B:304:ARG:HH22	1.85	0.41
2:B:77:TYR:CE1	2:B:141:ARG:HB2	2.55	0.41
1:C:227:LEU:HA	1:C:227:LEU:HD23	1.92	0.41
1:C:274:GLU:HG3	1:C:310:TYR:CE2	2.55	0.41
1:E:350:THR:O	1:E:353:LYS:HB2	2.20	0.41
2:B:187:ASN:OD1	2:B:187:ASN:C	2.59	0.41
2:B:33:LEU:HD22	2:B:54:ALA:HB1	2.02	0.41
2:B:47:ARG:HH11	2:B:98:SER:HB2	1.86	0.41
2:D:21:LEU:CD1	2:D:21:LEU:N	2.83	0.41
1:E:303:GLN:HB3	1:E:304:PRO:HD3	2.02	0.41
1:G:311:LEU:C	1:G:311:LEU:HD23	2.41	0.41
2:H:258:ASN:CG	2:H:259:GLY:H	2.22	0.41
2:H:44:GLU:O	2:H:47:ARG:HG3	2.20	0.41
1:I:263:THR:HG21	1:I:280:LEU:HB2	2.02	0.41
2:B:115:HIS:HA	2:B:116:PRO:HD3	1.88	0.41
2:B:37:PRO:C	2:B:39:ARG:N	2.73	0.41
1:C:328:ASP:O	1:C:329:ASN:CB	2.69	0.41
2:D:84:THR:HG22	2:D:112:GLY:O	2.20	0.41
2:D:63:SER:O	2:D:66:VAL:HG22	2.20	0.41
2:F:58:LEU:HA	2:F:58:LEU:HD23	1.92	0.41
1:G:344:LEU:HA	1:G:348:LYS:HB2	2.02	0.41
1:I:106:VAL:HG11	1:I:116:ALA:HB1	2.02	0.41
2:J:129:LEU:HB2	2:J:184:MET:HE3	2.02	0.41
2:J:329:LEU:HD12	2:J:329:LEU:HA	1.88	0.41
1:K:101:ASP:HA	1:K:104:ARG:HH11	1.85	0.41
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.55	0.41
1:C:329:ASN:O	1:C:330:LYS:C	2.58	0.41
1:C:65:LEU:O	1:C:69:ARG:HG3	2.20	0.41
1:C:207:GLN:OE1	2:D:216:LEU:HD13	2.21	0.41
2:F:37:PRO:C	2:F:39:ARG:N	2.74	0.41
1:G:223:VAL:HG11	1:G:240:ARG:HB2	2.01	0.41
2:H:198:SER:OG	2:H:202:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:MET:HE2	2:H:347:SER:HB3	2.02	0.41
2:J:145:GLU:HA	2:J:145:GLU:OE2	2.21	0.41
2:J:294:ASN:O	2:J:298:ILE:HG13	2.21	0.41
2:L:73:ILE:HD13	2:L:137:ASP:HB2	2.02	0.41
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.55	0.41
1:C:117:PHE:CE2	1:C:146:LYS:HE2	2.56	0.41
2:D:269:ASP:HB3	2:D:272:TYR:CD2	2.54	0.41
1:E:329:ASN:CB	1:E:332:ASP:HB3	2.48	0.41
2:H:303:ASP:OD1	2:H:306:VAL:HG13	2.21	0.41
2:H:334:GLU:HB3	2:H:337:ILE:HD12	2.03	0.41
2:L:156:LEU:HD12	2:L:170:ASN:ND2	2.36	0.41
2:H:193:MET:HG3	2:H:233:MET:HE2	2.01	0.41
2:J:207:ASP:O	2:J:208:ASN:HB2	2.20	0.41
1:A:189:ILE:HD11	1:A:205:HIS:CD2	2.51	0.41
1:A:308:SER:HB2	1:A:309:PRO:HD2	2.02	0.41
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.83	0.41
2:B:249:LYS:HB3	2:B:285:ILE:HD13	2.02	0.41
2:B:357:LEU:HD22	2:B:361:TRP:CZ2	2.56	0.41
1:C:262:TYR:O	1:C:266:MET:HG2	2.20	0.41
2:D:243:LYS:HB3	2:D:243:LYS:NZ	2.35	0.41
1:E:207:GLN:HG2	1:E:242:PHE:CE2	2.56	0.41
2:H:311:LYS:HB3	2:H:321:HIS:NE2	2.36	0.41
1:G:88:VAL:HG12	2:H:36:LEU:HD11	2.03	0.41
1:I:79:PRO:HA	1:I:101:ASP:OD1	2.20	0.41
2:L:269:ASP:HB3	2:L:272:TYR:CD2	2.54	0.41
2:L:329:LEU:HA	2:L:329:LEU:HD12	1.93	0.41
1:E:106:VAL:HG11	1:E:116:ALA:CB	2.51	0.41
2:F:138:ASP:OD1	2:F:140:SER:CB	2.68	0.41
2:H:122:ILE:HG22	2:H:163:ALA:HA	2.01	0.41
2:H:230:LEU:HD22	2:H:239:VAL:HG21	2.03	0.41
2:H:339:LYS:HG2	2:H:348:THR:CG2	2.50	0.41
1:I:231:VAL:HG22	1:I:231:VAL:O	2.21	0.41
1:K:156:ILE:CD1	1:K:184:GLN:NE2	2.82	0.41
1:C:180:LYS:HE3	1:E:212:GLU:O	2.21	0.41
1:C:284:LEU:O	1:C:287:ARG:HG2	2.20	0.41
2:D:110:ASN:CB	2:D:111:PRO:HD2	2.50	0.41
2:H:294:ASN:O	2:H:298:ILE:HG13	2.21	0.41
1:I:296:LEU:HD12	1:I:296:LEU:O	2.21	0.41
1:K:165:ASN:O	1:K:168:VAL:HG22	2.21	0.41
2:L:152:ARG:HD3	2:L:189:SER:O	2.21	0.41
2:F:269:ASP:OD2	2:F:311:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:359:GLN:CA	2:J:359:GLN:HE21	2.22	0.41
2:B:320:LEU:HD11	3:M:5:LEU:HD11	2.03	0.41
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.56	0.41
2:D:329:LEU:HA	2:D:329:LEU:HD12	1.92	0.41
2:D:39:ARG:HG3	2:D:40:TYR:CD1	2.56	0.41
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.20	0.41
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.56	0.41
2:H:290:ASN:OD1	2:H:290:ASN:C	2.59	0.41
1:I:124:ILE:HD13	1:I:134:TRP:CH2	2.55	0.41
1:I:359:ILE:HA	1:I:359:ILE:HD13	1.89	0.41
2:J:103:ILE:HG23	2:J:104:PRO:HD2	2.03	0.41
1:K:328:ASP:O	1:K:329:ASN:CB	2.69	0.41
2:L:110:ASN:CB	2:L:111:PRO:HD2	2.43	0.41
2:D:263:ARG:HB2	2:D:266:LYS:HG3	2.03	0.40
2:H:255:ARG:HD3	2:H:261:HIS:NE2	2.37	0.40
2:H:334:GLU:OE1	2:H:334:GLU:HA	2.21	0.40
1:K:263:THR:HG21	1:K:280:LEU:HB2	2.03	0.40
1:K:60:SER:OG	1:K:61:PRO:HD2	2.21	0.40
1:K:88:VAL:HG12	1:K:88:VAL:O	2.21	0.40
2:D:133:ILE:CD1	2:D:354:LEU:HD13	2.51	0.40
1:G:308:SER:O	1:G:312:ILE:HG12	2.22	0.40
2:J:359:GLN:O	2:J:362:LYS:N	2.55	0.40
1:K:106:VAL:HG11	1:K:116:ALA:CB	2.51	0.40
1:A:331:GLU:O	1:A:335:ASN:ND2	2.54	0.40
2:B:138:ASP:OD1	2:B:140:SER:HB3	2.21	0.40
2:B:329:LEU:HA	2:B:329:LEU:HD12	1.95	0.40
1:C:92:TYR:O	1:C:97:ARG:NH2	2.52	0.40
1:E:340:LEU:HA	1:E:343:ILE:HD12	2.03	0.40
2:F:249:LYS:HB3	2:F:285:ILE:HD13	2.03	0.40
1:G:231:VAL:HG22	1:G:231:VAL:O	2.22	0.40
1:G:334:LEU:O	1:G:338:LEU:HG	2.21	0.40
1:G:71:GLU:O	1:G:115:ARG:NH1	2.55	0.40
1:I:65:LEU:HD12	1:I:67:ARG:CZ	2.52	0.40
1:K:151:GLU:OE1	1:K:151:GLU:HA	2.22	0.40
1:C:303:GLN:CB	1:C:304:PRO:HD3	2.52	0.40
2:D:68:ASN:OD1	2:D:70:ASP:HB2	2.22	0.40
1:E:136:PHE:CE2	1:E:140:LEU:HD11	2.57	0.40
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.91	0.40
1:K:329:ASN:HB3	1:K:332:ASP:CB	2.50	0.40
2:B:357:LEU:CD2	2:B:361:TRP:HE1	2.34	0.40
2:B:86:ASP:N	2:B:86:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:ILE:HD11	1:G:205:HIS:CD2	2.49	0.40
2:H:59:ASP:OD2	2:H:59:ASP:C	2.60	0.40
2:H:64:LEU:HA	2:H:64:LEU:HD23	1.90	0.40
1:I:165:ASN:O	1:I:168:VAL:HG22	2.22	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%)	22 (7%)	3 (1%)	15	45
1	C	312/377 (83%)	287 (92%)	22 (7%)	3 (1%)	15	45
1	E	312/377 (83%)	287 (92%)	22 (7%)	3 (1%)	15	45
1	G	312/377 (83%)	288 (92%)	21 (7%)	3 (1%)	15	45
1	I	312/377 (83%)	288 (92%)	21 (7%)	3 (1%)	15	45
1	K	312/377 (83%)	287 (92%)	21 (7%)	4 (1%)	12	37
2	B	344/377 (91%)	326 (95%)	16 (5%)	2 (1%)	25	58
2	D	344/377 (91%)	324 (94%)	19 (6%)	1 (0%)	41	71
2	F	344/377 (91%)	328 (95%)	14 (4%)	2 (1%)	25	58
2	H	344/377 (91%)	318 (92%)	23 (7%)	3 (1%)	17	48
2	J	344/377 (91%)	324 (94%)	16 (5%)	4 (1%)	13	40
2	L	344/377 (91%)	326 (95%)	17 (5%)	1 (0%)	41	71
3	M	3/6 (50%)	3 (100%)	0	0	100	100
3	N	3/6 (50%)	3 (100%)	0	0	100	100
3	O	3/6 (50%)	3 (100%)	0	0	100	100
3	P	3/6 (50%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	3/6 (50%)	3 (100%)	0	0	100	100
3	R	3/6 (50%)	3 (100%)	0	0	100	100
All	All	3954/4560 (87%)	3688 (93%)	234 (6%)	32 (1%)	19	51

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
2	B	258	ASN
1	C	326	GLN
2	D	258	ASN
2	F	258	ASN
2	F	362	LYS
1	G	326	GLN
2	H	66	VAL
2	H	258	ASN
1	I	326	GLN
2	J	258	ASN
2	L	258	ASN
1	C	217	ASP
1	E	217	ASP
1	G	217	ASP
1	I	217	ASP
1	K	217	ASP
1	K	326	GLN
1	K	329	ASN
1	A	217	ASP
1	C	196	ASP
1	E	196	ASP
1	E	326	GLN
2	H	333	GLU
1	A	196	ASP
1	G	196	ASP
1	I	196	ASP
2	J	34	GLN
1	K	196	ASP
2	B	66	VAL
2	J	360	SER
2	J	66	VAL

### 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	282/338 (83%)	270 (96%)	12 (4%)	29	62
1	C	286/338 (85%)	277 (97%)	9 (3%)	40	74
1	E	289/338 (86%)	279 (96%)	10 (4%)	36	70
1	G	285/338 (84%)	278 (98%)	7 (2%)	47	78
1	I	285/338 (84%)	278 (98%)	7 (2%)	47	78
1	K	292/338 (86%)	282 (97%)	10 (3%)	37	71
2	B	291/326 (89%)	279 (96%)	12 (4%)	30	64
2	D	291/326 (89%)	278 (96%)	13 (4%)	27	61
2	F	295/326 (90%)	283 (96%)	12 (4%)	30	64
2	H	288/326 (88%)	276 (96%)	12 (4%)	30	63
2	J	291/326 (89%)	273 (94%)	18 (6%)	18	47
2	L	295/326 (90%)	282 (96%)	13 (4%)	28	61
3	M	5/6 (83%)	5 (100%)	0	100	100
3	N	5/6 (83%)	5 (100%)	0	100	100
3	O	5/6 (83%)	5 (100%)	0	100	100
3	P	5/6 (83%)	5 (100%)	0	100	100
3	Q	5/6 (83%)	4 (80%)	1 (20%)	1	4
3	R	5/6 (83%)	5 (100%)	0	100	100
All	All	3500/4020 (87%)	3364 (96%)	136 (4%)	32	66

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	71	GLU
1	A	107	LEU
1	A	173	ARG
1	A	184	GLN
1	A	194	ASN

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	214	ARG
1	A	225	GLN
1	A	287	ARG
1	A	348	LYS
1	A	354	GLU
2	B	21	LEU
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU
2	B	255	ARG
2	B	261	HIS
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	353	ARG
2	B	357	LEU
1	C	60	SER
1	C	71	GLU
1	C	107	LEU
1	C	184	GLN
1	C	194	ASN
1	C	195	GLN
1	C	211	GLN
1	C	287	ARG
1	C	324	GLU
2	D	21	LEU
2	D	110	ASN
2	D	151	LEU
2	D	216	LEU
2	D	232	LEU
2	D	236	LEU
2	D	255	ARG
2	D	258	ASN
2	D	261	HIS
2	D	329	LEU
2	D	331	LEU
2	D	349	ARG
2	D	357	LEU
1	E	71	GLU
1	E	81	ASN

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Mol	Chain	Res	Type
1	E	97	ARG
1	E	107	LEU
1	E	211	GLN
1	E	214	ARG
1	E	265	GLU
1	E	324	GLU
1	E	326	GLN
1	E	364	GLN
2	F	21	LEU
2	F	24	ARG
2	F	30	GLN
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	258	ASN
2	F	261	HIS
2	F	329	LEU
2	F	331	LEU
1	G	71	GLU
1	G	107	LEU
1	G	194	ASN
1	G	211	GLN
1	G	224	ASP
1	G	225	GLN
1	G	287	ARG
2	H	21	LEU
2	H	91	ASP
2	H	151	LEU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	261	HIS
2	H	296	ASN
2	H	329	LEU
2	H	331	LEU
2	H	339	LYS
1	I	71	GLU
1	I	107	LEU
1	I	184	GLN

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Mol	Chain	Res	Type
1	I	261	GLN
1	I	287	ARG
1	I	332	ASP
1	I	353	LYS
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	237	GLU
2	J	255	ARG
2	J	258	ASN
2	J	261	HIS
2	J	281	LYS
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	341	HIS
2	J	349	ARG
2	J	353	ARG
1	K	67	ARG
1	K	71	GLU
1	K	80	GLN
1	K	107	LEU
1	K	142	ARG
1	K	150	GLU
1	K	211	GLN
1	K	287	ARG
1	K	320	GLU
1	K	348	LYS
2	L	106	ASN
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	237	GLU
2	L	255	ARG
2	L	258	ASN
2	L	261	HIS
2	L	329	LEU

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Mol	Chain	Res	Type
2	L	331	LEU
2	L	353	ARG
2	L	360	SER
3	Q	5	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	A	194	ASN
1	A	225	GLN
1	A	278	ASN
1	A	285	GLN
1	A	325	ASN
1	A	367	HIS
2	B	208	ASN
1	C	108	GLN
1	C	153	ASN
1	C	184	GLN
1	C	201	HIS
1	C	218	ASN
1	C	225	GLN
1	C	298	GLN
1	C	367	HIS
2	D	34	GLN
2	D	246	ASN
1	E	81	ASN
1	E	184	GLN
1	E	285	GLN
1	E	297	ASN
1	E	298	GLN
1	E	364	GLN
1	E	367	HIS
2	F	208	ASN
2	F	246	ASN
2	F	258	ASN
1	G	80	GLN
1	G	81	ASN
1	G	108	GLN
1	G	184	GLN
1	G	201	HIS
1	G	225	GLN

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Mol	Chain	Res	Type
1	G	234	ASN
1	G	278	ASN
1	G	285	GLN
1	G	297	ASN
1	G	303	GLN
1	G	325	ASN
1	G	335	ASN
2	H	208	ASN
2	H	246	ASN
2	H	265	ASN
2	H	296	ASN
1	I	81	ASN
1	I	89	GLN
1	I	162	GLN
1	I	184	GLN
1	I	218	ASN
1	I	225	GLN
1	I	261	GLN
1	I	285	GLN
1	I	367	HIS
2	J	30	GLN
2	J	208	ASN
2	J	246	ASN
2	J	258	ASN
2	J	359	GLN
1	K	184	GLN
1	K	201	HIS
1	K	205	HIS
1	K	218	ASN
1	K	285	GLN
1	K	298	GLN
1	K	325	ASN
1	K	326	GLN
1	K	367	HIS
2	L	106	ASN
2	L	208	ASN
2	L	212	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 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	$\# Z  > 2$
5	MGM	H	380	-	26,28,28	1.05	2 (7%)	33,37,37	1.91	6 (18%)
5	MGM	J	379	-	26,28,28	1.10	2 (7%)	33,37,37	1.94	7 (21%)
5	MGM	D	380	-	26,28,28	1.07	2 (7%)	33,37,37	1.97	5 (15%)
5	MGM	B	379	-	26,28,28	1.04	2 (7%)	33,37,37	2.02	6 (18%)
7	MES	F	380	-	12,12,12	9.05	8 (66%)	14,16,16	2.51	5 (35%)
5	MGM	F	381	-	26,28,28	1.17	3 (11%)	33,37,37	1.90	7 (21%)
5	MGM	L	379	-	26,28,28	1.17	2 (7%)	33,37,37	1.99	7 (21%)

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
5	MGM	H	380	-	-	12/31/31/31	-
5	MGM	J	379	-	-	12/31/31/31	-
5	MGM	D	380	-	-	10/31/31/31	-
5	MGM	B	379	-	-	9/31/31/31	-
7	MES	F	380	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGM	F	381	-	-	13/31/31/31	-
5	MGM	L	379	-	-	11/31/31/31	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	380	MES	C8-S	-23.66	1.43	1.77
7	F	380	MES	O2S-S	12.31	1.81	1.45
7	F	380	MES	O1S-S	11.76	1.79	1.45
7	F	380	MES	O3S-S	9.25	1.80	1.47
7	F	380	MES	C7-C8	-4.63	1.40	1.52
5	L	379	MGM	C7-C8	3.03	1.40	1.33
5	J	379	MGM	C7-C8	2.82	1.39	1.33
7	F	380	MES	C3-C2	-2.80	1.39	1.50
5	F	381	MGM	C7-C8	2.57	1.39	1.33
7	F	380	MES	C5-C6	-2.54	1.40	1.50
5	D	380	MGM	C7-C8	2.52	1.39	1.33
7	F	380	MES	C7-N4	-2.42	1.41	1.47
5	H	380	MGM	C7-C8	2.40	1.38	1.33
5	D	380	MGM	C12-C13	2.40	1.38	1.33
5	B	379	MGM	C7-C8	2.39	1.38	1.33
5	H	380	MGM	C12-C13	2.32	1.38	1.33
5	J	379	MGM	C12-C13	2.23	1.38	1.33
5	F	381	MGM	C5-C6	2.21	1.57	1.53
5	F	381	MGM	C12-C13	2.14	1.38	1.33
5	L	379	MGM	C12-C13	2.06	1.37	1.33
5	B	379	MGM	C12-C13	2.05	1.37	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	379	MGM	C1-C2-N3	7.26	131.01	113.31
5	D	380	MGM	C1-C2-N3	7.04	130.48	113.31
5	H	380	MGM	C1-C2-N3	6.56	129.29	113.31
5	L	379	MGM	C1-C2-N3	6.28	128.62	113.31
5	F	381	MGM	C1-C2-N3	5.99	127.91	113.31
7	F	380	MES	O3S-S-C8	5.79	115.14	105.77
5	J	379	MGM	C1-C2-N3	5.62	127.01	113.31
5	D	380	MGM	C4-N3-C2	5.53	125.71	110.62
5	B	379	MGM	C4-N3-C2	5.45	125.50	110.62
5	H	380	MGM	C4-N3-C2	5.06	124.43	110.62
5	L	379	MGM	C4-N3-C2	4.96	124.17	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	379	MGM	C4-N3-C2	4.74	123.56	110.62
5	F	381	MGM	C4-N3-C2	4.69	123.44	110.62
5	L	379	MGM	O1-C1-C2	4.60	116.22	107.27
7	F	380	MES	O1S-S-C8	4.26	112.04	106.92
5	J	379	MGM	C5-C6-C7	3.97	116.98	111.12
5	B	379	MGM	O1-C1-C2	3.96	114.97	107.27
5	D	380	MGM	O1-C1-C2	3.93	114.92	107.27
5	H	380	MGM	O1-C1-C2	3.74	114.54	107.27
5	J	379	MGM	O1-C1-C2	3.68	114.44	107.27
5	F	381	MGM	O1-C1-C2	3.64	114.35	107.27
7	F	380	MES	O2S-S-C8	3.54	111.18	106.92
5	F	381	MGM	C2-N3-C5	3.20	124.84	111.92
5	L	379	MGM	C2-N3-C5	3.15	124.63	111.92
5	J	379	MGM	C2-N3-C5	3.07	124.31	111.92
5	H	380	MGM	C2-N3-C5	3.06	124.27	111.92
5	J	379	MGM	O1B-PB-O3A	2.98	114.64	104.64
5	L	379	MGM	O1B-PB-O3A	2.79	114.01	104.64
5	F	381	MGM	C5-C6-C7	2.69	115.09	111.12
5	F	381	MGM	O1B-PB-O3A	2.68	113.63	104.64
5	D	380	MGM	C2-N3-C5	2.60	122.42	111.92
7	F	380	MES	O3S-S-O2S	-2.56	105.01	111.27
5	B	379	MGM	C2-N3-C5	2.56	122.26	111.92
5	L	379	MGM	C5-C6-C7	2.51	114.82	111.12
7	F	380	MES	O2S-S-O1S	-2.48	105.35	113.95
5	B	379	MGM	O1B-PB-O3A	2.46	112.88	104.64
5	H	380	MGM	O1B-PB-O3A	2.42	112.76	104.64
5	D	380	MGM	O1B-PB-O3A	2.36	112.54	104.64
5	J	379	MGM	C10-C8-C9	-2.29	111.42	115.27
5	F	381	MGM	C10-C8-C9	-2.16	111.64	115.27
5	L	379	MGM	C10-C8-C9	-2.15	111.65	115.27
5	B	379	MGM	C10-C8-C9	-2.06	111.80	115.27
5	H	380	MGM	C10-C8-C9	-2.00	111.90	115.27

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	380	MGM	C6-C5-N3-C2
5	H	380	MGM	C1-C2-N3-C4
5	H	380	MGM	O1-C1-C2-N3
5	H	380	MGM	PA-O3A-PB-O1B
5	J	379	MGM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	J	379	MGM	N3-C5-C6-C7
5	J	379	MGM	C6-C5-N3-C2
5	J	379	MGM	C1-C2-N3-C4
5	J	379	MGM	PA-O3A-PB-O1B
5	D	380	MGM	C1-C2-N3-C4
5	D	380	MGM	O1-C1-C2-N3
5	D	380	MGM	PA-O3A-PB-O1B
5	F	381	MGM	N3-C5-C6-C7
5	F	381	MGM	C6-C5-N3-C2
5	F	381	MGM	C1-C2-N3-C4
5	F	381	MGM	PA-O3A-PB-O1B
5	B	379	MGM	C1-C2-N3-C4
5	B	379	MGM	O1-C1-C2-N3
5	B	379	MGM	PA-O3A-PB-O1B
7	F	380	MES	C7-C8-S-O1S
5	L	379	MGM	C5-C6-C7-C8
5	L	379	MGM	C6-C5-N3-C2
5	L	379	MGM	C1-C2-N3-C4
5	L	379	MGM	O1-C1-C2-N3
5	L	379	MGM	PA-O3A-PB-O1B
5	D	380	MGM	C6-C5-N3-C4
5	B	379	MGM	C6-C5-N3-C4
5	H	380	MGM	C10-C8-C9-C11
5	F	381	MGM	C10-C8-C9-C11
5	F	381	MGM	C7-C8-C9-C11
5	J	379	MGM	C10-C8-C9-C11
5	H	380	MGM	C7-C8-C9-C11
5	J	379	MGM	C7-C8-C9-C11
5	L	379	MGM	C10-C8-C9-C11
5	F	381	MGM	C5-C6-C7-C8
5	D	380	MGM	C10-C8-C9-C11
5	J	379	MGM	C2-C1-O1-PA
5	F	381	MGM	C2-C1-O1-PA
7	F	380	MES	C7-C8-S-O2S
5	L	379	MGM	C2-C1-O1-PA
5	B	379	MGM	C10-C8-C9-C11
5	L	379	MGM	C7-C8-C9-C11
5	D	380	MGM	C7-C8-C9-C11
5	B	379	MGM	C7-C8-C9-C11
5	J	379	MGM	C14-C13-C15-C16
5	F	381	MGM	C14-C13-C15-C16
5	L	379	MGM	N3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	D	380	MGM	C14-C13-C15-C16
5	H	380	MGM	C14-C13-C15-C16
5	H	380	MGM	PA-O3A-PB-O3B
5	D	380	MGM	PA-O3A-PB-O3B
5	F	381	MGM	PA-O3A-PB-O3B
5	B	379	MGM	C14-C13-C15-C16
5	H	380	MGM	PA-O3A-PB-O2B
5	J	379	MGM	PA-O3A-PB-O2B
5	D	380	MGM	PA-O3A-PB-O2B
5	F	381	MGM	PA-O3A-PB-O2B
5	B	379	MGM	PA-O3A-PB-O2B
5	L	379	MGM	PA-O3A-PB-O2B
5	H	380	MGM	C12-C13-C15-C16
5	H	380	MGM	C9-C11-C12-C13
5	J	379	MGM	C9-C11-C12-C13
5	B	379	MGM	C9-C11-C12-C13
5	D	380	MGM	C9-C11-C12-C13
5	F	381	MGM	C9-C11-C12-C13
5	L	379	MGM	C9-C11-C12-C13
5	H	380	MGM	C2-C1-O1-PA
5	J	379	MGM	O1-C1-C2-N3
5	F	381	MGM	O1-C1-C2-N3

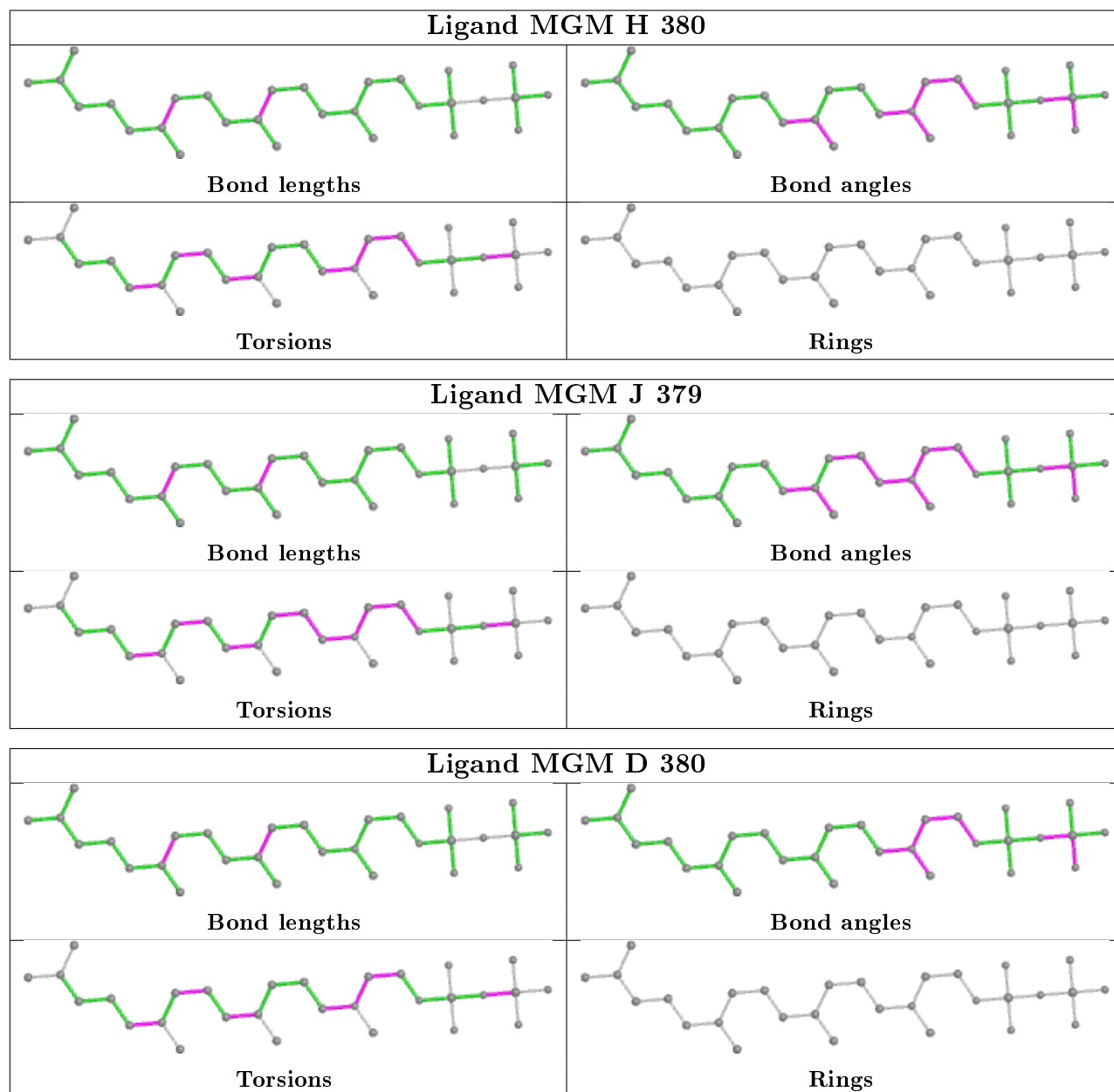
There are no ring outliers.

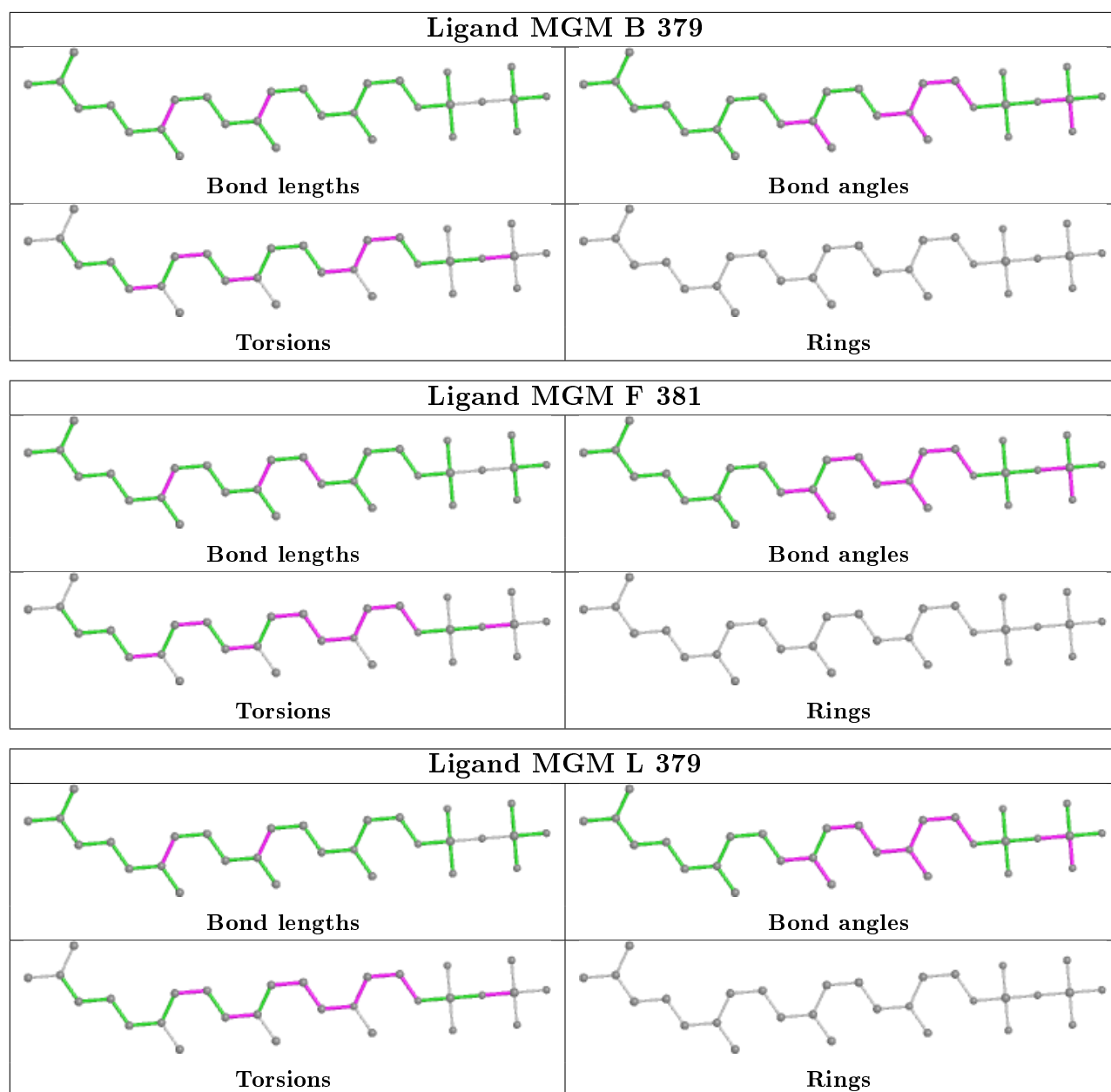
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	380	MGM	2	0
5	J	379	MGM	3	0
5	D	380	MGM	2	0
5	B	379	MGM	2	0
5	F	381	MGM	4	0
5	L	379	MGM	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	314/377 (83%)	0.22	11 (3%) 44 38	62, 84, 117, 131	0
1	C	314/377 (83%)	0.25	14 (4%) 33 29	61, 81, 110, 131	0
1	E	314/377 (83%)	0.18	9 (2%) 51 47	59, 82, 108, 127	0
1	G	314/377 (83%)	0.32	14 (4%) 33 29	64, 84, 110, 132	0
1	I	314/377 (83%)	0.11	8 (2%) 57 55	55, 80, 111, 125	0
1	K	314/377 (83%)	-0.05	2 (0%) 89 89	53, 68, 95, 107	0
2	B	346/377 (91%)	0.04	6 (1%) 70 69	61, 76, 97, 122	0
2	D	346/377 (91%)	0.04	8 (2%) 60 58	59, 72, 94, 109	0
2	F	346/377 (91%)	-0.00	4 (1%) 79 79	55, 69, 95, 117	0
2	H	346/377 (91%)	0.28	13 (3%) 40 36	65, 85, 109, 130	0
2	J	346/377 (91%)	-0.01	7 (2%) 65 63	57, 76, 102, 122	0
2	L	346/377 (91%)	-0.07	3 (0%) 84 84	52, 66, 85, 109	0
3	M	5/6 (83%)	-0.01	0 100 100	63, 66, 79, 93	1 (20%)
3	N	5/6 (83%)	0.18	0 100 100	67, 69, 78, 93	1 (20%)
3	O	5/6 (83%)	0.41	0 100 100	64, 65, 75, 91	1 (20%)
3	P	5/6 (83%)	0.44	0 100 100	77, 80, 91, 106	1 (20%)
3	Q	5/6 (83%)	0.33	0 100 100	63, 67, 75, 92	1 (20%)
3	R	5/6 (83%)	0.07	0 100 100	59, 60, 73, 88	1 (20%)
All	All	3990/4560 (87%)	0.11	99 (2%) 57 55	52, 77, 105, 132	6 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	361	TRP	5.9
1	E	306	HIS	5.9
1	A	306	HIS	5.7

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Mol	Chain	Res	Type	RSRZ
2	H	108	SER	5.1
1	C	306	HIS	4.9
2	J	108	SER	4.7
1	I	306	HIS	4.5
2	H	363	THR	4.0
1	G	306	HIS	4.0
2	H	304	ARG	3.7
2	B	363	THR	3.6
1	C	55	PHE	3.6
2	H	112	GLY	3.6
2	J	363	THR	3.6
1	G	55	PHE	3.5
1	E	302	LEU	3.5
1	C	334	LEU	3.5
1	G	333	ILE	3.4
2	D	112	GLY	3.4
1	I	55	PHE	3.2
2	J	360	SER	3.2
1	K	326	GLN	3.2
2	F	363	THR	3.2
1	C	307	SER	3.1
1	C	336	LYS	3.1
2	L	108	SER	3.1
2	D	113	THR	3.1
1	E	75	ILE	3.0
2	D	363	THR	3.0
1	I	305	SER	3.0
2	H	305	LEU	3.0
1	A	367	HIS	3.0
2	B	362	LYS	2.9
1	G	367	HIS	2.9
1	E	303	GLN	2.9
1	G	82	ASP	2.8
1	G	327	CYS	2.8
1	A	302	LEU	2.8
1	A	304	PRO	2.8
1	E	305	SER	2.8
1	C	327	CYS	2.7
1	I	327	CYS	2.7
2	J	112	GLY	2.7
2	D	111	PRO	2.7
2	H	362	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	112	GLY	2.7
2	H	87	ARG	2.6
2	D	114	ALA	2.6
1	C	333	ILE	2.6
1	G	56	LEU	2.6
1	C	329	ASN	2.6
1	G	78	VAL	2.6
2	H	190	GLY	2.6
1	A	329	ASN	2.5
1	E	304	PRO	2.5
1	C	324	GLU	2.5
1	G	305	SER	2.5
1	G	330	LYS	2.5
1	E	55	PHE	2.5
1	I	326	GLN	2.4
2	L	361	TRP	2.4
2	B	107	PRO	2.4
1	G	302	LEU	2.4
2	B	361	TRP	2.4
2	J	361	TRP	2.4
1	G	329	ASN	2.4
1	C	331	GLU	2.4
2	B	108	SER	2.4
1	G	334	LEU	2.4
1	C	367	HIS	2.3
2	H	132	LEU	2.3
1	E	327	CYS	2.3
1	A	333	ILE	2.3
2	D	108	SER	2.3
2	H	179	SER	2.3
1	K	306	HIS	2.3
2	H	114	ALA	2.3
2	F	73	ILE	2.3
2	F	113	THR	2.3
1	A	330	LYS	2.3
2	J	357	LEU	2.3
2	H	111	PRO	2.3
1	I	302	LEU	2.3
1	A	305	SER	2.2
2	B	112	GLY	2.2
1	A	332	ASP	2.2
1	C	75	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	361	TRP	2.2
2	L	113	THR	2.2
1	C	330	LYS	2.1
1	G	75	ILE	2.1
2	D	305	LEU	2.1
2	J	85	GLU	2.1
1	I	270	VAL	2.1
1	I	225	GLN	2.1
1	E	331	GLU	2.1
1	A	307	SER	2.0
1	A	300	LEU	2.0
1	C	328	ASP	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	MES	F	380	12/12	0.92	0.30	114,119,120,120	0
5	MGM	H	380	29/29	0.93	0.29	76,81,99,101	0
6	CL	D	379	1/1	0.94	0.12	74,74,74,74	0
6	CL	H	379	1/1	0.96	0.15	87,87,87,87	0
5	MGM	D	380	29/29	0.96	0.26	66,76,89,90	0
6	CL	F	379	1/1	0.96	0.18	72,72,72,72	0
5	MGM	J	379	29/29	0.97	0.22	56,68,79,81	0
5	MGM	F	381	29/29	0.97	0.24	59,67,87,89	0
5	MGM	L	379	29/29	0.97	0.23	53,66,76,78	0
5	MGM	B	379	29/29	0.97	0.23	67,73,89,90	0
4	ZN	B	378	1/1	0.99	0.15	66,66,66,66	0

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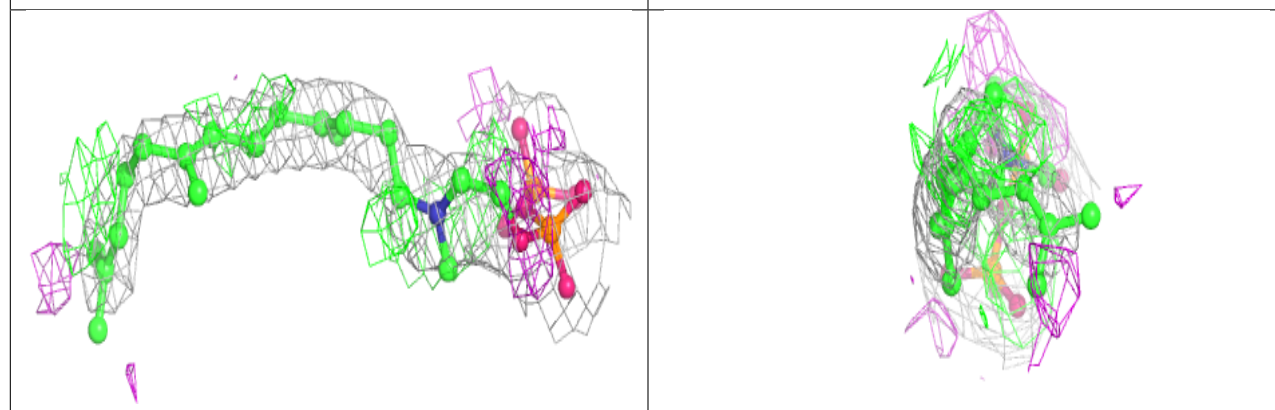
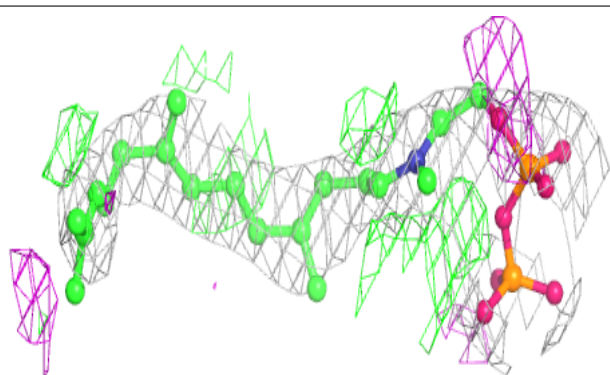
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	F	378	1/1	0.99	0.14	63,63,63,63	0
4	ZN	L	378	1/1	1.00	0.16	65,65,65,65	0
4	ZN	D	378	1/1	1.00	0.19	72,72,72,72	0
4	ZN	H	378	1/1	1.00	0.14	82,82,82,82	0
4	ZN	J	378	1/1	1.00	0.17	67,67,67,67	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.

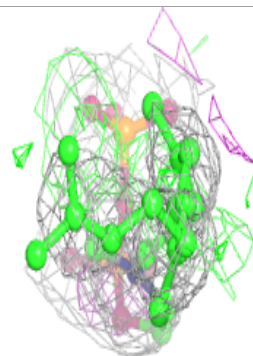
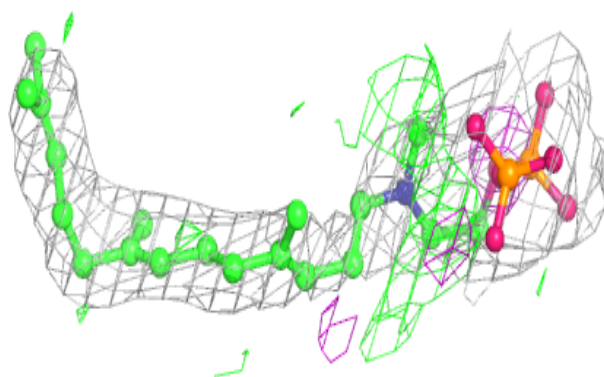
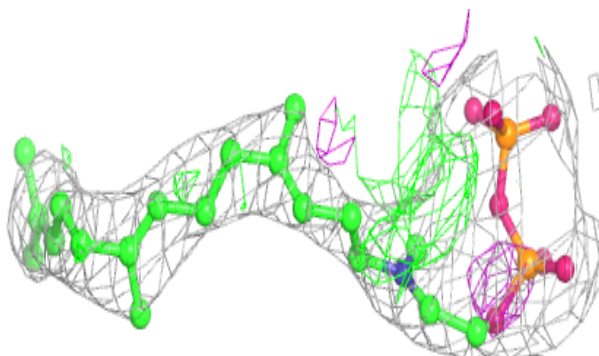
**Electron density around MGM H 380:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

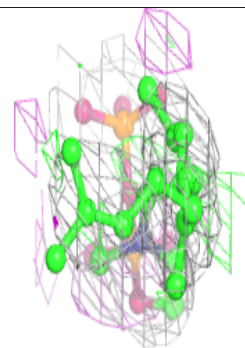
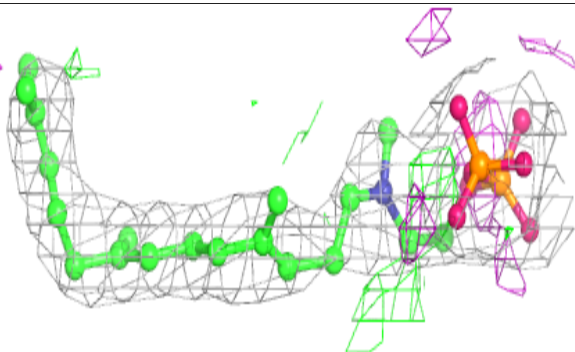
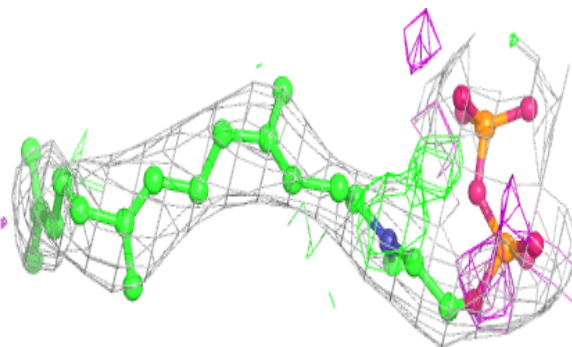


**Electron density around MGM D 380:**

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

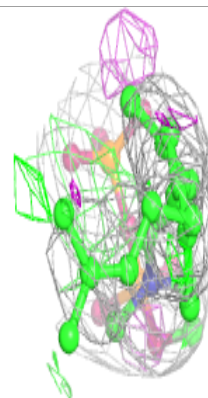
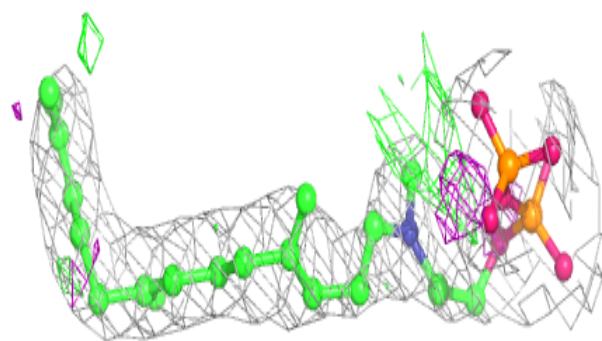
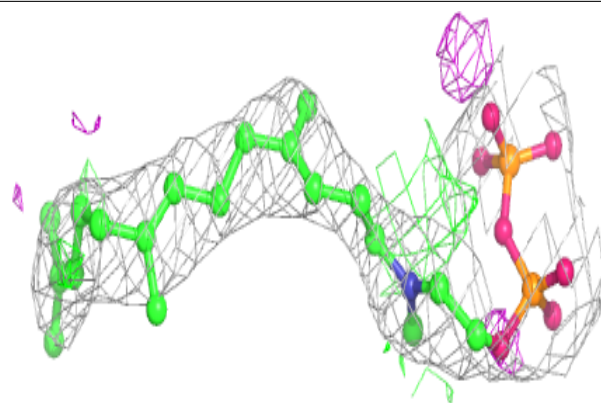
**Electron density around MGM J 379:**

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

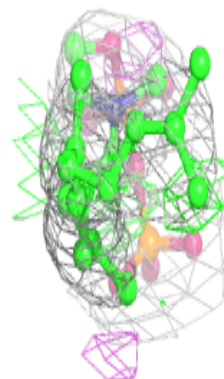
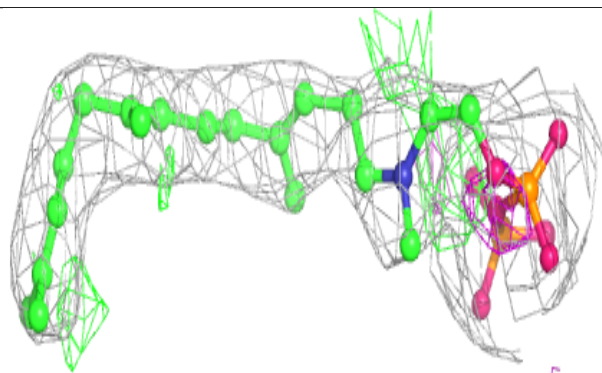
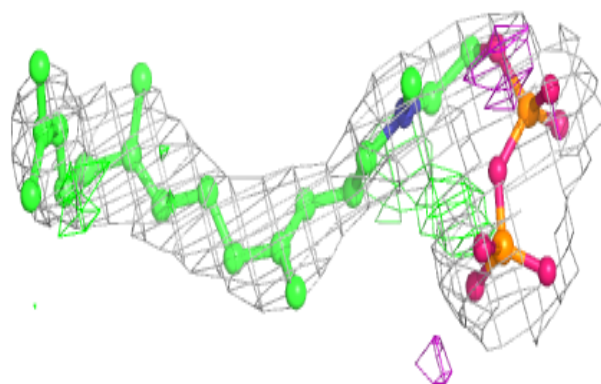


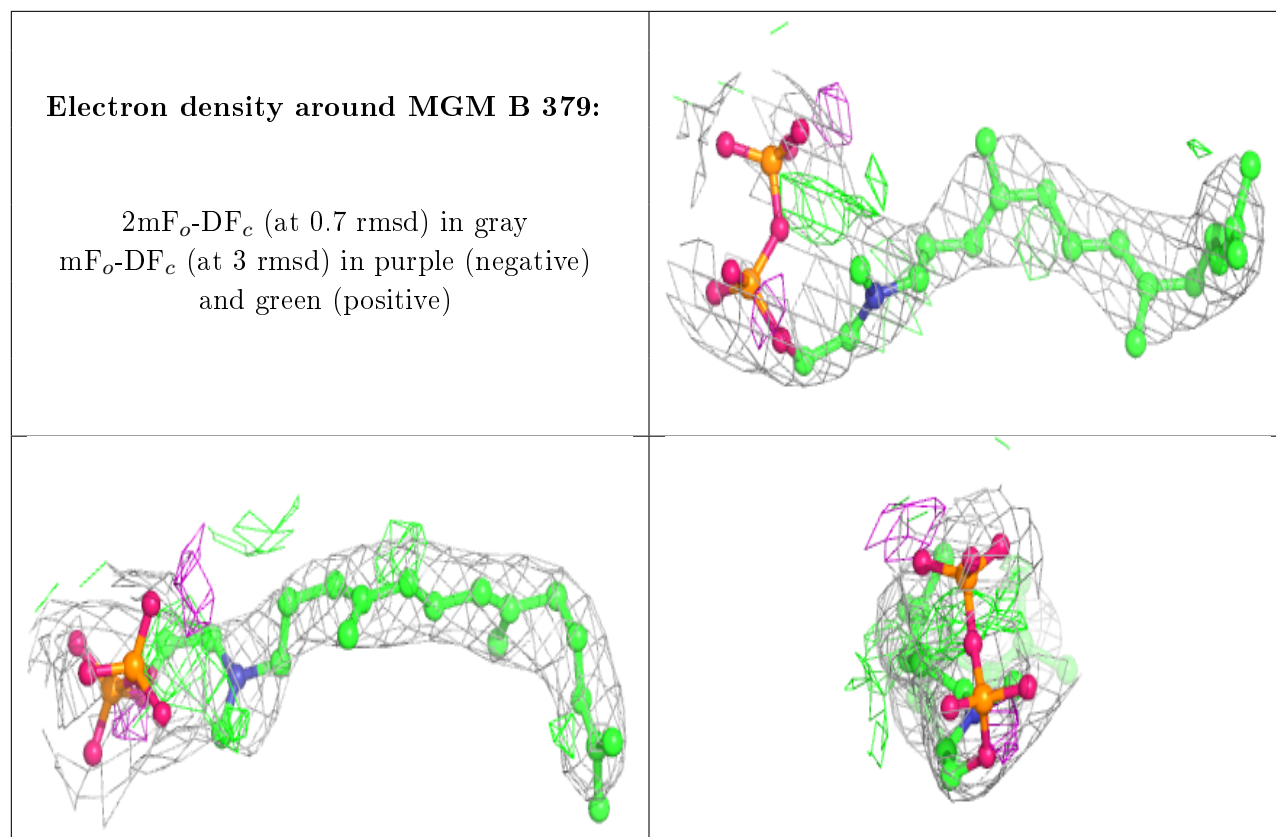
**Electron density around MGM F 381:**

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

**Electron density around MGM L 379:**

$2mF_o-DF_c$  (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.