



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:56 pm BST

PDB ID : 1TNU
Title : Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a GCINCKVL Peptide Derived from RhoB
Authors : Reid, T.S.; Terry, K.L.; Casey, P.J.; Beese, L.S.
Deposited on : 2004-06-11
Resolution : 2.70 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 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

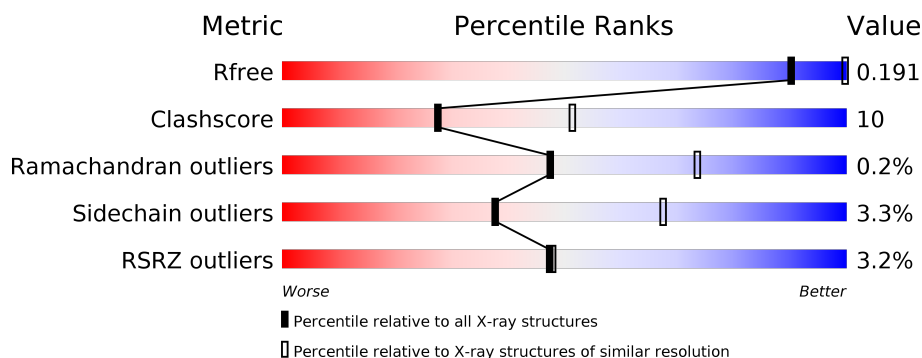
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	377	<div> <div>3%</div> <div>61% 20% 17%</div> </div>
1	C	377	<div> <div>2%</div> <div>64% 18% 17%</div> </div>
1	E	377	<div> <div>3%</div> <div>61% 21% 17%</div> </div>
1	G	377	<div> <div>2%</div> <div>62% 20% 17%</div> </div>
1	I	377	<div> <div>3%</div> <div>67% 16% 17%</div> </div>
1	K	377	<div> <div>%</div> <div>65% 18% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	9	
3	N	9	
3	O	9	
3	P	9	
3	Q	9	
3	R	9	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33463 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			

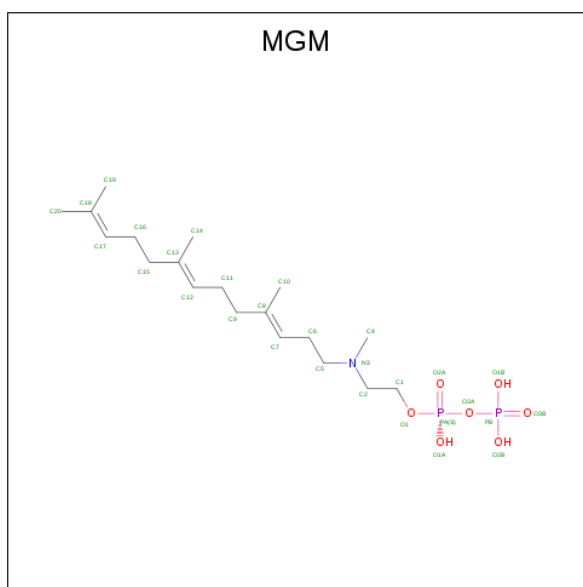
- Molecule 3 is a protein called Transforming protein RhoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	S	0	0	0
			45	27	8	8	2			
3	N	6	Total	C	N	O	S	0	0	0
			45	27	8	8	2			
3	O	6	Total	C	N	O	S	0	0	0
			45	27	8	8	2			
3	P	6	Total	C	N	O	S	0	0	0
			45	27	8	8	2			
3	Q	6	Total	C	N	O	S	0	0	0
			45	27	8	8	2			
3	R	6	Total	C	N	O	S	0	0	0
			45	27	8	8	2			

- 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: C₁₉H₃₇NO₇P₂).

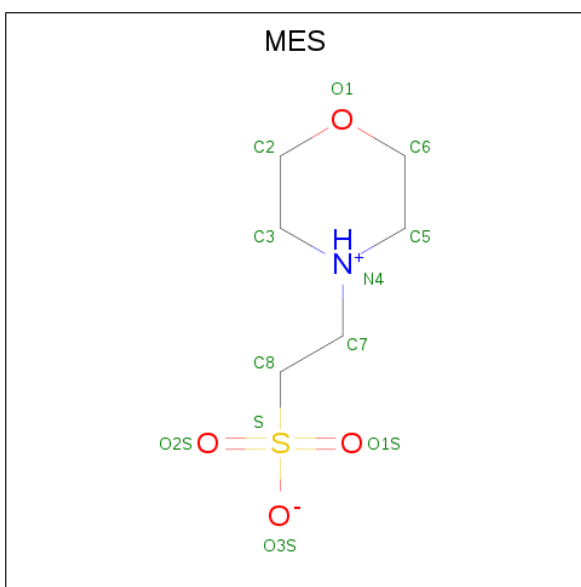


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	D	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	F	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	H	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	J	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	L	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

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

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

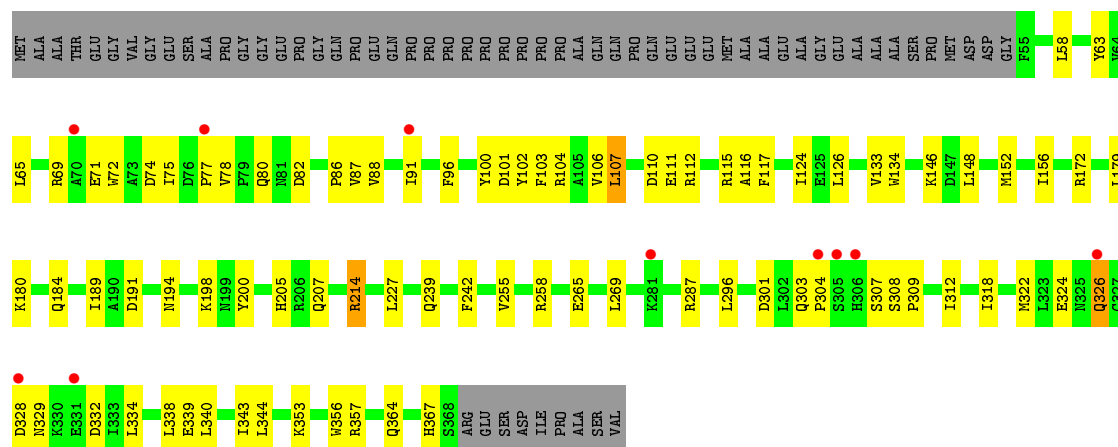
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	46	Total	O	0	0
			46	46		
8	B	44	Total	O	0	0
			44	44		
8	C	48	Total	O	0	0
			48	48		
8	D	81	Total	O	0	0
			81	81		
8	E	52	Total	O	0	0
			52	52		
8	F	80	Total	O	0	0
			80	80		
8	G	51	Total	O	0	0
			51	51		
8	H	45	Total	O	0	0
			45	45		
8	I	68	Total	O	0	0
			68	68		
8	J	47	Total	O	0	0
			47	47		
8	K	135	Total	O	0	0
			135	135		

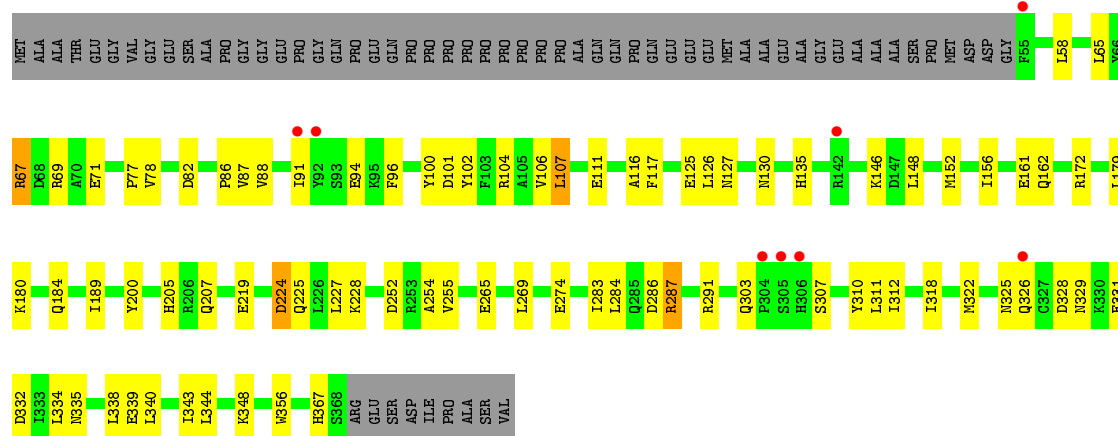
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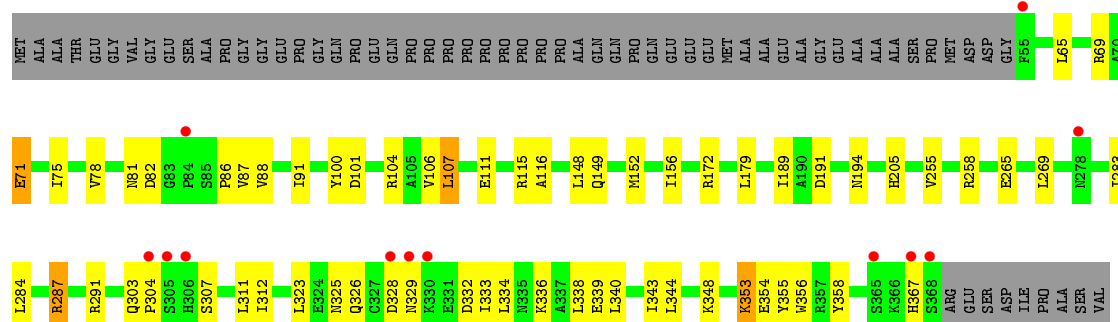
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	103	Total 103	O 103	0	0
8	M	7	Total 7	O 7	0	0
8	N	2	Total 2	O 2	0	0
8	O	3	Total 3	O 3	0	0
8	P	4	Total 4	O 4	0	0
8	Q	3	Total 3	O 3	0	0
8	R	3	Total 3	O 3	0	0



- Molecule 1: geranylgeranyltransferase type I alpha subunit

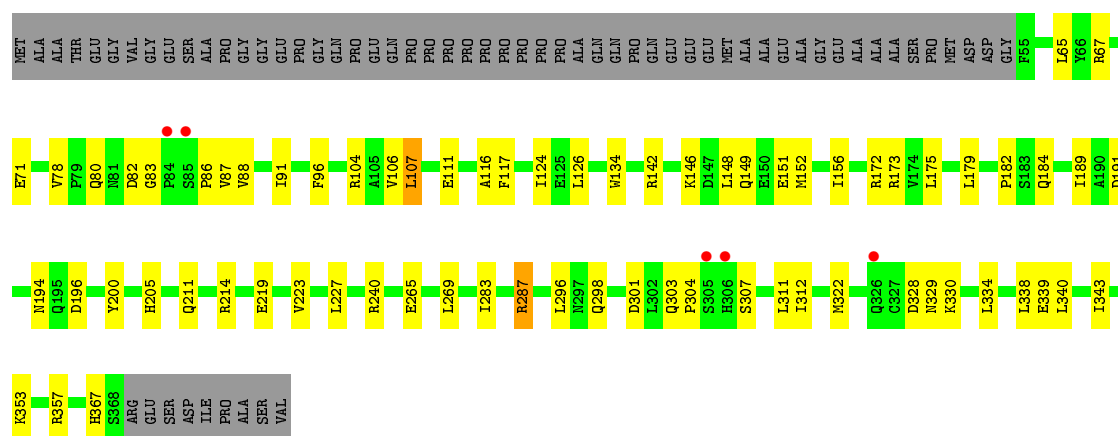


- Molecule 1: geranylgeranyltransferase type I alpha subunit

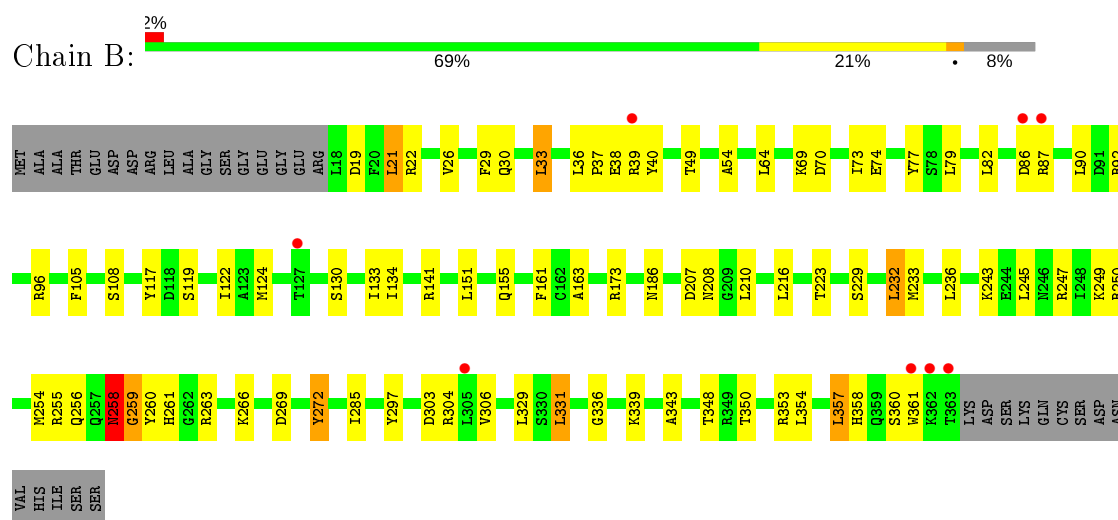


- Molecule 1: geranylgeranyltransferase type I alpha subunit

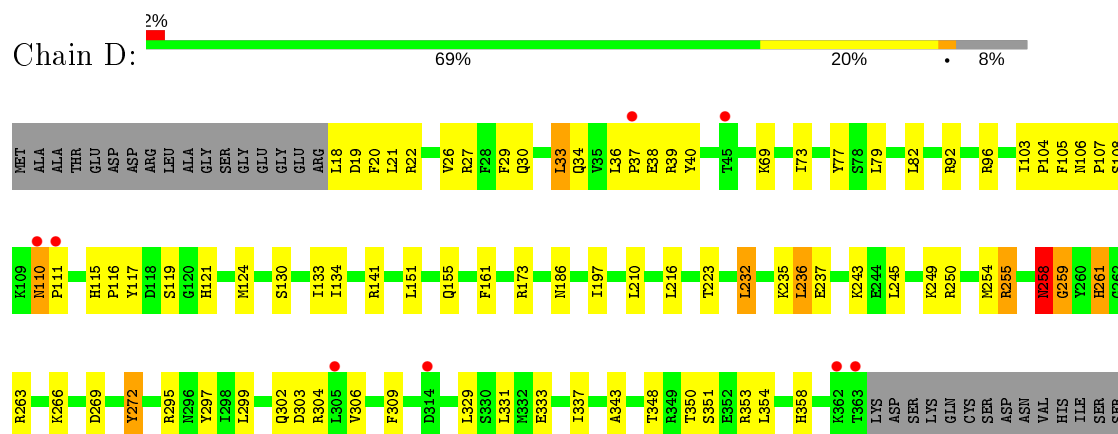




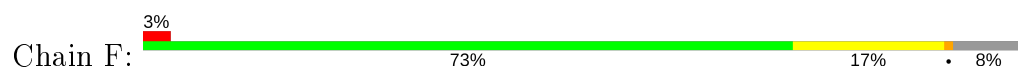
• Molecule 2: Geranylgeranyl transferase type I beta subunit

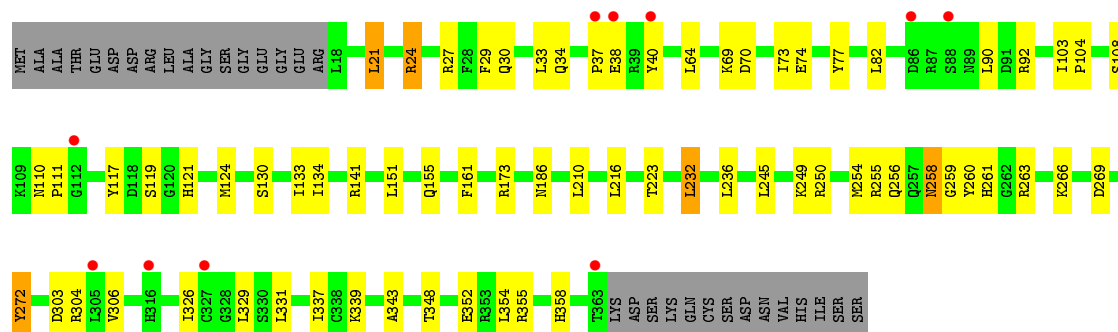


• Molecule 2: Geranylgeranyl transferase type I beta subunit

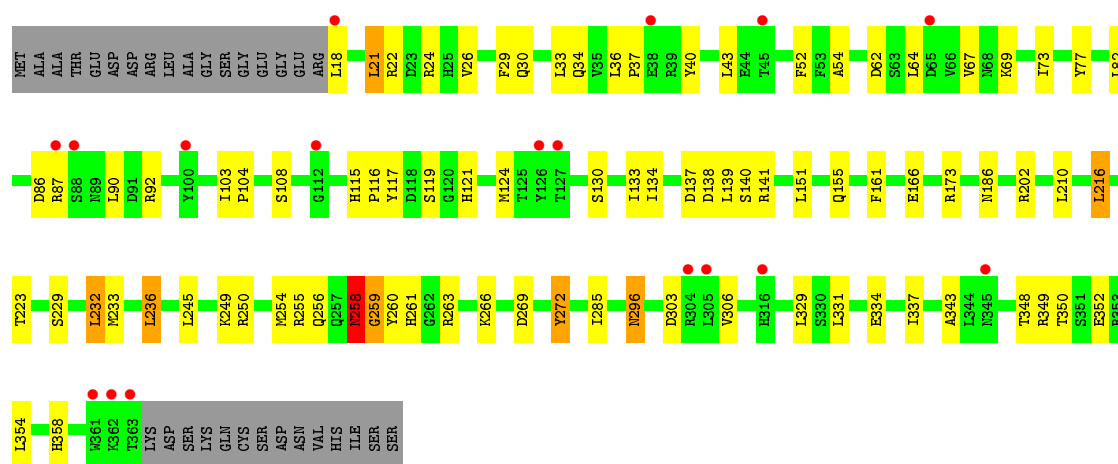


• Molecule 2: Geranylgeranyl transferase type I beta subunit

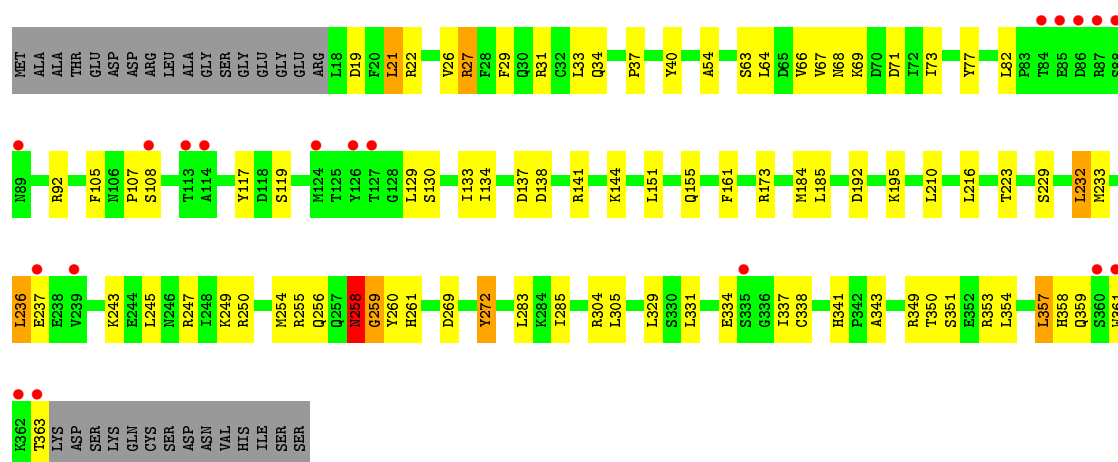




• Molecule 2: Geranylgeranyl transferase type I beta subunit

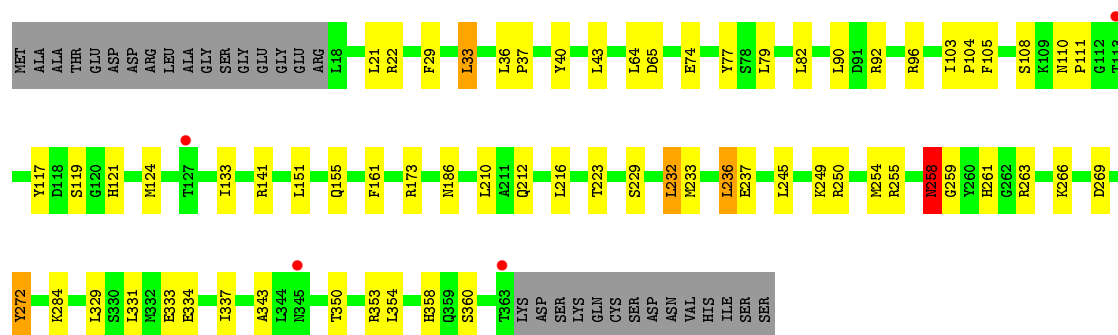


• Molecule 2: Geranylgeranyl transferase type I beta subunit

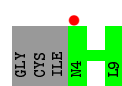


• Molecule 2: Geranylgeranyl transferase type I beta subunit

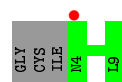




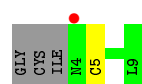
- Molecule 3: Transforming protein RhoB



- Molecule 3: Transforming protein RhoB



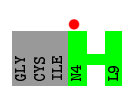
- Molecule 3: Transforming protein RhoB



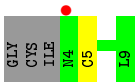
- Molecule 3: Transforming protein RhoB



- Molecule 3: Transforming protein RhoB



- Molecule 3: Transforming protein RhoB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	270.36Å 266.55Å 184.82Å 90.00° 131.58° 90.00°	Depositor
Resolution (Å)	29.94 – 2.70 30.09 – 2.61	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.94-2.70) 88.9 (30.09-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.212 0.172 , 0.191	Depositor DCC
R_{free} test set	10738 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.079 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33463	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: 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	0.37	0/2721	0.54	0/3698
1	E	0.36	0/2730	0.53	0/3710
1	G	0.37	0/2717	0.53	0/3692
1	I	0.36	0/2714	0.53	0/3690
1	K	0.40	0/2741	0.55	0/3722
2	B	0.37	0/2765	0.59	2/3741 (0.1%)
2	D	0.38	0/2768	0.60	2/3743 (0.1%)
2	F	0.39	0/2779	0.61	2/3757 (0.1%)
2	H	0.36	0/2755	0.59	2/3727 (0.1%)
2	J	0.37	0/2769	0.60	2/3744 (0.1%)
2	L	0.40	0/2781	0.62	2/3759 (0.1%)
3	M	0.43	0/44	0.54	0/56
3	N	0.39	0/44	0.56	0/56
3	O	0.43	0/44	0.58	0/56
3	P	0.41	0/44	0.58	0/56
3	Q	0.47	0/44	0.57	0/56
3	R	0.39	0/44	0.61	0/56
All	All	0.37	0/33206	0.57	12/44996 (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	2
2	F	0	1
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	D	258	ASN	N-CA-C	-5.70	95.62	111.00
2	J	259	GLY	N-CA-C	-5.67	98.92	113.10
2	H	259	GLY	N-CA-C	-5.67	98.92	113.10
2	D	259	GLY	N-CA-C	-5.66	98.96	113.10
2	L	259	GLY	N-CA-C	-5.64	99.01	113.10
2	B	259	GLY	N-CA-C	-5.57	99.18	113.10
2	F	259	GLY	N-CA-C	-5.56	99.20	113.10
2	B	258	ASN	N-CA-C	-5.51	96.11	111.00
2	F	258	ASN	N-CA-C	-5.51	96.12	111.00
2	L	258	ASN	N-CA-C	-5.51	96.12	111.00
2	H	258	ASN	N-CA-C	-5.49	96.18	111.00
2	J	258	ASN	N-CA-C	-5.47	96.22	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	D	297	TYR	Sidechain
2	F	272	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	74	1
1	C	2655	0	2562	52	1
1	E	2664	0	2570	63	0
1	G	2651	0	2563	57	0
1	I	2648	0	2547	50	0
1	K	2675	0	2594	54	0
2	B	2703	0	2606	60	0
2	D	2706	0	2616	53	0
2	F	2717	0	2635	44	0
2	H	2694	0	2589	62	0
2	J	2708	0	2613	57	0
2	L	2719	0	2639	38	0
3	M	45	0	47	0	0
3	N	45	0	47	0	0
3	O	45	0	47	1	0
3	P	45	0	47	1	0
3	Q	45	0	47	0	0
3	R	45	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	1	0
5	F	29	0	34	3	0
5	H	29	0	34	2	0
5	J	29	0	34	1	0
5	L	29	0	34	2	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	46	0	0	3	0
8	B	44	0	0	0	0
8	C	48	0	0	0	0
8	D	81	0	0	0	0
8	E	52	0	0	1	0
8	F	80	0	0	1	0
8	G	51	0	0	1	0
8	H	45	0	0	0	0
8	I	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	47	0	0	0	0
8	K	135	0	0	5	0
8	L	103	0	0	1	0
8	M	7	0	0	0	0
8	N	2	0	0	0	0
8	O	3	0	0	1	0
8	P	4	0	0	1	0
8	Q	3	0	0	0	0
8	R	3	0	0	1	0
All	All	33463	0	31559	642	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (642) 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:E:156:ILE:HG12	1:E:172:ARG:HH12	1.05	1.16
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.06	1.15
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.06	1.13
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.97	1.08
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.13	1.07
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.13	1.03
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.19	1.02
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.82	0.94
1:E:255:VAL:HG13	1:E:258:ARG:NH2	1.81	0.94
2:F:352:GLU:HG2	2:F:355:ARG:HH12	1.35	0.90
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.91	0.86
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.90	0.85
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.91	0.85
1:C:353:LYS:HE3	1:K:339:GLU:HG3	1.59	0.84
1:I:156:ILE:CG1	1:I:172:ARG:HH12	1.93	0.80
1:A:348:LYS:HA	1:A:348:LYS:HE2	1.64	0.79
1:I:353:LYS:HG2	1:I:354:GLU:N	1.97	0.79
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.93	0.78
1:A:152:MET:O	1:A:156:ILE:HG13	1.83	0.78
1:G:152:MET:O	1:G:156:ILE:HG13	1.85	0.77
1:G:65:LEU:HD12	1:G:67:ARG:NH1	2.00	0.77
1:K:152:MET:O	1:K:156:ILE:HG13	1.84	0.77
2:H:348:THR:O	2:H:352:GLU:HG2	1.85	0.77
1:I:152:MET:O	1:I:156:ILE:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.68	0.76
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.69	0.75
1:A:339:GLU:O	1:A:343:ILE:HG13	1.88	0.74
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.70	0.73
3:R:5:CYS:HB2	8:R:748:HOH:O	1.86	0.73
1:E:152:MET:O	1:E:156:ILE:HG13	1.89	0.72
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.71	0.72
1:C:339:GLU:O	1:C:343:ILE:HG13	1.90	0.71
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.70	0.71
1:K:91:ILE:O	1:K:91:ILE:HD12	1.91	0.71
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.02	0.70
2:H:69:LYS:O	2:H:73:ILE:HG13	1.91	0.70
1:E:82:ASP:HB2	1:E:86:PRO:HB3	1.72	0.70
1:G:252:ASP:OD2	1:G:255:VAL:HG23	1.92	0.70
1:I:91:ILE:HD12	1:I:91:ILE:O	1.90	0.70
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.74	0.69
2:F:339:LYS:O	2:F:348:THR:HG23	1.92	0.69
1:A:91:ILE:O	1:A:91:ILE:HD12	1.92	0.69
1:C:152:MET:O	1:C:156:ILE:HG13	1.91	0.69
1:C:78:VAL:HG21	1:C:108:GLN:NE2	2.08	0.69
2:B:87:ARG:HH12	2:B:90:LEU:HD11	1.58	0.68
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.74	0.68
1:A:287:ARG:O	1:A:291:ARG:HD3	1.93	0.68
2:D:37:PRO:HB2	2:D:39:ARG:HG2	1.76	0.68
1:G:339:GLU:O	1:G:343:ILE:HG13	1.94	0.68
2:J:359:GLN:HA	2:J:359:GLN:NE2	2.08	0.68
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.23	0.68
1:E:339:GLU:O	1:E:343:ILE:HG13	1.94	0.68
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.76	0.68
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.76	0.68
2:B:26:VAL:O	2:B:30:GLN:HG3	1.93	0.68
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.28	0.67
1:E:91:ILE:O	1:E:91:ILE:HD12	1.95	0.67
1:C:329:ASN:HB3	1:C:332:ASP:HB3	1.76	0.67
2:J:359:GLN:HA	2:J:359:GLN:HE21	1.59	0.67
1:G:91:ILE:HD12	1:G:91:ILE:O	1.95	0.66
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.78	0.66
1:I:339:GLU:O	1:I:343:ILE:HG13	1.96	0.66
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.77	0.66
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.77	0.66
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:ASN:HB3	2:F:111:PRO:HD2	1.78	0.65
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.78	0.65
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.31	0.65
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.62	0.65
3:O:5:CYS:HB2	8:O:755:HOH:O	1.97	0.65
2:B:69:LYS:O	2:B:73:ILE:HG13	1.98	0.64
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.80	0.64
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.79	0.64
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.62	0.63
1:E:329:ASN:HB3	1:E:332:ASP:HB3	1.78	0.63
1:C:91:ILE:HD12	1:C:91:ILE:O	1.99	0.63
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.80	0.63
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.34	0.62
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.79	0.62
2:H:229:SER:O	2:H:233:MET:HG3	1.99	0.62
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.81	0.62
2:D:69:LYS:O	2:D:73:ILE:HG13	1.99	0.62
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.65	0.62
1:A:184:GLN:HG3	8:A:379:HOH:O	1.99	0.62
1:K:156:ILE:HD11	1:K:184:GLN:HE21	1.64	0.62
1:G:100:TYR:O	1:G:104:ARG:HG3	2.00	0.61
1:A:258:ARG:HH11	1:A:258:ARG:HB3	1.66	0.61
1:C:303:GLN:O	1:C:307:SER:HB2	2.00	0.61
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.82	0.61
1:G:156:ILE:HG12	1:G:172:ARG:NH1	1.99	0.61
1:G:334:LEU:HD22	1:G:367:HIS:O	1.99	0.61
2:D:303:ASP:OD1	2:D:306:VAL:HG13	1.99	0.61
1:K:339:GLU:O	1:K:343:ILE:HG13	1.98	0.61
2:H:296:ASN:HD22	2:H:296:ASN:C	2.03	0.61
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.83	0.61
1:A:283:ILE:O	1:A:287:ARG:HD3	2.00	0.61
2:H:18:LEU:N	2:H:18:LEU:HD22	2.16	0.61
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.36	0.61
2:F:69:LYS:O	2:F:73:ILE:HG13	2.01	0.60
1:G:252:ASP:OD2	1:G:254:ALA:HB3	2.01	0.60
2:D:354:LEU:HD11	2:D:358:HIS:NE2	2.17	0.60
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.84	0.60
2:F:30:GLN:HG2	8:F:456:HOH:O	2.02	0.60
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.84	0.59
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.84	0.59
1:I:107:LEU:HD22	2:J:117:TYR:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:351:SER:O	2:J:354:LEU:HB3	2.03	0.59
2:B:229:SER:O	2:B:233:MET:HG3	2.02	0.59
1:I:328:ASP:O	1:I:329:ASN:HB2	2.02	0.59
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.85	0.59
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.66	0.59
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.84	0.59
1:G:65:LEU:HD12	1:G:67:ARG:HH12	1.65	0.59
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.84	0.59
1:A:303:GLN:O	1:A:307:SER:HB2	2.02	0.58
1:A:255:VAL:HG13	1:A:258:ARG:HH12	1.68	0.58
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.85	0.58
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.68	0.58
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.04	0.58
2:J:269:ASP:HB3	2:J:272:TYR:HD2	1.69	0.58
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.84	0.58
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.38	0.58
1:K:334:LEU:HD22	1:K:367:HIS:O	2.03	0.58
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.68	0.58
1:C:328:ASP:O	1:C:329:ASN:HB2	2.03	0.58
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.67	0.58
1:E:334:LEU:HD22	1:E:367:HIS:O	2.02	0.58
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.84	0.58
1:A:258:ARG:NH1	1:A:258:ARG:HB3	2.19	0.58
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.19	0.58
1:I:334:LEU:HD22	1:I:367:HIS:O	2.04	0.58
2:J:144:LYS:HG2	2:J:185:LEU:HD22	1.86	0.58
2:F:269:ASP:HB3	2:F:272:TYR:HD2	1.69	0.58
2:H:349:ARG:O	2:H:352:GLU:HB2	2.04	0.58
1:I:303:GLN:HB3	1:I:304:PRO:HD3	1.86	0.58
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.69	0.57
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.92	0.57
1:K:330:LYS:HE3	1:K:367:HIS:HB3	1.86	0.57
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.85	0.57
1:E:301:ASP:O	1:E:304:PRO:HD2	2.04	0.57
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.70	0.57
1:A:214:ARG:O	1:A:214:ARG:HG3	2.04	0.57
1:C:334:LEU:HD22	1:C:367:HIS:O	2.04	0.57
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.39	0.57
1:G:287:ARG:O	1:G:291:ARG:HD3	2.04	0.57
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.86	0.57
2:F:303:ASP:OD1	2:F:306:VAL:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:TYR:O	1:I:104:ARG:HG3	2.04	0.57
1:E:318:ILE:HG22	1:E:322:MET:HE2	1.85	0.57
1:E:78:VAL:O	1:E:104:ARG:HD2	2.04	0.57
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.40	0.57
1:E:100:TYR:O	1:E:104:ARG:HG3	2.05	0.57
1:A:78:VAL:O	1:A:104:ARG:HD2	2.05	0.56
2:B:269:ASP:HB3	2:B:272:TYR:HD2	1.70	0.56
1:E:214:ARG:O	1:E:214:ARG:HG3	2.03	0.56
1:G:303:GLN:O	1:G:307:SER:HB2	2.05	0.56
2:H:245:LEU:O	2:H:249:LYS:HG3	2.05	0.56
1:A:265:GLU:O	1:A:269:LEU:HD13	2.05	0.56
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.40	0.56
2:H:210:LEU:HB2	2:H:223:THR:HA	1.86	0.56
1:I:340:LEU:HD23	1:I:343:ILE:HD12	1.87	0.56
2:H:133:ILE:HG22	2:H:350:THR:HG23	1.87	0.56
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.86	0.56
1:E:340:LEU:HD23	1:E:343:ILE:HD12	1.87	0.56
1:G:67:ARG:NH2	1:G:94:GLU:OE1	2.39	0.56
1:A:255:VAL:HA	1:A:258:ARG:NH1	2.21	0.56
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.36	0.56
1:A:287:ARG:HG3	1:A:292:TYR:OH	2.05	0.56
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.88	0.56
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.40	0.55
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.88	0.55
1:A:255:VAL:HA	1:A:258:ARG:HH12	1.71	0.55
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.88	0.55
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.72	0.55
2:L:269:ASP:HB3	2:L:272:TYR:HD2	1.70	0.55
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.88	0.55
2:D:354:LEU:HD11	2:D:358:HIS:HE2	1.72	0.55
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.42	0.55
2:D:210:LEU:HB2	2:D:223:THR:HA	1.88	0.54
1:E:303:GLN:O	1:E:307:SER:HB2	2.07	0.54
2:J:258:ASN:OD1	2:J:259:GLY:N	2.35	0.54
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.42	0.54
2:L:210:LEU:HB2	2:L:223:THR:HA	1.89	0.54
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.73	0.54
1:E:265:GLU:O	1:E:269:LEU:HD13	2.08	0.54
2:J:210:LEU:HB2	2:J:223:THR:HA	1.88	0.54
2:L:133:ILE:HG22	2:L:350:THR:HG23	1.89	0.54
1:A:107:LEU:HD22	2:B:117:TYR:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:O	1:A:329:ASN:HB2	2.07	0.54
1:A:334:LEU:HD22	1:A:367:HIS:O	2.07	0.54
1:C:78:VAL:O	1:C:104:ARG:HD2	2.08	0.54
1:C:156:ILE:CG1	1:C:172:ARG:HH12	2.06	0.54
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.89	0.54
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.89	0.54
1:K:265:GLU:O	1:K:269:LEU:HD13	2.08	0.54
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.73	0.54
2:F:339:LYS:NZ	2:F:339:LYS:HB3	2.23	0.54
2:J:358:HIS:O	2:J:361:TRP:HB2	2.08	0.54
1:A:191:ASP:O	1:A:194:ASN:HB2	2.08	0.54
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.43	0.54
1:A:296:LEU:HD22	1:A:322:MET:HE3	1.91	0.53
2:F:210:LEU:HB2	2:F:223:THR:HA	1.88	0.53
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.72	0.53
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.43	0.53
1:G:82:ASP:HB2	1:G:86:PRO:HB3	1.90	0.53
2:J:359:GLN:CA	2:J:359:GLN:HE21	2.17	0.53
1:A:303:GLN:HB3	1:A:304:PRO:HD3	1.89	0.53
1:C:214:ARG:HG2	1:C:214:ARG:O	2.08	0.53
2:D:269:ASP:HB3	2:D:272:TYR:HD2	1.72	0.53
2:H:269:ASP:HB3	2:H:272:TYR:HD2	1.72	0.53
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.44	0.53
1:I:78:VAL:O	1:I:104:ARG:HD2	2.08	0.53
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.43	0.53
1:I:82:ASP:HB2	1:I:86:PRO:HB3	1.91	0.53
1:K:303:GLN:O	1:K:307:SER:HB2	2.09	0.53
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.44	0.53
1:C:78:VAL:HG21	1:C:108:GLN:HE22	1.73	0.53
1:G:156:ILE:CG1	1:G:172:ARG:HH12	2.03	0.53
1:C:287:ARG:O	1:C:291:ARG:HD3	2.09	0.52
1:I:106:VAL:HG13	1:I:111:GLU:HB3	1.91	0.52
2:B:29:PHE:O	2:B:33:LEU:HD22	2.09	0.52
2:D:82:LEU:HD11	2:D:108:SER:HA	1.92	0.52
1:E:353:LYS:NZ	1:E:357:ARG:HH12	2.07	0.52
1:I:283:ILE:O	1:I:287:ARG:HD3	2.10	0.52
1:A:252:ASP:OD2	1:A:255:VAL:HG23	2.09	0.52
2:H:303:ASP:OD1	2:H:306:VAL:HG13	2.09	0.52
1:G:265:GLU:O	1:G:269:LEU:HD13	2.10	0.52
1:I:255:VAL:HG13	1:I:258:ARG:NH2	2.25	0.52
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:LYS:O	2:B:348:THR:HG23	2.09	0.52
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.10	0.52
2:D:353:ARG:O	2:D:353:ARG:HD2	2.10	0.52
1:E:106:VAL:HG13	1:E:111:GLU:HB3	1.92	0.52
1:G:224:ASP:O	1:G:228:LYS:HG3	2.09	0.52
1:I:323:LEU:HB3	1:I:367:HIS:CD2	2.45	0.52
2:J:22:ARG:O	2:J:26:VAL:HG23	2.09	0.52
1:G:328:ASP:O	1:G:329:ASN:HB2	2.09	0.52
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.52
1:A:71:GLU:CD	1:A:71:GLU:H	2.13	0.51
1:E:107:LEU:HD22	2:F:117:TYR:CD2	2.45	0.51
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.45	0.51
2:F:70:ASP:O	2:F:74:GLU:HG2	2.10	0.51
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.92	0.51
2:B:210:LEU:HB2	2:B:223:THR:HA	1.91	0.51
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.26	0.51
2:H:138:ASP:OD1	2:H:140:SER:HB3	2.11	0.51
1:E:74:ASP:OD1	1:E:75:ILE:HG12	2.11	0.51
1:E:326:GLN:N	1:E:326:GLN:HE21	2.09	0.51
2:F:24:ARG:HB2	2:F:24:ARG:HH11	1.76	0.51
1:G:106:VAL:HG13	1:G:111:GLU:HB3	1.93	0.51
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.83	0.51
1:A:284:LEU:O	1:A:287:ARG:HG2	2.11	0.50
2:B:82:LEU:HD11	2:B:108:SER:HA	1.92	0.50
2:B:22:ARG:NH1	2:B:22:ARG:HG2	2.26	0.50
1:E:207:GLN:HG2	1:E:242:PHE:CE2	2.47	0.50
1:K:357:ARG:HD2	8:K:433:HOH:O	2.11	0.50
1:C:265:GLU:O	1:C:269:LEU:HD13	2.11	0.50
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.26	0.50
2:F:352:GLU:CG	2:F:355:ARG:HH12	2.17	0.50
1:I:69:ARG:HB3	1:I:71:GLU:OE1	2.12	0.50
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.92	0.50
1:A:261:GLN:O	1:A:265:GLU:HG2	2.12	0.50
1:C:283:ILE:O	1:C:287:ARG:HD3	2.12	0.50
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.92	0.50
2:B:258:ASN:OD1	2:B:259:GLY:N	2.39	0.49
2:D:245:LEU:O	2:D:249:LYS:HG3	2.12	0.49
2:L:82:LEU:HD11	2:L:108:SER:HA	1.94	0.49
2:J:64:LEU:O	2:J:67:VAL:HG22	2.12	0.49
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.47	0.49
1:K:184:GLN:HG2	8:K:384:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:GLN:CA	1:E:326:GLN:HE21	2.24	0.49
1:G:334:LEU:O	1:G:338:LEU:HG	2.13	0.49
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.47	0.49
1:K:283:ILE:O	1:K:287:ARG:HD3	2.12	0.49
1:K:301:ASP:O	1:K:304:PRO:HD2	2.13	0.49
2:B:250:ARG:O	2:B:254:MET:HG2	2.11	0.49
1:I:284:LEU:O	1:I:287:ARG:HG2	2.12	0.49
2:D:115:HIS:ND1	2:D:116:PRO:HD2	2.27	0.49
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.95	0.49
1:E:110:ASP:OD2	1:E:112:ARG:NE	2.34	0.49
2:L:79:LEU:O	2:L:96:ARG:HG3	2.12	0.49
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.48	0.49
1:G:311:LEU:HD23	1:G:311:LEU:C	2.33	0.49
2:H:258:ASN:OD1	2:H:259:GLY:N	2.39	0.49
2:B:245:LEU:O	2:B:249:LYS:HG3	2.13	0.49
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.48	0.48
1:E:318:ILE:HG22	1:E:322:MET:CE	2.42	0.48
2:F:30:GLN:O	2:F:34:GLN:HG3	2.12	0.48
1:I:265:GLU:O	1:I:269:LEU:HD13	2.12	0.48
2:J:27:ARG:HH11	2:J:27:ARG:HG3	1.78	0.48
2:L:353:ARG:HD2	2:L:353:ARG:O	2.12	0.48
1:A:106:VAL:HG13	1:A:111:GLU:HB3	1.95	0.48
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.48	0.48
2:F:92:ARG:HB3	2:F:119:SER:CB	2.43	0.48
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.29	0.48
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.48
2:H:296:ASN:C	2:H:296:ASN:ND2	2.67	0.48
1:I:303:GLN:O	1:I:307:SER:HB2	2.13	0.48
2:D:155:GLN:HB2	2:D:161:PHE:CE2	2.48	0.48
2:F:29:PHE:O	2:F:33:LEU:HD22	2.12	0.48
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.49	0.48
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.49	0.48
1:I:191:ASP:O	1:I:194:ASN:HB2	2.13	0.48
1:E:156:ILE:HD11	1:E:172:ARG:HH22	1.79	0.48
2:L:37:PRO:HD2	2:L:40:TYR:CD1	2.49	0.48
1:A:91:ILE:HD11	2:B:38:GLU:H	1.78	0.48
2:F:326:ILE:HG23	2:F:337:ILE:HD13	1.94	0.48
2:H:130:SER:O	2:H:134:ILE:HG13	2.14	0.48
2:J:229:SER:O	2:J:233:MET:HG3	2.13	0.48
1:G:283:ILE:O	1:G:287:ARG:HD3	2.14	0.48
1:C:92:TYR:O	1:C:97:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82:LEU:HD11	2:H:108:SER:HA	1.96	0.47
2:J:82:LEU:HD11	2:J:108:SER:HA	1.96	0.47
2:F:155:GLN:HB2	2:F:161:PHE:CE2	2.50	0.47
1:G:78:VAL:O	1:G:104:ARG:HD2	2.14	0.47
2:B:155:GLN:HB2	2:B:161:PHE:CE2	2.49	0.47
2:D:110:ASN:HB3	2:D:111:PRO:HD2	1.97	0.47
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.97	0.47
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.80	0.47
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.49	0.47
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.48	0.47
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.15	0.47
2:H:29:PHE:O	2:H:33:LEU:HD22	2.15	0.47
2:J:130:SER:O	2:J:134:ILE:HG13	2.15	0.47
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.44	0.47
1:A:214:ARG:O	1:A:214:ARG:CG	2.62	0.47
1:G:77:PRO:HB3	1:G:102:TYR:CE1	2.50	0.47
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.15	0.47
1:I:106:VAL:HG11	1:I:116:ALA:HB1	1.97	0.47
2:J:133:ILE:CD1	2:J:354:LEU:HD13	2.43	0.47
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.96	0.47
2:B:130:SER:O	2:B:134:ILE:HG13	2.14	0.47
1:I:106:VAL:HG11	1:I:116:ALA:CB	2.45	0.47
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.50	0.47
1:K:191:ASP:O	1:K:194:ASN:HB2	2.15	0.47
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.80	0.47
1:C:107:LEU:HD22	2:D:117:TYR:CD2	2.50	0.47
1:C:219:GLU:HA	1:C:219:GLU:OE1	2.15	0.47
2:D:79:LEU:O	2:D:96:ARG:HG3	2.14	0.47
2:H:21:LEU:HD23	2:H:24:ARG:HD2	1.97	0.47
2:H:33:LEU:HD22	2:H:54:ALA:HB1	1.96	0.47
2:J:27:ARG:NH1	2:J:27:ARG:HG3	2.29	0.47
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.50	0.47
1:A:334:LEU:O	1:A:338:LEU:HG	2.14	0.47
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.50	0.47
2:D:173:ARG:HG2	5:D:380:MGM:H112	1.96	0.47
2:D:130:SER:O	2:D:134:ILE:HG13	2.15	0.46
1:E:106:VAL:HG11	1:E:116:ALA:HB1	1.97	0.46
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.50	0.46
1:A:296:LEU:HD12	1:A:296:LEU:O	2.16	0.46
2:B:258:ASN:CG	2:B:259:GLY:H	2.18	0.46
2:B:303:ASP:OD1	2:B:306:VAL:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:ASP:N	2:H:86:ASP:OD2	2.41	0.46
1:I:255:VAL:HG13	1:I:258:ARG:HH21	1.79	0.46
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.98	0.46
2:F:245:LEU:O	2:F:249:LYS:HG3	2.15	0.46
1:I:75:ILE:CG1	1:I:115:ARG:NH2	2.79	0.46
2:L:29:PHE:O	2:L:33:LEU:HD22	2.16	0.46
1:C:106:VAL:HG13	1:C:111:GLU:HB3	1.97	0.46
2:D:77:TYR:CE1	2:D:141:ARG:HB2	2.50	0.46
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.50	0.46
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.97	0.46
2:H:64:LEU:O	2:H:67:VAL:HG22	2.16	0.46
1:I:325:ASN:O	1:I:326:GLN:C	2.54	0.46
1:A:105:ALA:O	1:A:109:ARG:HG3	2.16	0.46
1:C:112:ARG:O	1:C:144:LEU:HD21	2.15	0.46
1:C:311:LEU:HD23	1:C:311:LEU:C	2.36	0.46
2:F:339:LYS:NZ	2:F:339:LYS:CB	2.79	0.46
2:J:21:LEU:HD11	2:J:304:ARG:NH2	2.30	0.46
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.50	0.46
2:B:207:ASP:O	2:B:208:ASN:HB2	2.16	0.46
2:D:302:GLN:HB2	2:D:309:PHE:CE2	2.51	0.46
1:E:106:VAL:HG11	1:E:116:ALA:CB	2.46	0.46
2:F:250:ARG:O	2:F:254:MET:HG2	2.15	0.46
1:I:100:TYR:C	1:I:104:ARG:NH1	2.69	0.46
1:K:219:GLU:OE1	1:K:219:GLU:HA	2.16	0.46
1:C:138:ARG:O	1:C:142:ARG:HG3	2.16	0.46
2:D:29:PHE:O	2:D:33:LEU:HD22	2.16	0.46
1:E:100:TYR:C	1:E:104:ARG:NH1	2.69	0.46
1:I:311:LEU:C	1:I:311:LEU:HD23	2.36	0.46
2:J:33:LEU:CD2	2:J:54:ALA:HB1	2.46	0.46
2:J:92:ARG:HB3	2:J:119:SER:CB	2.45	0.46
1:C:232:ARG:NH2	1:C:272:HIS:O	2.49	0.46
2:D:30:GLN:O	2:D:34:GLN:HG3	2.16	0.46
1:E:214:ARG:O	1:E:214:ARG:CG	2.64	0.46
2:F:82:LEU:HD11	2:F:108:SER:HA	1.96	0.46
1:A:92:TYR:O	1:A:97:ARG:NH2	2.48	0.46
2:B:70:ASP:O	2:B:74:GLU:HG2	2.15	0.46
1:C:296:LEU:HD22	1:C:322:MET:HE3	1.98	0.46
2:H:250:ARG:O	2:H:254:MET:HG2	2.17	0.46
2:H:133:ILE:HD13	2:H:354:LEU:HD13	1.97	0.46
2:B:92:ARG:HB3	2:B:119:SER:CB	2.47	0.45
2:D:105:PHE:CE2	2:D:107:PRO:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:SER:O	2:F:134:ILE:HG13	2.15	0.45
2:H:249:LYS:HB3	2:H:285:ILE:HD13	1.98	0.45
1:I:333:ILE:HA	1:I:336:LYS:HG3	1.98	0.45
1:I:81:ASN:HD21	2:J:105:PHE:H	1.64	0.45
2:J:133:ILE:HG22	2:J:350:THR:CG2	2.46	0.45
1:G:58:LEU:HB2	1:G:125:GLU:OE2	2.16	0.45
2:H:137:ASP:OD1	2:H:139:LEU:N	2.41	0.45
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.51	0.45
2:J:105:PHE:CE2	2:J:107:PRO:HD3	2.51	0.45
1:A:274:GLU:HG2	1:A:278:ASN:HD21	1.81	0.45
1:E:334:LEU:O	1:E:338:LEU:HG	2.16	0.45
1:I:287:ARG:O	1:I:291:ARG:HD3	2.17	0.45
2:D:92:ARG:HB3	2:D:119:SER:CB	2.45	0.45
1:E:296:LEU:HD22	1:E:322:MET:CE	2.46	0.45
2:H:52:PHE:HE1	2:H:130:SER:HG	1.64	0.45
2:J:77:TYR:HE2	2:J:137:ASP:OD2	2.00	0.45
1:A:301:ASP:O	1:A:304:PRO:HD2	2.17	0.45
2:F:103:ILE:HG23	2:F:104:PRO:HD2	1.98	0.45
2:J:359:GLN:C	2:J:361:TRP:N	2.70	0.45
1:K:328:ASP:O	1:K:329:ASN:HB2	2.17	0.45
2:L:236:LEU:HD22	2:L:245:LEU:HD21	1.99	0.45
1:E:191:ASP:O	1:E:194:ASN:HB2	2.17	0.45
1:G:106:VAL:HG11	1:G:116:ALA:HB1	1.99	0.45
2:J:134:ILE:HG12	2:J:350:THR:HG21	1.99	0.45
2:J:236:LEU:HD22	2:J:245:LEU:HD21	1.97	0.45
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.81	0.45
2:D:250:ARG:O	2:D:254:MET:HG2	2.17	0.45
1:E:200:TYR:CB	5:F:380:MGM:HC12	2.47	0.45
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.82	0.45
1:I:332:ASP:O	1:I:336:LYS:HG3	2.16	0.45
2:B:256:GLN:HB2	2:B:260:TYR:CE2	2.53	0.45
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.82	0.45
2:H:115:HIS:ND1	2:H:116:PRO:HD2	2.31	0.45
2:L:155:GLN:HB2	2:L:161:PHE:CE2	2.52	0.45
2:B:173:ARG:HG2	5:B:379:MGM:H112	1.99	0.44
2:J:359:GLN:C	2:J:361:TRP:H	2.20	0.44
1:A:344:LEU:HA	1:A:348:LYS:HB2	2.00	0.44
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.53	0.44
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.99	0.44
1:I:149:GLN:NE2	1:I:179:LEU:HD13	2.32	0.44
2:J:63:SER:O	2:J:66:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD23	1:A:311:LEU:C	2.37	0.44
2:B:19:ASP:OD2	2:B:19:ASP:N	2.51	0.44
1:G:274:GLU:HG3	1:G:310:TYR:CE2	2.52	0.44
2:H:24:ARG:HG2	2:H:24:ARG:HH11	1.82	0.44
1:K:156:ILE:HD11	1:K:184:GLN:NE2	2.29	0.44
1:A:258:ARG:CB	1:A:258:ARG:HH11	2.27	0.44
1:C:335:ASN:O	1:C:339:GLU:HG3	2.17	0.44
2:F:27:ARG:HA	2:F:30:GLN:HE21	1.82	0.44
1:C:117:PHE:CE2	1:C:146:LYS:HE2	2.52	0.44
1:C:323:LEU:O	1:C:330:LYS:HE3	2.17	0.44
2:J:283:LEU:O	2:J:285:ILE:HG23	2.17	0.44
1:K:106:VAL:HG13	1:K:111:GLU:HB3	1.99	0.44
1:G:107:LEU:HD22	2:H:117:TYR:CD2	2.52	0.44
2:J:129:LEU:HB2	2:J:184:MET:CE	2.48	0.44
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.53	0.44
1:C:65:LEU:O	1:C:69:ARG:HG3	2.17	0.44
2:D:18:LEU:HD12	2:D:304:ARG:NH1	2.32	0.44
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.52	0.44
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.47	0.44
2:J:19:ASP:OD2	2:J:19:ASP:N	2.49	0.44
2:B:232:LEU:HD13	2:B:343:ALA:HB1	1.99	0.44
1:E:328:ASP:O	1:E:329:ASN:HB2	2.18	0.44
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.86	0.44
2:H:77:TYR:CE1	2:H:141:ARG:HB2	2.51	0.44
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.53	0.44
1:G:88:VAL:HG13	2:H:36:LEU:HD11	2.00	0.44
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.82	0.44
1:K:214:ARG:O	1:K:214:ARG:HG2	2.18	0.44
1:I:334:LEU:O	1:I:338:LEU:HG	2.18	0.43
2:J:69:LYS:O	2:J:73:ILE:HG13	2.18	0.43
1:K:173:ARG:HD2	8:K:443:HOH:O	2.18	0.43
2:J:243:LYS:O	2:J:247:ARG:HG3	2.18	0.43
1:K:311:LEU:HD23	1:K:311:LEU:C	2.38	0.43
1:E:200:TYR:HB3	5:F:380:MGM:HC12	1.99	0.43
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.00	0.43
2:D:348:THR:HA	2:D:351:SER:OG	2.19	0.43
2:J:29:PHE:O	2:J:33:LEU:HD22	2.18	0.43
1:A:106:VAL:HG11	1:A:116:ALA:HB1	2.01	0.43
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.54	0.43
2:L:245:LEU:O	2:L:249:LYS:HG3	2.17	0.43
2:L:40:TYR:HB3	2:L:43:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:ILE:HD11	2:D:235:LYS:HD2	1.99	0.43
1:K:200:TYR:CB	5:L:379:MGM:HC12	2.48	0.43
1:A:322:MET:HB3	1:A:327:CYS:SG	2.59	0.43
2:F:263:ARG:HB2	2:F:266:LYS:HG3	2.01	0.43
1:G:286:ASP:HB2	8:G:406:HOH:O	2.17	0.43
1:G:344:LEU:HD13	1:G:356:TRP:CE2	2.54	0.43
2:J:155:GLN:HB2	2:J:161:PHE:CE2	2.53	0.43
2:B:133:ILE:CD1	2:B:354:LEU:HD13	2.47	0.43
2:B:357:LEU:HD22	2:B:361:TRP:NE1	2.33	0.43
1:C:328:ASP:O	1:C:329:ASN:CB	2.67	0.43
1:K:106:VAL:HG11	1:K:116:ALA:HB1	2.01	0.43
2:L:250:ARG:O	2:L:254:MET:HG2	2.19	0.43
1:E:77:PRO:HB3	1:E:102:TYR:CE1	2.54	0.43
1:E:328:ASP:O	1:E:329:ASN:CB	2.67	0.43
1:K:78:VAL:O	1:K:104:ARG:HD2	2.19	0.43
1:A:65:LEU:HD12	1:A:67:ARG:NH1	2.34	0.42
2:B:357:LEU:O	2:B:360:SER:HB2	2.19	0.42
2:F:173:ARG:HG2	5:F:380:MGM:H112	2.01	0.42
1:G:106:VAL:HG11	1:G:116:ALA:CB	2.48	0.42
1:G:227:LEU:HA	1:G:227:LEU:HD23	1.86	0.42
2:H:202:ARG:HG3	2:H:202:ARG:NH1	2.31	0.42
1:I:65:LEU:O	1:I:69:ARG:HG3	2.18	0.42
1:K:353:LYS:HB2	1:K:353:LYS:HE3	1.74	0.42
2:D:22:ARG:HG2	2:D:22:ARG:NH1	2.34	0.42
2:J:245:LEU:O	2:J:249:LYS:HG3	2.19	0.42
1:A:96:PHE:CE1	1:A:126:LEU:HB3	2.55	0.42
2:B:33:LEU:CD2	2:B:54:ALA:HB1	2.50	0.42
2:B:29:PHE:CD2	2:B:54:ALA:HA	2.54	0.42
1:C:91:ILE:HG13	2:D:36:LEU:O	2.19	0.42
2:D:258:ASN:OD1	2:D:259:GLY:N	2.45	0.42
2:H:40:TYR:HB3	2:H:43:LEU:HD12	2.01	0.42
2:J:173:ARG:HG2	5:J:379:MGM:H112	2.00	0.42
1:C:106:VAL:HG11	1:C:116:ALA:HB1	2.01	0.42
2:D:232:LEU:HD13	2:D:343:ALA:HB1	2.01	0.42
1:E:239:GLN:HA	1:E:239:GLN:OE1	2.19	0.42
1:G:318:ILE:HG22	1:G:322:MET:CE	2.50	0.42
1:G:331:GLU:O	1:G:335:ASN:ND2	2.53	0.42
1:A:124:ILE:HD13	1:A:134:TRP:CH2	2.55	0.42
1:A:83:GLY:HA3	2:B:105:PHE:CE1	2.54	0.42
2:B:33:LEU:HD22	2:B:54:ALA:HB1	2.02	0.42
2:D:19:ASP:OD2	2:D:19:ASP:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:ARG:HB2	2:D:266:LYS:HG3	2.01	0.42
1:E:326:GLN:H	1:E:326:GLN:HE21	1.66	0.42
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.55	0.42
1:G:284:LEU:O	1:G:287:ARG:HG2	2.19	0.42
1:K:124:ILE:HD13	1:K:134:TRP:CH2	2.54	0.42
1:K:334:LEU:O	1:K:338:LEU:HG	2.19	0.42
2:L:77:TYR:CE1	2:L:141:ARG:HB2	2.53	0.42
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.86	0.42
2:B:87:ARG:NH1	2:B:90:LEU:HD11	2.31	0.42
1:E:180:LYS:HD3	1:E:180:LYS:HA	1.86	0.42
1:E:91:ILE:HD11	2:F:38:GLU:H	1.83	0.42
2:B:37:PRO:O	2:B:39:ARG:N	2.53	0.42
1:C:124:ILE:HD13	1:C:134:TRP:CH2	2.55	0.42
2:L:92:ARG:HB3	2:L:119:SER:CB	2.49	0.42
1:A:83:GLY:HA3	2:B:105:PHE:CD1	2.54	0.42
2:D:255:ARG:HD3	2:D:261:HIS:CD2	2.54	0.42
1:C:91:ILE:HD11	2:D:38:GLU:H	1.85	0.42
2:F:90:LEU:HD23	2:F:90:LEU:HA	1.90	0.42
2:L:173:ARG:HG2	5:L:379:MGM:H112	2.02	0.42
1:A:106:VAL:HG11	1:A:116:ALA:CB	2.50	0.42
2:D:26:VAL:O	2:D:30:GLN:HG3	2.20	0.42
1:E:124:ILE:HD13	1:E:134:TRP:CH2	2.54	0.42
1:E:65:LEU:O	1:E:69:ARG:HG3	2.19	0.42
2:J:250:ARG:O	2:J:254:MET:HG2	2.19	0.42
1:K:223:VAL:HG11	1:K:240:ARG:HB2	2.00	0.42
1:A:200:TYR:HB3	5:B:379:MGM:HC12	2.02	0.42
2:B:64:LEU:HD23	2:B:64:LEU:HA	1.84	0.42
2:D:186:ASN:HB2	2:D:358:HIS:CE1	2.55	0.42
2:D:236:LEU:HD22	2:D:245:LEU:HD21	2.02	0.42
1:E:308:SER:HB2	1:E:309:PRO:HD2	2.01	0.42
1:I:344:LEU:HA	1:I:348:LYS:HB2	2.01	0.42
2:J:192:ASP:OD1	2:J:195:LYS:HG3	2.20	0.42
1:K:151:GLU:HG3	1:K:175:LEU:HD11	2.01	0.42
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.23	0.42
2:B:122:ILE:HG22	2:B:163:ALA:HA	2.02	0.41
2:B:86:ASP:OD2	2:B:86:ASP:N	2.53	0.41
1:C:58:LEU:HB2	1:C:125:GLU:OE2	2.20	0.41
1:I:258:ARG:HB3	1:I:258:ARG:HE	1.64	0.41
2:J:269:ASP:HB3	2:J:272:TYR:CD2	2.52	0.41
2:L:212:GLN:NE2	2:L:212:GLN:HA	2.35	0.41
2:D:243:LYS:HB3	2:D:243:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:ARG:NH1	2:H:24:ARG:HG2	2.35	0.41
2:H:26:VAL:O	2:H:30:GLN:HG3	2.20	0.41
1:K:296:LEU:HD22	1:K:322:MET:HE3	2.02	0.41
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.34	0.41
1:A:194:ASN:HA	1:A:194:ASN:HD22	1.51	0.41
1:K:196:ASP:HB3	8:K:493:HOH:O	2.20	0.41
1:E:72:TRP:CZ2	1:E:115:ARG:HB2	2.56	0.41
2:F:269:ASP:HB3	2:F:272:TYR:CD2	2.53	0.41
2:L:22:ARG:HG2	2:L:22:ARG:HH11	1.84	0.41
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.55	0.41
2:D:37:PRO:O	2:D:39:ARG:N	2.54	0.41
1:E:227:LEU:HD23	1:E:227:LEU:HA	1.90	0.41
1:G:96:PHE:CE1	1:G:126:LEU:HB3	2.55	0.41
2:J:21:LEU:HD11	2:J:304:ARG:HH22	1.85	0.41
1:A:66:TYR:CE1	1:A:119:LEU:HD13	2.56	0.41
1:A:173:ARG:HD2	8:A:399:HOH:O	2.20	0.41
2:B:243:LYS:O	2:B:247:ARG:HG3	2.20	0.41
2:B:249:LYS:HB3	2:B:285:ILE:HD13	2.03	0.41
2:B:331:LEU:HD12	2:B:331:LEU:HA	1.91	0.41
1:G:219:GLU:OE1	1:G:219:GLU:HA	2.20	0.41
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.86	0.41
2:L:229:SER:O	2:L:233:MET:HG3	2.20	0.41
1:K:91:ILE:HG13	2:L:36:LEU:O	2.21	0.41
1:A:91:ILE:HG13	2:B:36:LEU:O	2.21	0.41
1:E:77:PRO:HB2	1:E:101:ASP:HB3	2.02	0.41
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.35	0.41
1:G:325:ASN:O	1:G:326:GLN:C	2.59	0.41
1:K:65:LEU:HD12	1:K:67:ARG:NH1	2.36	0.41
2:L:333:GLU:HA	8:L:470:HOH:O	2.20	0.41
1:A:104:ARG:NH2	8:A:388:HOH:O	2.53	0.41
1:C:96:PHE:CE1	1:C:126:LEU:HB3	2.56	0.41
1:C:303:GLN:HB3	1:C:304:PRO:HD3	2.03	0.41
2:D:106:ASN:O	2:D:108:SER:N	2.51	0.41
2:F:92:ARG:HB3	2:F:119:SER:HB3	2.02	0.41
2:H:263:ARG:HB2	2:H:266:LYS:HG3	2.02	0.41
2:J:361:TRP:C	2:J:363:THR:H	2.23	0.41
1:K:106:VAL:HG11	1:K:116:ALA:CB	2.49	0.41
1:K:227:LEU:HD23	1:K:227:LEU:HA	1.88	0.41
1:A:281:LYS:HB2	1:A:281:LYS:HE3	1.89	0.41
2:B:79:LEU:O	2:B:96:ARG:HG3	2.21	0.41
1:C:284:LEU:O	1:C:287:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:LYS:HE2	8:E:383:HOH:O	2.20	0.41
1:G:127:ASN:ND2	1:G:130:ASN:HB2	2.36	0.41
2:H:36:LEU:HA	2:H:37:PRO:HD3	1.87	0.41
3:P:7:LYS:HD3	8:P:65:HOH:O	2.21	0.41
2:B:263:ARG:HB2	2:B:266:LYS:HG3	2.01	0.41
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.03	0.41
1:I:81:ASN:ND2	2:J:105:PHE:H	2.18	0.41
2:L:121:HIS:HB3	2:L:124:MET:HG2	2.03	0.41
1:A:323:LEU:HB3	1:A:367:HIS:CD2	2.56	0.41
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.03	0.41
2:H:115:HIS:HA	2:H:116:PRO:HD3	1.89	0.41
2:H:21:LEU:N	2:H:21:LEU:CD1	2.84	0.41
1:K:149:GLN:HG3	8:K:492:HOH:O	2.20	0.41
1:A:296:LEU:HD22	1:A:322:MET:CE	2.50	0.40
1:C:106:VAL:HG11	1:C:116:ALA:CB	2.51	0.40
2:H:121:HIS:HB3	2:H:124:MET:HG2	2.03	0.40
2:H:18:LEU:N	2:H:18:LEU:CD2	2.83	0.40
2:L:263:ARG:HB2	2:L:266:LYS:HG3	2.02	0.40
1:C:340:LEU:HD23	1:C:343:ILE:HD12	2.02	0.40
1:E:326:GLN:CA	1:E:326:GLN:NE2	2.84	0.40
2:F:266:LYS:HE3	2:F:266:LYS:HB3	1.93	0.40
2:F:37:PRO:HD2	2:F:40:TYR:HE1	1.81	0.40
2:H:103:ILE:HG23	2:H:104:PRO:HD2	2.02	0.40
2:H:62:ASP:OD1	2:H:349:ARG:NH2	2.54	0.40
1:I:355:TYR:O	1:I:358:TYR:HB3	2.21	0.40
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.53	0.40
1:K:340:LEU:HD23	1:K:343:ILE:HD12	2.03	0.40
2:L:269:ASP:HB3	2:L:272:TYR:CD2	2.54	0.40
2:L:90:LEU:HD23	2:L:90:LEU:HA	1.87	0.40
1:A:61:PRO:HG3	1:K:298:GLN:HE22	1.86	0.40
2:B:49:THR:HG23	2:B:124:MET:SD	2.61	0.40
2:B:133:ILE:HG22	2:B:350:THR:HG23	2.04	0.40
2:H:173:ARG:HG2	5:H:380:MGM:H112	2.04	0.40
1:G:200:TYR:CB	5:H:380:MGM:HC12	2.52	0.40
1:K:156:ILE:CD1	1:K:172:ARG:HH22	2.33	0.40
2:L:64:LEU:HD23	2:L:64:LEU:HA	1.83	0.40
2:D:258:ASN:CG	2:D:259:GLY:H	2.23	0.40
2:H:236:LEU:HD22	2:H:245:LEU:HD21	2.03	0.40
2:J:68:ASN:ND2	2:J:71:ASP:OD2	2.55	0.40
1:E:344:LEU:HD13	1:E:356:TRP:CE2	2.56	0.40
1:G:161:GLU:HG2	1:G:162:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:HIS:CD2	2:H:166:GLU:HG2	2.56	0.40
2:H:22:ARG:NH1	2:H:22:ARG:HG2	2.37	0.40
2:L:22:ARG:HG2	2:L:22:ARG:NH1	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:OE1	1:C:60:SER:OG[4_556]	2.19	0.01

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%)	25 (8%)	0	100	100
1	C	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	41	66
1	E	312/377 (83%)	287 (92%)	25 (8%)	0	100	100
1	G	312/377 (83%)	291 (93%)	21 (7%)	0	100	100
1	I	312/377 (83%)	285 (91%)	27 (9%)	0	100	100
1	K	312/377 (83%)	292 (94%)	20 (6%)	0	100	100
2	B	344/377 (91%)	331 (96%)	12 (4%)	1 (0%)	41	66
2	D	344/377 (91%)	331 (96%)	11 (3%)	2 (1%)	25	50
2	F	344/377 (91%)	330 (96%)	13 (4%)	1 (0%)	41	66
2	H	344/377 (91%)	328 (95%)	15 (4%)	1 (0%)	41	66
2	J	344/377 (91%)	328 (95%)	14 (4%)	2 (1%)	25	50
2	L	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	41	66
3	M	4/9 (44%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	4/9 (44%)	4 (100%)	0	0	100	100
3	O	4/9 (44%)	4 (100%)	0	0	100	100
3	P	4/9 (44%)	4 (100%)	0	0	100	100
3	Q	4/9 (44%)	4 (100%)	0	0	100	100
3	R	4/9 (44%)	4 (100%)	0	0	100	100
All	All	3960/4578 (86%)	3736 (94%)	215 (5%)	9 (0%)	47	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
2	D	258	ASN
2	J	34	GLN
2	J	258	ASN
2	F	258	ASN
2	H	258	ASN
2	L	258	ASN
2	D	333	GLU
1	C	329	ASN

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%)	275 (98%)	7 (2%)	47	76
1	C	286/338 (85%)	277 (97%)	9 (3%)	40	69
1	E	289/338 (86%)	280 (97%)	9 (3%)	40	69
1	G	285/338 (84%)	279 (98%)	6 (2%)	53	80
1	I	285/338 (84%)	281 (99%)	4 (1%)	67	86
1	K	292/338 (86%)	285 (98%)	7 (2%)	49	77
2	B	291/326 (89%)	280 (96%)	11 (4%)	33	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	291/326 (89%)	277 (95%)	14 (5%)	25	53
2	F	295/326 (90%)	285 (97%)	10 (3%)	37	66
2	H	288/326 (88%)	278 (96%)	10 (4%)	36	65
2	J	291/326 (89%)	276 (95%)	15 (5%)	23	49
2	L	295/326 (90%)	280 (95%)	15 (5%)	24	50
3	M	6/8 (75%)	6 (100%)	0	100	100
3	N	6/8 (75%)	6 (100%)	0	100	100
3	O	6/8 (75%)	6 (100%)	0	100	100
3	P	6/8 (75%)	6 (100%)	0	100	100
3	Q	6/8 (75%)	6 (100%)	0	100	100
3	R	6/8 (75%)	6 (100%)	0	100	100
All	All	3506/4032 (87%)	3389 (97%)	117 (3%)	38	67

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	107	LEU
1	A	184	GLN
1	A	194	ASN
1	A	214	ARG
1	A	287	ARG
1	A	354	GLU
2	B	21	LEU
2	B	33	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	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	60	SER
1	C	71	GLU
1	C	107	LEU
1	C	184	GLN

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Mol	Chain	Res	Type
1	C	194	ASN
1	C	211	GLN
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	110	ASN
2	D	151	LEU
2	D	216	LEU
2	D	232	LEU
2	D	236	LEU
2	D	237	GLU
2	D	255	ARG
2	D	258	ASN
2	D	261	HIS
2	D	329	LEU
2	D	331	LEU
1	E	71	GLU
1	E	80	GLN
1	E	107	LEU
1	E	184	GLN
1	E	214	ARG
1	E	287	ARG
1	E	324	GLU
1	E	326	GLN
1	E	364	GLN
2	F	21	LEU
2	F	24	ARG
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	261	HIS
2	F	329	LEU
2	F	331	LEU
1	G	67	ARG
1	G	107	LEU
1	G	184	GLN
1	G	224	ASP

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Mol	Chain	Res	Type
1	G	225	GLN
1	G	287	ARG
2	H	21	LEU
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
1	I	71	GLU
1	I	107	LEU
1	I	287	ARG
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	261	HIS
2	J	329	LEU
2	J	331	LEU
2	J	341	HIS
2	J	353	ARG
2	J	357	LEU
1	K	71	GLU
1	K	80	GLN
1	K	107	LEU
1	K	142	ARG
1	K	182	PRO
1	K	211	GLN
1	K	287	ARG
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	151	LEU

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Mol	Chain	Res	Type
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	284	LYS
2	L	329	LEU
2	L	331	LEU
2	L	360	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	184	GLN
1	A	194	ASN
1	A	225	GLN
1	A	278	ASN
1	A	367	HIS
1	C	108	GLN
1	C	153	ASN
1	C	170	HIS
1	C	184	GLN
1	C	218	ASN
1	C	298	GLN
1	C	364	GLN
2	D	246	ASN
1	E	149	GLN
1	E	184	GLN
1	E	297	ASN
1	E	326	GLN
1	E	335	ASN
1	E	364	GLN
1	E	367	HIS
2	F	30	GLN
2	F	246	ASN
1	G	81	ASN
1	G	89	GLN
1	G	184	GLN
1	G	225	GLN

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Mol	Chain	Res	Type
1	G	297	ASN
1	G	325	ASN
1	G	335	ASN
2	H	296	ASN
1	I	81	ASN
1	I	89	GLN
1	I	149	GLN
1	I	184	GLN
1	I	218	ASN
1	I	261	GLN
1	I	335	ASN
1	I	367	HIS
2	J	246	ASN
2	J	359	GLN
1	K	135	HIS
1	K	184	GLN
1	K	205	HIS
1	K	298	GLN
1	K	367	HIS
2	L	212	GLN
3	M	4	ASN
3	N	4	ASN
3	O	4	ASN
3	P	4	ASN
3	Q	4	ASN
3	R	4	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	F	380	-	26,28,28	0.96	1 (3%)	33,37,37	2.04	5 (15%)
5	MGM	D	380	-	26,28,28	0.97	2 (7%)	33,37,37	2.01	5 (15%)
5	MGM	B	379	-	26,28,28	0.92	2 (7%)	33,37,37	2.04	6 (18%)
5	MGM	L	379	-	26,28,28	0.98	2 (7%)	33,37,37	1.99	5 (15%)
5	MGM	J	379	-	26,28,28	0.96	2 (7%)	33,37,37	1.98	5 (15%)
7	MES	F	381	-	12,12,12	9.13	8 (66%)	14,16,16	2.47	5 (35%)
5	MGM	H	380	-	26,28,28	0.88	1 (3%)	33,37,37	1.98	5 (15%)

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	F	380	-	-	9/31/31/31	-
5	MGM	D	380	-	-	9/31/31/31	-
5	MGM	B	379	-	-	10/31/31/31	-
5	MGM	L	379	-	-	9/31/31/31	-
5	MGM	J	379	-	-	9/31/31/31	-
7	MES	F	381	-	-	3/6/14/14	0/1/1/1
5	MGM	H	380	-	-	10/31/31/31	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	381	MES	C8-S	-24.15	1.43	1.77
7	F	381	MES	O2S-S	12.22	1.81	1.45
7	F	381	MES	O1S-S	11.64	1.79	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	381	MES	O3S-S	9.10	1.79	1.47
7	F	381	MES	C7-C8	-4.71	1.39	1.52
7	F	381	MES	C3-C2	-2.75	1.39	1.50
7	F	381	MES	C7-N4	-2.56	1.41	1.47
7	F	381	MES	C5-C6	-2.49	1.40	1.50
5	L	379	MGM	C7-C8	2.36	1.38	1.33
5	D	380	MGM	C7-C8	2.31	1.38	1.33
5	L	379	MGM	C12-C13	2.23	1.38	1.33
5	H	380	MGM	C7-C8	2.22	1.38	1.33
5	F	380	MGM	C7-C8	2.17	1.38	1.33
5	J	379	MGM	C12-C13	2.12	1.38	1.33
5	B	379	MGM	C7-C8	2.11	1.38	1.33
5	B	379	MGM	C12-C13	2.09	1.38	1.33
5	D	380	MGM	C12-C13	2.08	1.38	1.33
5	J	379	MGM	C7-C8	2.04	1.37	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	379	MGM	C1-C2-N3	7.27	131.02	113.31
5	F	380	MGM	C1-C2-N3	7.22	130.91	113.31
5	D	380	MGM	C1-C2-N3	6.98	130.33	113.31
5	L	379	MGM	C1-C2-N3	6.93	130.20	113.31
5	H	380	MGM	C1-C2-N3	6.90	130.14	113.31
5	J	379	MGM	C1-C2-N3	6.89	130.10	113.31
5	J	379	MGM	C4-N3-C2	5.48	125.58	110.62
5	L	379	MGM	C4-N3-C2	5.43	125.44	110.62
5	D	380	MGM	C4-N3-C2	5.40	125.36	110.62
5	B	379	MGM	C4-N3-C2	5.40	125.36	110.62
5	H	380	MGM	C4-N3-C2	5.36	125.25	110.62
5	F	380	MGM	C4-N3-C2	5.35	125.22	110.62
7	F	381	MES	O3S-S-C8	5.26	114.27	105.77
7	F	381	MES	O1S-S-C8	4.53	112.37	106.92
5	F	380	MGM	O1-C1-C2	4.21	115.46	107.27
5	B	379	MGM	O1-C1-C2	4.13	115.31	107.27
5	L	379	MGM	O1-C1-C2	3.96	114.97	107.27
5	D	380	MGM	O1-C1-C2	3.89	114.84	107.27
5	H	380	MGM	O1-C1-C2	3.82	114.71	107.27
7	F	381	MES	O2S-S-C8	3.79	111.48	106.92
5	J	379	MGM	O1-C1-C2	3.59	114.26	107.27
5	J	379	MGM	O1B-PB-O3A	3.08	114.95	104.64
5	L	379	MGM	O1B-PB-O3A	3.06	114.89	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	380	MGM	O1B-PB-O3A	2.99	114.66	104.64
5	F	380	MGM	O1B-PB-O3A	2.92	114.43	104.64
5	D	380	MGM	O1B-PB-O3A	2.92	114.41	104.64
5	B	379	MGM	O1B-PB-O3A	2.72	113.76	104.64
5	D	380	MGM	C2-N3-C5	2.65	122.62	111.92
5	L	379	MGM	C2-N3-C5	2.64	122.57	111.92
5	H	380	MGM	C2-N3-C5	2.62	122.50	111.92
5	B	379	MGM	C2-N3-C5	2.62	122.49	111.92
5	F	380	MGM	C2-N3-C5	2.62	122.49	111.92
7	F	381	MES	O3S-S-O2S	-2.54	105.06	111.27
5	J	379	MGM	C2-N3-C5	2.51	122.04	111.92
7	F	381	MES	O2S-S-O1S	-2.47	105.41	113.95
5	B	379	MGM	C10-C8-C9	-2.01	111.89	115.27

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	380	MGM	C1-C2-N3-C4
5	F	380	MGM	O1-C1-C2-N3
5	F	380	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	B	379	MGM	C1-C2-N3-C4
5	B	379	MGM	O1-C1-C2-N3
5	B	379	MGM	PA-O3A-PB-O1B
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	J	379	MGM	C1-C2-N3-C4
5	J	379	MGM	O1-C1-C2-N3
5	J	379	MGM	PA-O3A-PB-O1B
5	H	380	MGM	C1-C2-N3-C4
5	H	380	MGM	O1-C1-C2-N3
5	H	380	MGM	PA-O3A-PB-O1B
7	F	381	MES	C7-C8-S-O3S
5	F	380	MGM	C6-C5-N3-C4
5	D	380	MGM	C6-C5-N3-C4
5	B	379	MGM	C6-C5-N3-C4
5	L	379	MGM	C6-C5-N3-C4
5	J	379	MGM	C6-C5-N3-C4

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Mol	Chain	Res	Type	Atoms
5	H	380	MGM	C6-C5-N3-C4
5	L	379	MGM	C6-C5-N3-C2
5	H	380	MGM	C10-C8-C9-C11
5	F	380	MGM	C10-C8-C9-C11
5	B	379	MGM	C10-C8-C9-C11
5	H	380	MGM	C7-C8-C9-C11
7	F	381	MES	C7-C8-S-O1S
7	F	381	MES	C7-C8-S-O2S
5	D	380	MGM	C10-C8-C9-C11
5	L	379	MGM	C10-C8-C9-C11
5	J	379	MGM	C10-C8-C9-C11
5	F	380	MGM	C7-C8-C9-C11
5	B	379	MGM	C7-C8-C9-C11
5	D	380	MGM	C6-C5-N3-C2
5	D	380	MGM	C7-C8-C9-C11
5	J	379	MGM	C7-C8-C9-C11
5	F	380	MGM	C6-C5-N3-C2
5	J	379	MGM	C6-C5-N3-C2
5	H	380	MGM	C6-C5-N3-C2
5	L	379	MGM	C7-C8-C9-C11
5	F	380	MGM	PA-O3A-PB-O2B
5	D	380	MGM	PA-O3A-PB-O2B
5	B	379	MGM	PA-O3A-PB-O2B
5	L	379	MGM	PA-O3A-PB-O2B
5	J	379	MGM	PA-O3A-PB-O2B
5	H	380	MGM	PA-O3A-PB-O2B
5	L	379	MGM	C9-C11-C12-C13
5	J	379	MGM	C9-C11-C12-C13
5	H	380	MGM	C9-C11-C12-C13
5	F	380	MGM	C9-C11-C12-C13
5	D	380	MGM	C9-C11-C12-C13
5	B	379	MGM	C9-C11-C12-C13
5	B	379	MGM	C6-C5-N3-C2
5	B	379	MGM	C14-C13-C15-C16
5	H	380	MGM	C14-C13-C15-C16

There are no ring outliers.

6 monomers are involved in 11 short contacts:

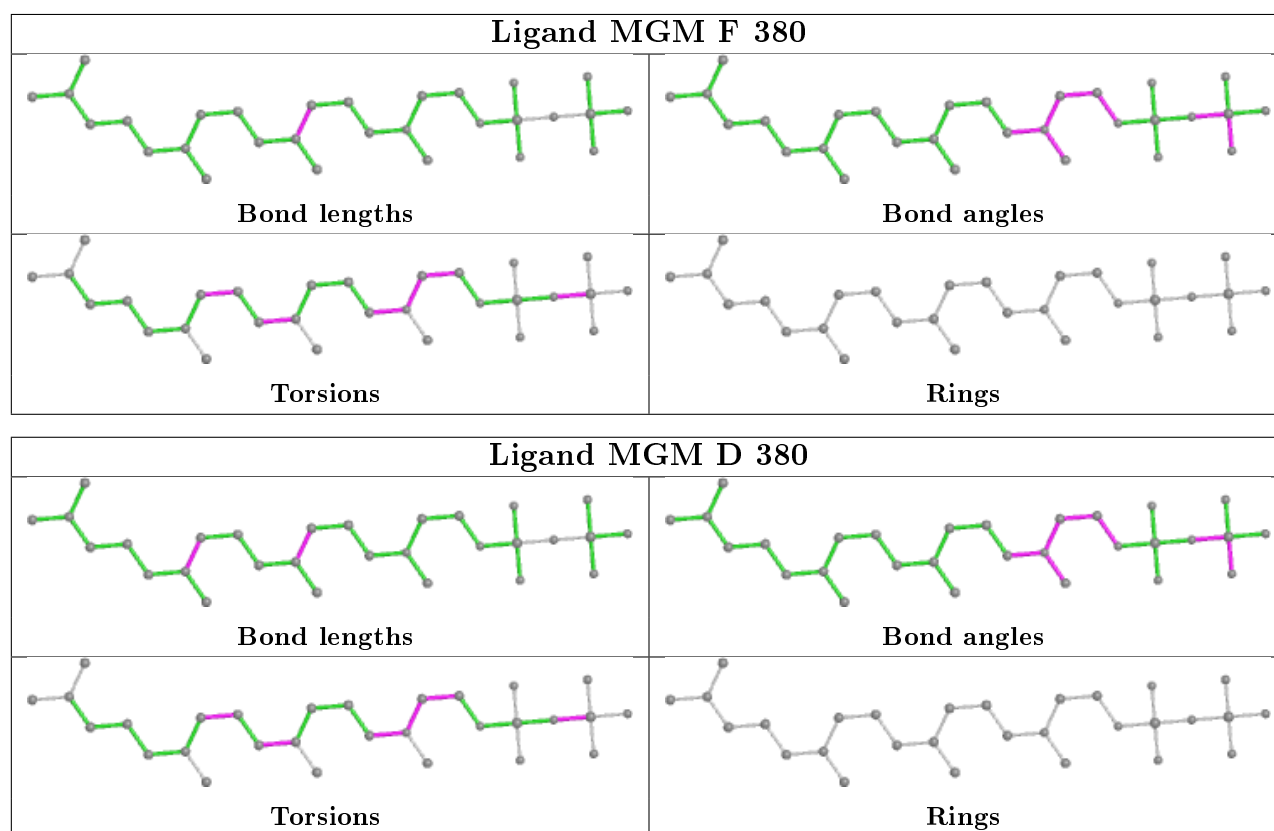
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	380	MGM	3	0
5	D	380	MGM	1	0

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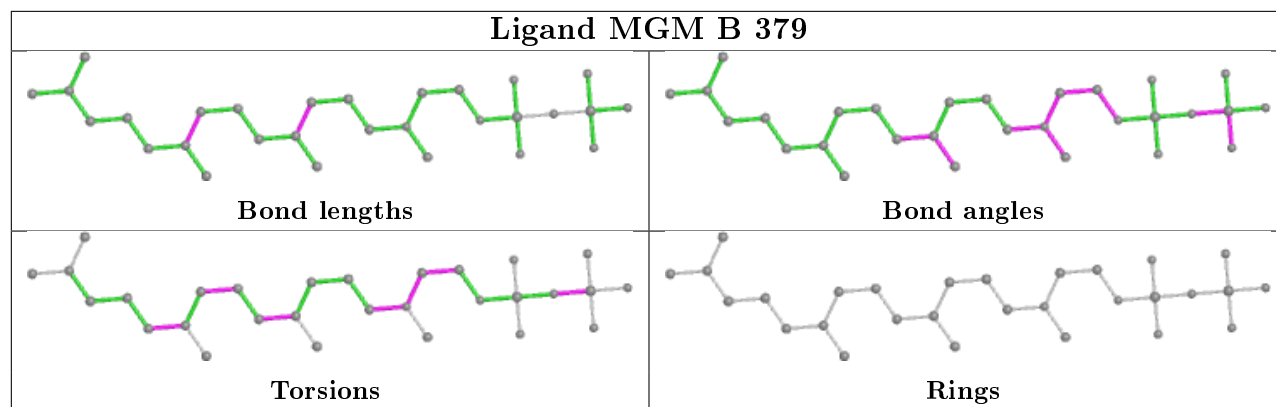
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	379	MGM	2	0
5	L	379	MGM	2	0
5	J	379	MGM	1	0
5	H	380	MGM	2	0

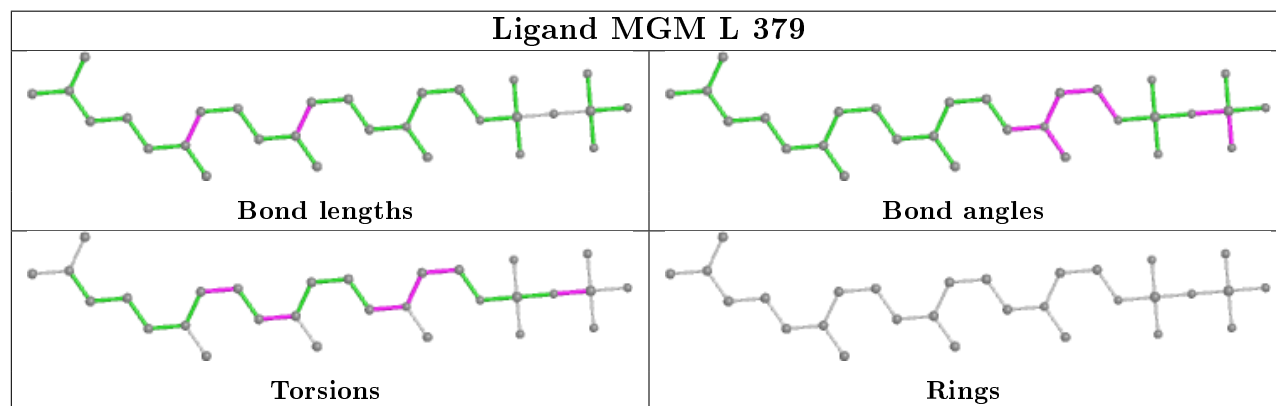
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



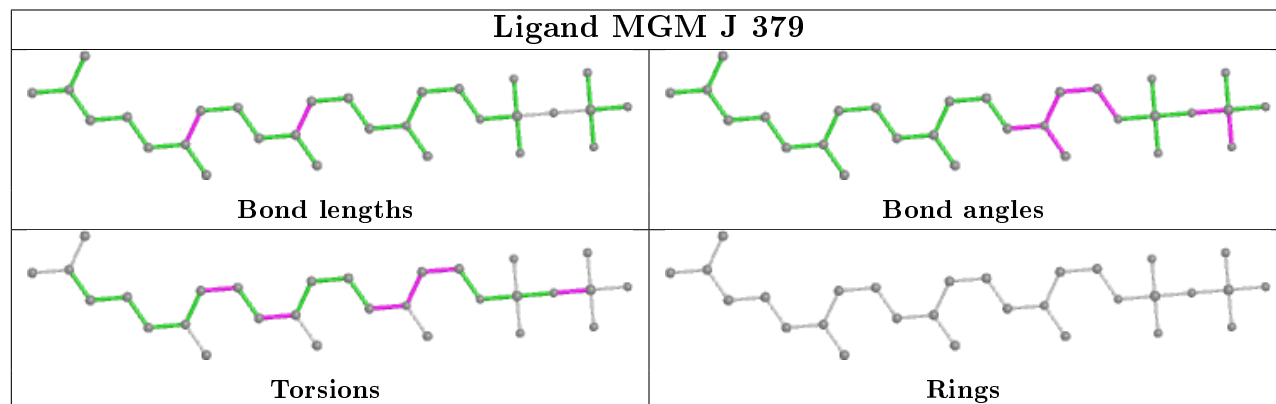
Ligand MGM B 379



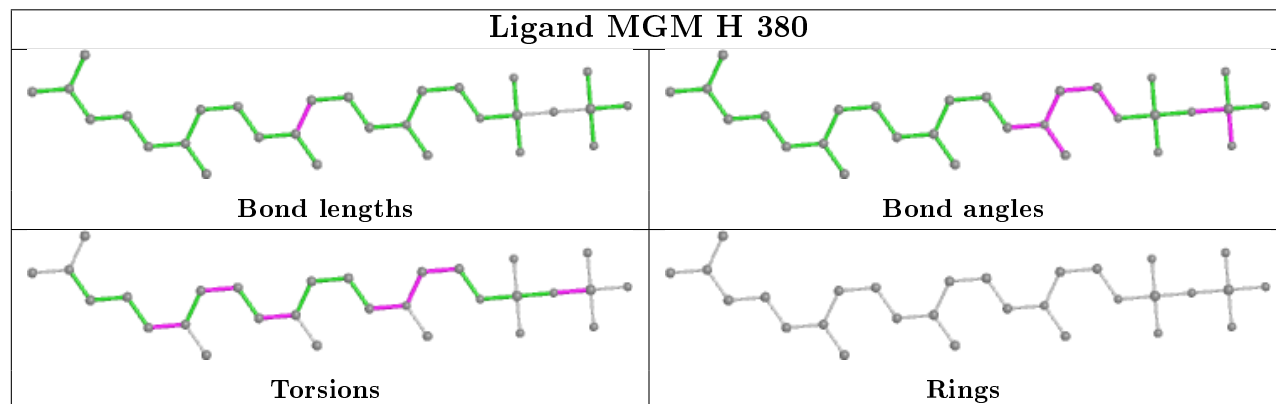
Ligand MGM L 379



Ligand MGM J 379



Ligand MGM H 380



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/377 (83%)	0.02	13 (4%) 37 36	45, 67, 100, 113	0
1	C	314/377 (83%)	-0.01	8 (2%) 57 59	44, 64, 93, 114	0
1	E	314/377 (83%)	0.03	10 (3%) 47 48	42, 65, 92, 110	0
1	G	314/377 (83%)	-0.01	8 (2%) 57 59	43, 63, 90, 112	0
1	I	314/377 (83%)	0.07	12 (3%) 40 39	42, 67, 97, 111	0
1	K	314/377 (83%)	-0.29	5 (1%) 72 74	35, 51, 77, 89	0
2	B	346/377 (91%)	-0.03	8 (2%) 60 62	43, 59, 80, 105	0
2	D	346/377 (91%)	-0.05	8 (2%) 60 62	42, 55, 78, 92	0
2	F	346/377 (91%)	-0.03	10 (2%) 51 52	38, 52, 78, 100	0
2	H	346/377 (91%)	0.17	17 (4%) 29 28	44, 64, 88, 110	0
2	J	346/377 (91%)	0.11	19 (5%) 25 24	43, 63, 89, 109	0
2	L	346/377 (91%)	-0.08	4 (1%) 79 80	35, 48, 68, 91	0
3	M	6/9 (66%)	0.75	1 (16%) 1 1	49, 65, 80, 94	0
3	N	6/9 (66%)	0.90	1 (16%) 1 1	52, 65, 82, 94	0
3	O	6/9 (66%)	0.89	1 (16%) 1 1	52, 63, 79, 92	0
3	P	6/9 (66%)	0.82	1 (16%) 1 1	53, 70, 85, 97	0
3	Q	6/9 (66%)	0.74	1 (16%) 1 1	46, 63, 79, 88	0
3	R	6/9 (66%)	1.13	1 (16%) 1 1	43, 65, 78, 88	0
All	All	3996/4578 (87%)	0.00	128 (3%) 47 48	35, 59, 88, 114	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	4	ASN	5.2
3	M	4	ASN	5.1
3	R	4	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
3	O	4	ASN	4.6
3	N	4	ASN	4.4
1	C	306	HIS	4.3
2	B	363	THR	4.3
1	G	55	PHE	4.2
1	E	306	HIS	4.1
2	L	363	THR	4.0
1	I	305	SER	3.9
1	G	306	HIS	3.9
2	H	363	THR	3.9
1	I	306	HIS	3.8
1	C	55	PHE	3.7
2	F	363	THR	3.7
1	I	329	ASN	3.6
1	A	328	ASP	3.6
2	B	362	LYS	3.6
1	A	330	LYS	3.5
1	I	328	ASP	3.5
2	J	363	THR	3.4
1	I	368	SER	3.4
1	G	304	PRO	3.4
2	J	85	GLU	3.4
2	H	361	TRP	3.4
1	A	304	PRO	3.4
2	F	305	LEU	3.3
2	J	86	ASP	3.3
2	D	363	THR	3.3
2	J	84	THR	3.3
1	I	304	PRO	3.2
2	H	112	GLY	3.2
2	H	305	LEU	3.1
3	Q	4	ASN	3.1
1	K	326	GLN	3.1
2	H	362	LYS	3.1
2	F	88	SER	3.0
2	H	304	ARG	3.0
1	E	326	GLN	3.0
1	I	367	HIS	3.0
2	J	108	SER	3.0
2	J	360	SER	3.0
2	F	112	GLY	3.0
2	B	86	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	306	HIS	2.9
2	H	316	HIS	2.9
1	I	84	PRO	2.9
2	F	37	PRO	2.9
1	E	91	ILE	2.9
2	H	38	GLU	2.8
1	E	304	PRO	2.8
1	E	70	ALA	2.8
1	A	368	SER	2.8
1	C	330	LYS	2.8
1	A	329	ASN	2.7
2	H	127	THR	2.7
1	K	305	SER	2.7
1	G	326	GLN	2.7
2	D	305	LEU	2.7
2	J	127	THR	2.7
1	C	91	ILE	2.6
1	C	304	PRO	2.6
2	D	110	ASN	2.6
1	E	305	SER	2.6
1	G	305	SER	2.6
2	D	314	ASP	2.5
1	G	91	ILE	2.5
2	H	65	ASP	2.5
2	D	362	LYS	2.5
1	C	329	ASN	2.5
1	E	77	PRO	2.5
1	I	365	SER	2.4
1	E	281	LYS	2.4
2	H	345	ASN	2.4
2	B	87	ARG	2.4
1	C	305	SER	2.4
2	J	88	SER	2.4
2	L	113	THR	2.4
2	H	100	TYR	2.3
2	J	124	MET	2.3
1	I	330	LYS	2.3
2	B	305	LEU	2.3
2	F	38	GLU	2.3
2	D	111	PRO	2.3
2	F	316	HIS	2.3
2	J	87	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	127	THR	2.3
2	H	45	THR	2.3
2	J	361	TRP	2.2
2	J	126	TYR	2.2
2	J	114	ALA	2.2
1	A	281	LYS	2.2
1	K	85	SER	2.2
1	E	331	GLU	2.2
1	K	84	PRO	2.2
1	K	306	HIS	2.2
2	B	361	TRP	2.2
1	G	142	ARG	2.2
2	F	327	CYS	2.2
1	A	326	GLN	2.2
1	E	328	ASP	2.2
2	F	86	ASP	2.2
2	H	87	ARG	2.2
2	H	88	SER	2.2
2	H	18	LEU	2.2
2	B	127	THR	2.2
2	J	113	THR	2.2
1	A	367	HIS	2.1
2	D	37	PRO	2.1
1	I	55	PHE	2.1
2	J	335	SER	2.1
1	A	301	ASP	2.1
1	A	305	SER	2.1
2	F	40	TYR	2.1
2	J	239	VAL	2.1
2	J	362	LYS	2.1
1	A	91	ILE	2.1
2	H	126	TYR	2.1
2	D	45	THR	2.1
2	J	89	ASN	2.1
2	L	345	ASN	2.1
1	A	314	PHE	2.1
2	B	39	ARG	2.1
1	I	278	ASN	2.1
1	G	92	TYR	2.0
2	J	237	GLU	2.0
1	C	331	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

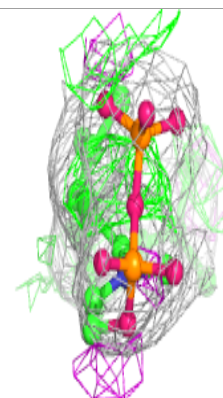
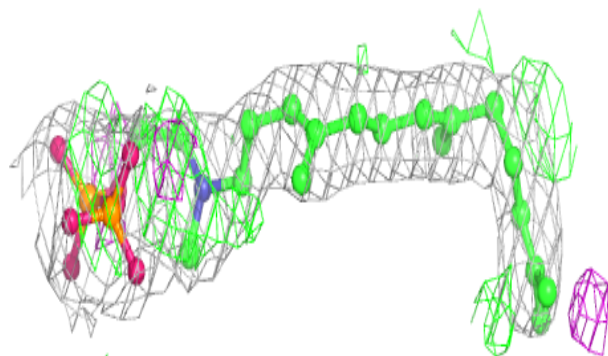
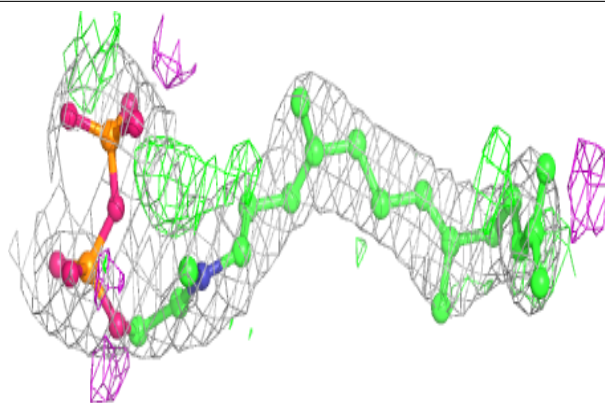
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MES	F	381	12/12	0.93	0.21	89,95,99,99	0
5	MGM	H	380	29/29	0.94	0.22	45,58,70,72	0
5	MGM	D	380	29/29	0.95	0.21	45,55,67,67	0
5	MGM	B	379	29/29	0.95	0.20	48,56,68,70	0
5	MGM	L	379	29/29	0.95	0.26	34,50,63,64	0
5	MGM	J	379	29/29	0.95	0.23	43,52,65,66	0
5	MGM	F	380	29/29	0.95	0.22	44,55,67,70	0
6	CL	H	379	1/1	0.97	0.08	62,62,62,62	0
6	CL	D	379	1/1	0.97	0.09	59,59,59,59	0
6	CL	F	379	1/1	0.98	0.07	55,55,55,55	0
4	ZN	J	378	1/1	0.99	0.09	58,58,58,58	0
4	ZN	D	378	1/1	0.99	0.09	53,53,53,53	0
4	ZN	H	378	1/1	0.99	0.10	59,59,59,59	0
4	ZN	B	378	1/1	1.00	0.07	54,54,54,54	0
4	ZN	L	378	1/1	1.00	0.07	50,50,50,50	0
4	ZN	F	378	1/1	1.00	0.07	51,51,51,51	0

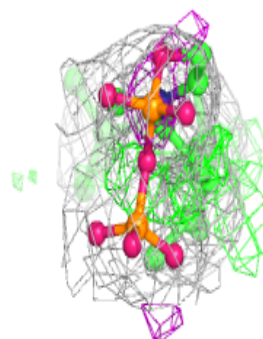
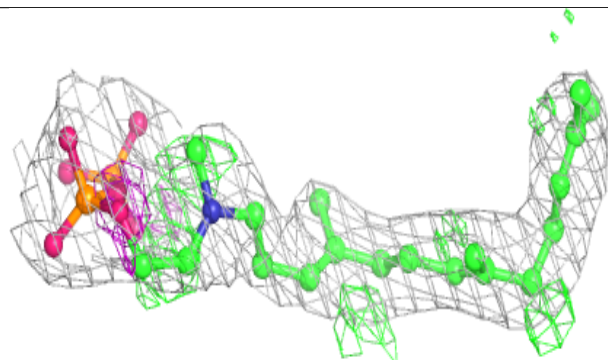
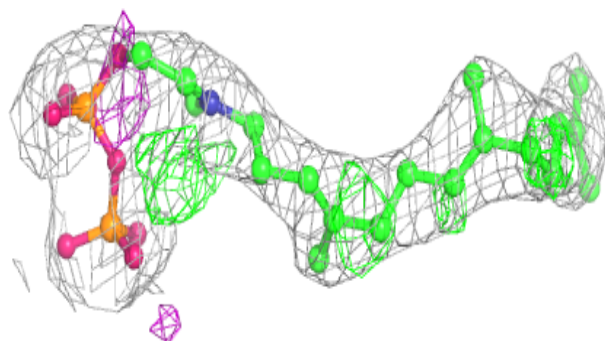
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGM H 380:

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

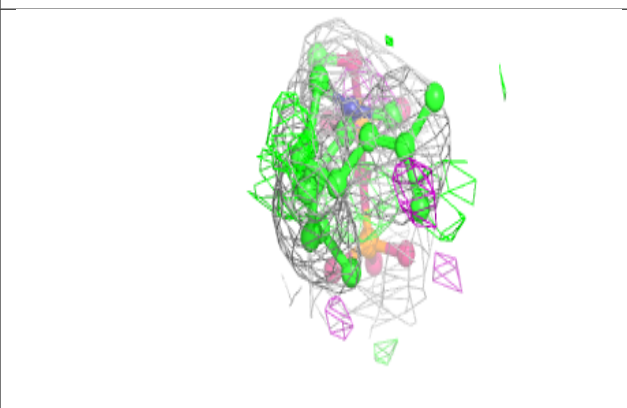
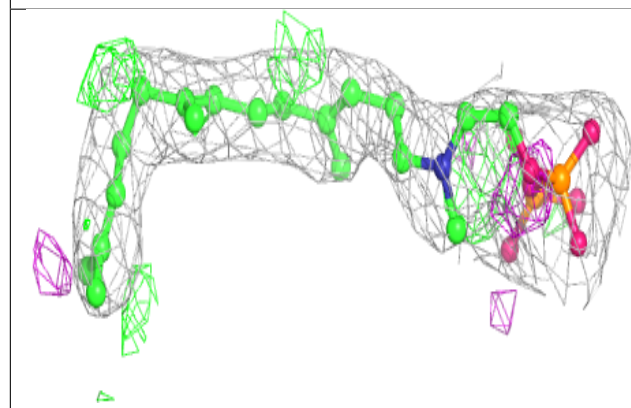
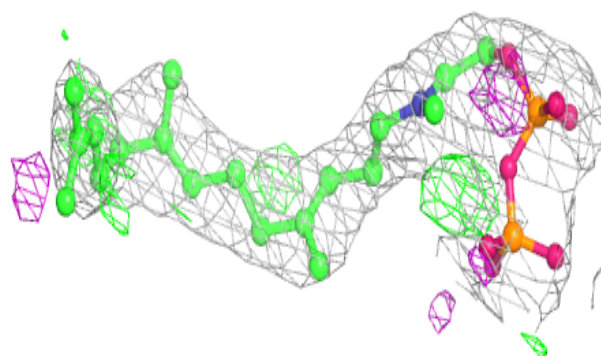
**Electron density around MGM D 380:**

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

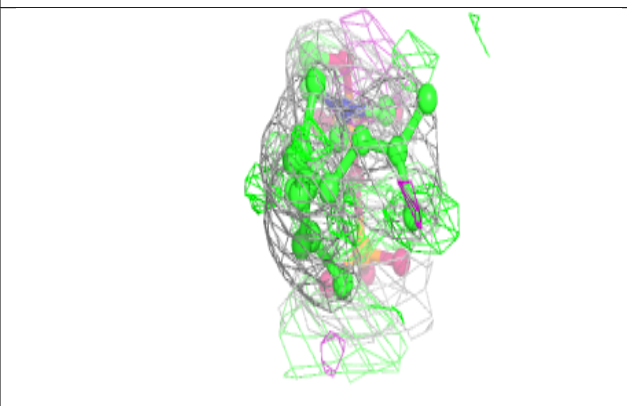
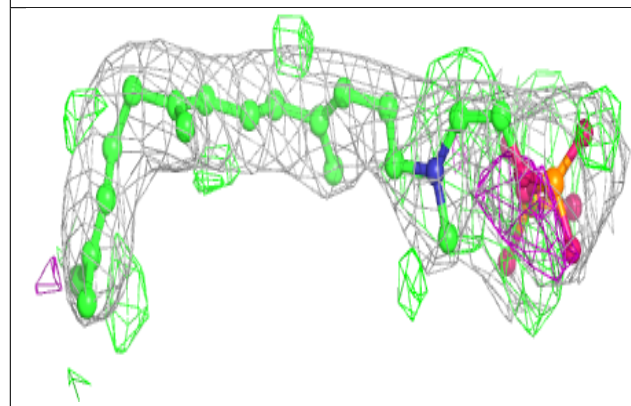
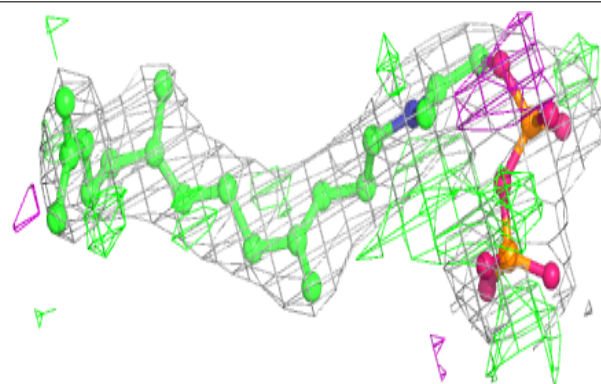


Electron density around MGM B 379:

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

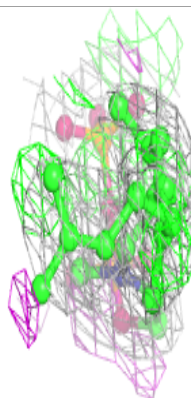
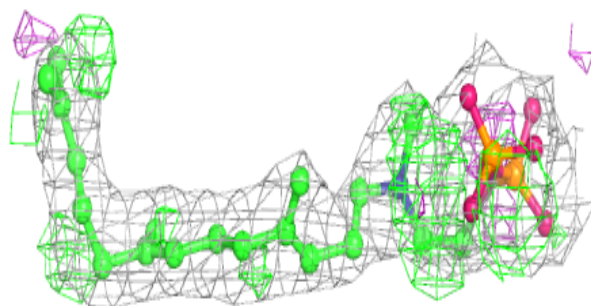
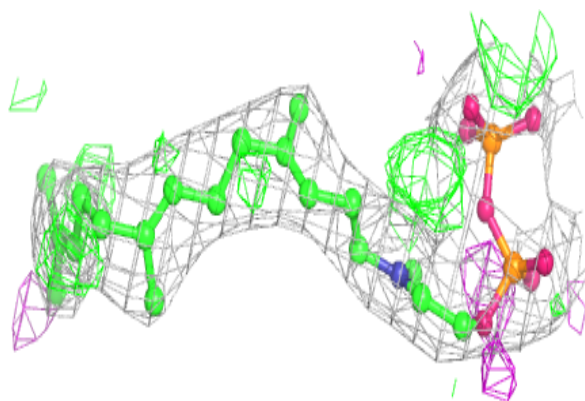
**Electron density around MGM L 379:**

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

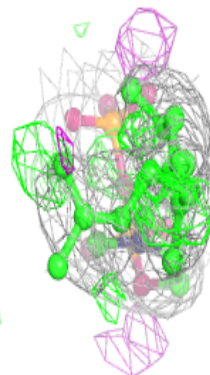
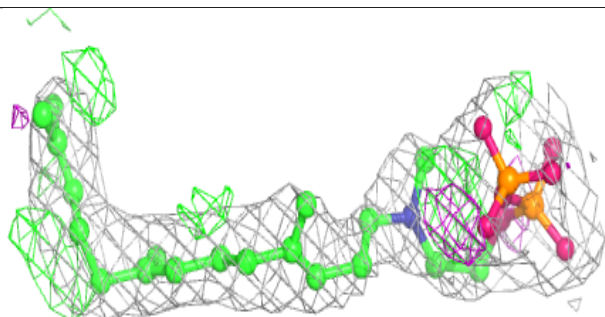
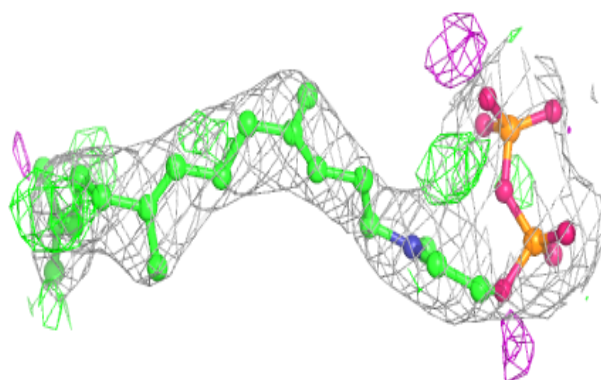


Electron density around MGM J 379:

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

**Electron density around MGM F 380:**

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



6.5 Other polymers

There are no such residues in this entry.