



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:09 am BST

PDB ID : 1TNO
Title : Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a KKKSKTKCVIM Peptide Derived from K-Ras4B
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

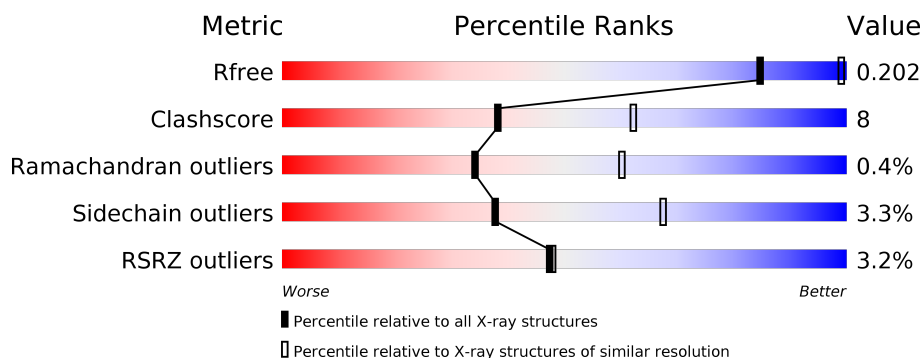
1 Overall quality at a glance

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> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	377	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	377	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	G	377	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>14%</div> <div>•</div> <div>17%</div> </div> </div>
1	I	377	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>
1	K	377	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>12%</div> <div>•</div> <div>17%</div> </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	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33292 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
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2643	1689	461	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2656	1694	465	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2671	1703	467	496	5			

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

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

- Molecule 3 is a protein called c-K-ras2 protein isoform b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	N	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	O	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	P	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	Q	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			
3	R	6	Total	C	N	O	S	0	0	0
			46	29	7	8	2			

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

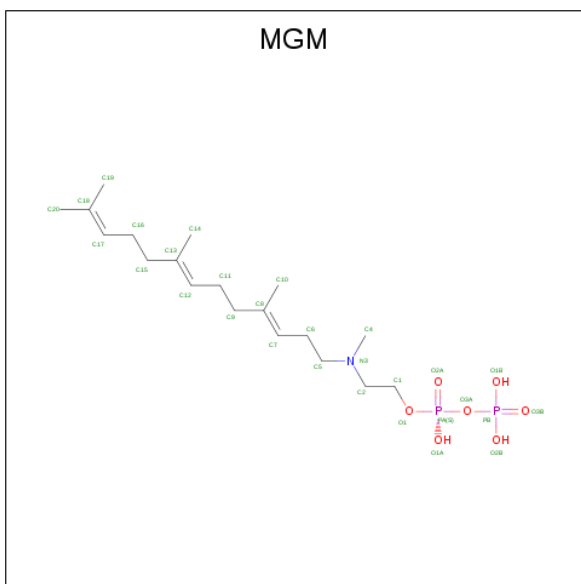
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 6 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
6	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	44	Total	O	0	0
			44	44		
8	B	34	Total	O	0	0
			34	34		
8	C	41	Total	O	0	0
			41	41		
8	D	51	Total	O	0	0
			51	51		
8	E	50	Total	O	0	0
			50	50		
8	F	58	Total	O	0	0
			58	58		
8	G	40	Total	O	0	0
			40	40		
8	H	31	Total	O	0	0
			31	31		

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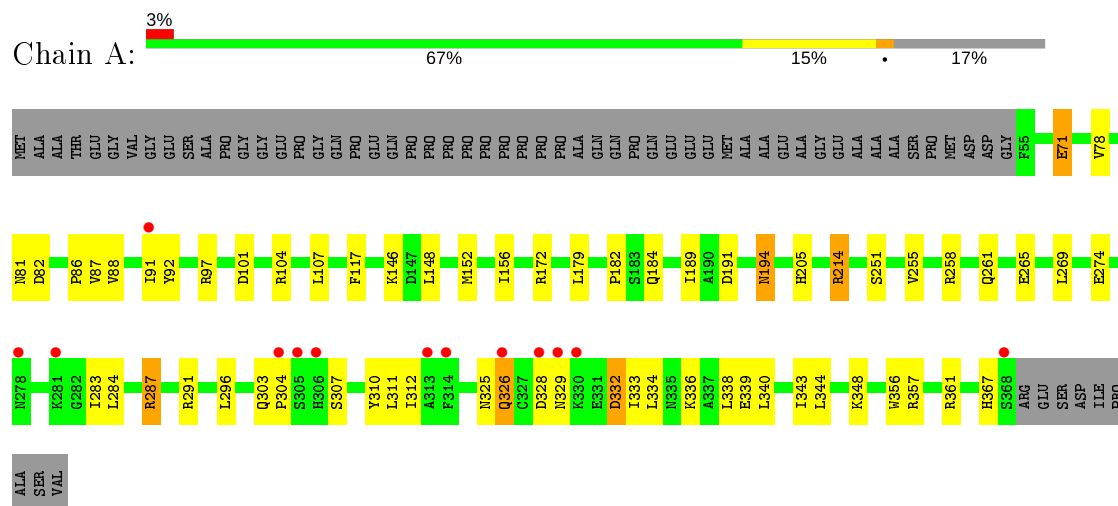
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	52	Total 52	O 52	0	0
8	J	47	Total 47	O 47	0	0
8	K	123	Total 123	O 123	0	0
8	L	93	Total 93	O 93	0	0
8	N	2	Total 2	O 2	0	0
8	O	2	Total 2	O 2	0	0
8	P	4	Total 4	O 4	0	0
8	Q	2	Total 2	O 2	0	0
8	R	4	Total 4	O 4	0	0

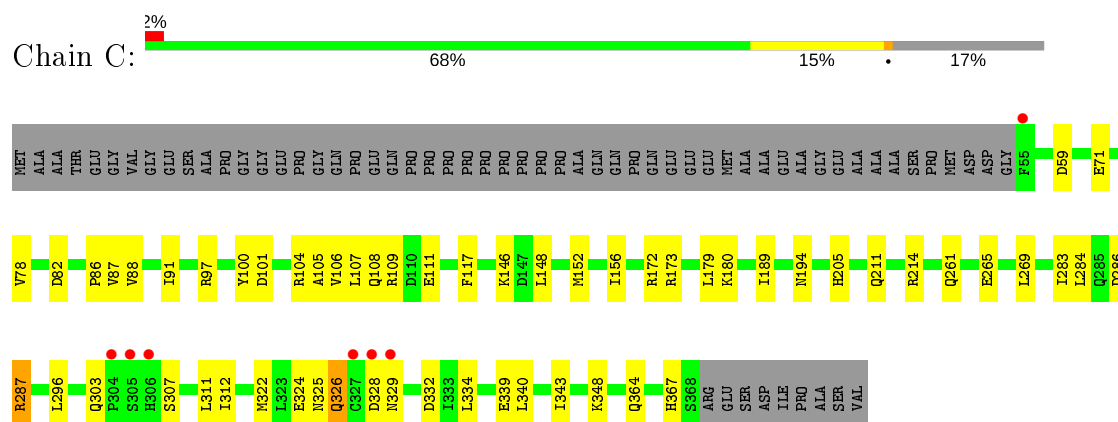
3 Residue-property plots

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.

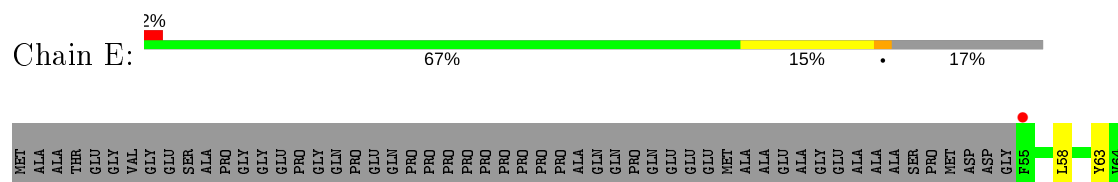
- Molecule 1: geranylgeranyltransferase type I alpha subunit

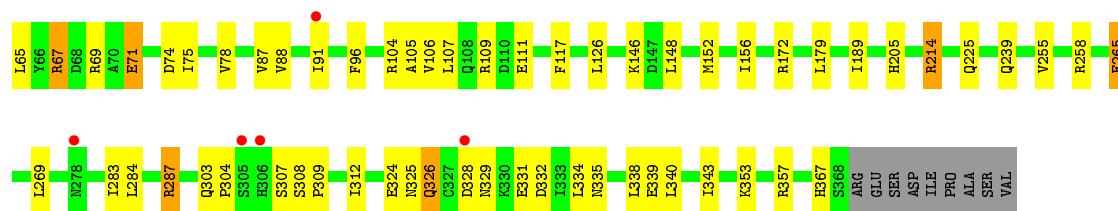


- Molecule 1: geranylgeranyltransferase type I alpha subunit

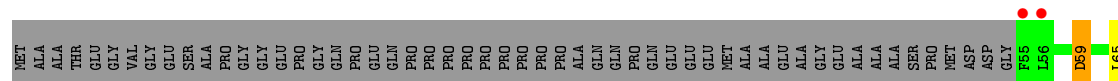


- Molecule 1: geranylgeranyltransferase type I alpha subunit

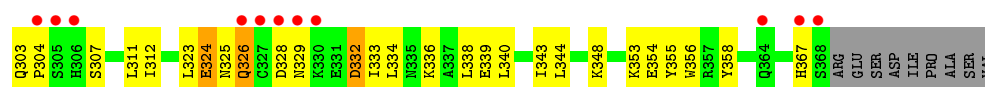
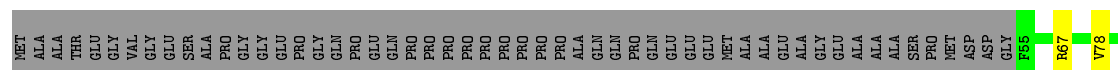




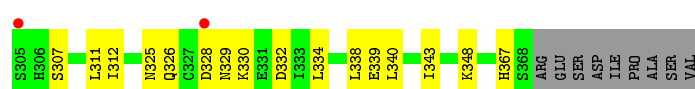
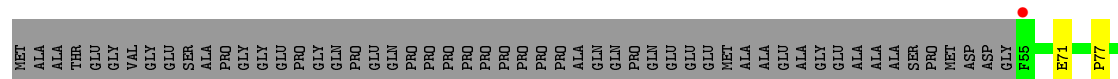
- Molecule 1: geranylgeranyltransferase type I alpha subunit



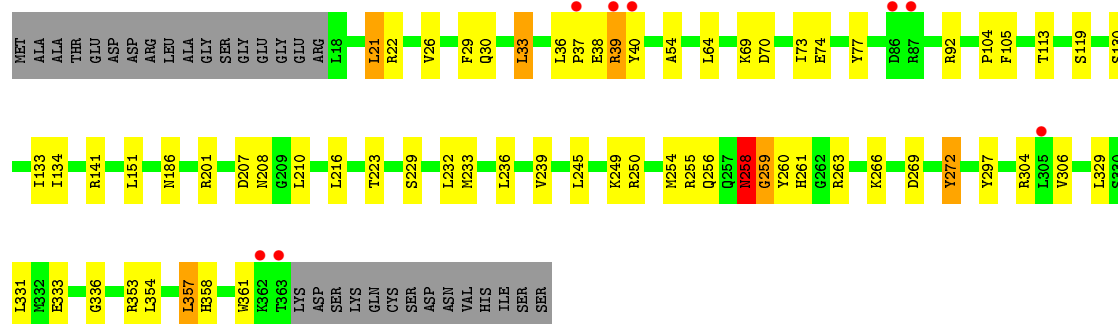
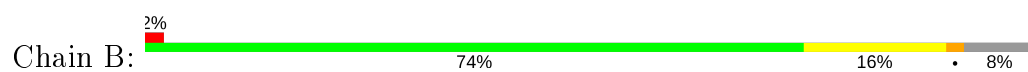
- Molecule 1: geranylgeranyltransferase type I alpha subunit



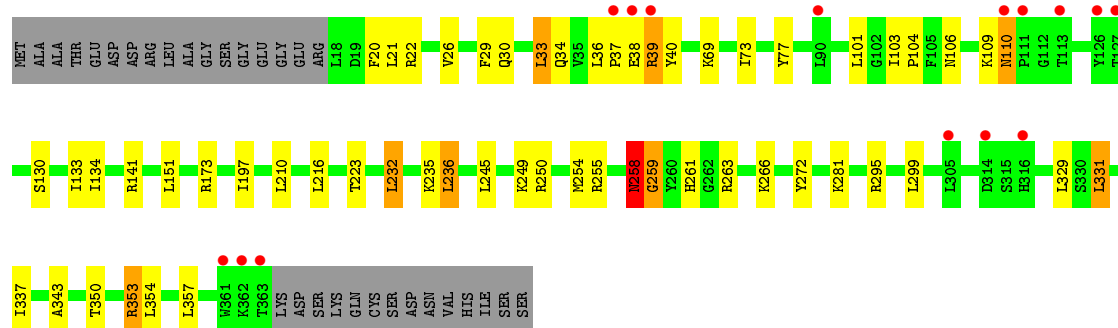
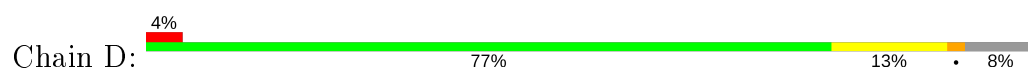
- Molecule 1: geranylgeranyltransferase type I alpha subunit



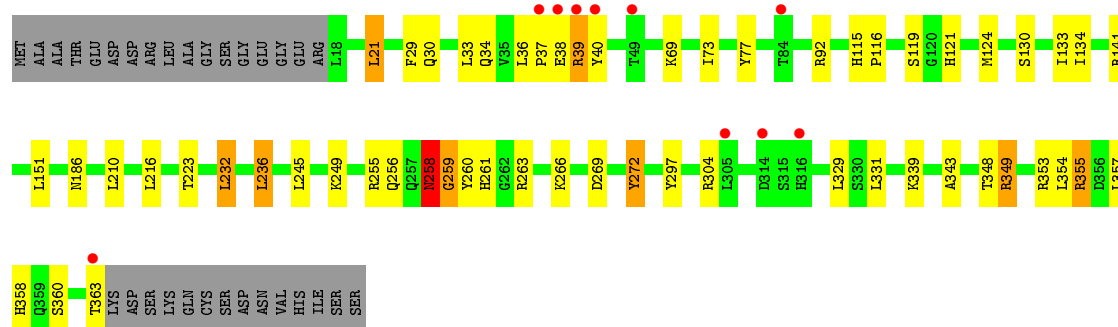
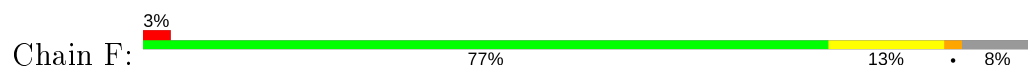
- Molecule 2: Geranylgeranyl transferase type I beta subunit



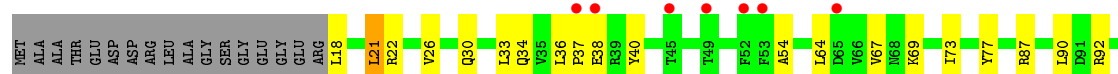
- Molecule 2: Geranylgeranyl transferase type I beta subunit

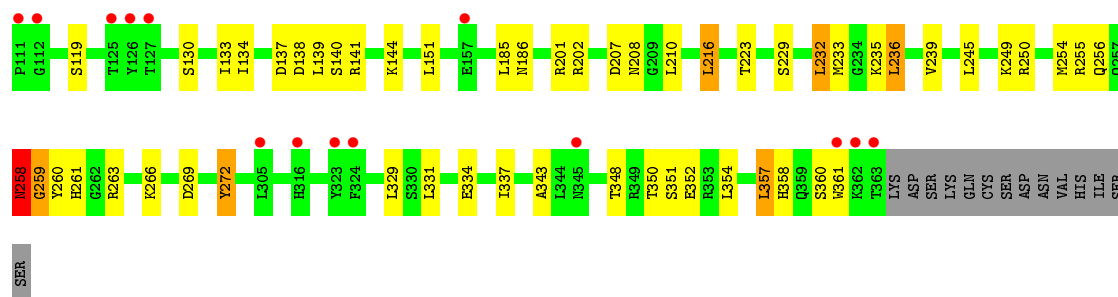


- Molecule 2: Geranylgeranyl transferase type I beta subunit

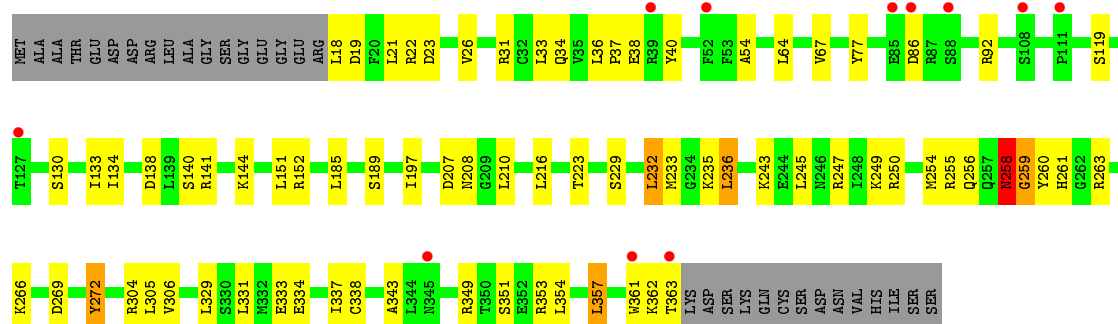


- Molecule 2: Geranylgeranyl transferase type I beta subunit

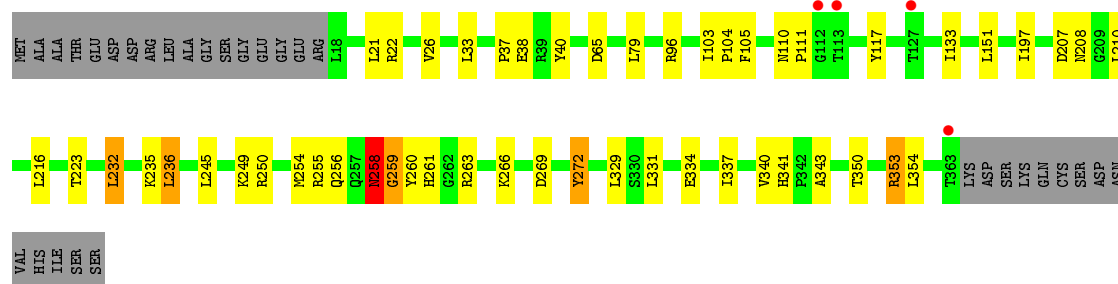
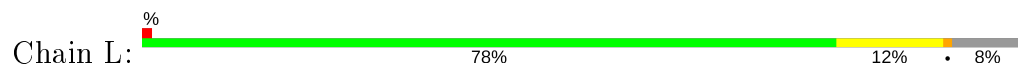




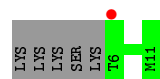
- Molecule 2: Geranylgeranyl transferase type I beta subunit



- Molecule 2: Geranylgeranyl transferase type I beta subunit



- Molecule 3: c-K-ras2 protein isoform b

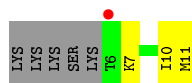
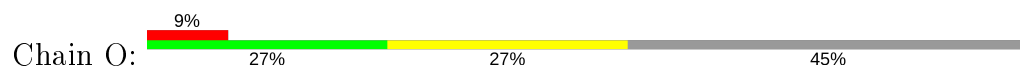


- Molecule 3: c-K-ras2 protein isoform b

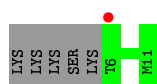




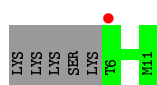
- Molecule 3: c-K-ras2 protein isoform b



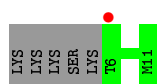
- Molecule 3: c-K-ras2 protein isoform b



- Molecule 3: c-K-ras2 protein isoform b



- Molecule 3: c-K-ras2 protein isoform b



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	272.53Å 268.48Å 185.94Å 90.00° 131.48° 90.00°	Depositor
Resolution (Å)	29.98 – 2.70 29.98 – 2.54	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.98-2.70) 85.5 (29.98-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.211 0.185 , 0.202	Depositor DCC
R_{free} test set	12637 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.089 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33292	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0/2695	0.52	0/3668
1	C	0.38	0/2709	0.54	0/3684
1	E	0.37	0/2708	0.54	0/3684
1	G	0.39	0/2699	0.54	0/3672
1	I	0.38	0/2722	0.53	0/3700
1	K	0.40	0/2737	0.55	0/3717
2	B	0.38	0/2759	0.59	2/3733 (0.1%)
2	D	0.38	0/2775	0.59	2/3752 (0.1%)
2	F	0.40	0/2780	0.61	2/3758 (0.1%)
2	H	0.36	0/2756	0.59	2/3729 (0.1%)
2	J	0.37	0/2773	0.59	2/3750 (0.1%)
2	L	0.41	0/2785	0.61	2/3764 (0.1%)
3	M	0.51	0/45	0.68	0/57
3	N	0.53	0/45	0.69	0/57
3	O	0.51	0/45	0.79	0/57
3	P	0.49	0/45	0.67	0/57
3	Q	0.57	0/45	0.73	0/57
3	R	0.55	0/45	0.70	0/57
All	All	0.38	0/33168	0.57	12/44953 (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	-5.91	98.33	113.10
2	L	259	GLY	N-CA-C	-5.89	98.37	113.10
2	F	259	GLY	N-CA-C	-5.76	98.69	113.10
2	H	259	GLY	N-CA-C	-5.76	98.71	113.10
2	B	259	GLY	N-CA-C	-5.68	98.90	113.10
2	D	259	GLY	N-CA-C	-5.67	98.93	113.10
2	D	258	ASN	N-CA-C	-5.58	95.93	111.00
2	H	258	ASN	N-CA-C	-5.40	96.43	111.00
2	B	258	ASN	N-CA-C	-5.29	96.70	111.00
2	J	258	ASN	N-CA-C	-5.29	96.71	111.00
2	L	258	ASN	N-CA-C	-5.28	96.75	111.00
2	F	258	ASN	N-CA-C	-5.14	97.11	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	2629	0	2520	52	0
1	C	2643	0	2540	39	0
1	E	2642	0	2534	40	0
1	G	2633	0	2524	45	0
1	I	2656	0	2560	42	0
1	K	2671	0	2588	38	0
2	B	2697	0	2600	45	0
2	D	2713	0	2628	43	0
2	F	2718	0	2635	35	0
2	H	2694	0	2590	49	0
2	J	2711	0	2616	47	0
2	L	2723	0	2643	27	0
3	M	46	0	52	0	0
3	N	46	0	52	0	0
3	O	46	0	52	1	0
3	P	46	0	52	0	0
3	Q	46	0	52	0	0
3	R	46	0	52	0	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	12	0	13	0	0
5	F	12	0	13	0	0
6	B	29	0	34	0	0
6	D	29	0	34	1	0
6	F	29	0	34	0	0
6	H	29	0	34	1	0
6	J	29	0	34	0	0
6	L	29	0	34	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	A	44	0	0	1	0
8	B	34	0	0	0	0
8	C	41	0	0	2	0
8	D	51	0	0	0	0
8	E	50	0	0	0	0
8	F	58	0	0	0	0
8	G	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	31	0	0	0	0
8	I	52	0	0	1	0
8	J	47	0	0	0	0
8	K	123	0	0	2	0
8	L	93	0	0	0	0
8	N	2	0	0	0	0
8	O	2	0	0	0	0
8	P	4	0	0	0	0
8	Q	2	0	0	0	0
8	R	4	0	0	0	0
All	All	33292	0	31520	485	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 8.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ILE:HG12	1:K:172:ARG:HH12	1.02	1.10
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.09	1.09
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.18	1.07
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.10	1.05
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.15	1.04
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.17	1.03
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.17	1.02
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.87	0.90
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.89	0.88
1:A:348:LYS:HA	1:A:348:LYS:HE2	1.64	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	1.84	0.77
1:I:152:MET:O	1:I:156:ILE:HG13	1.84	0.77
1:K:152:MET:O	1:K:156:ILE:HG13	1.85	0.76
2:F:355:ARG:HH11	2:F:355:ARG:HB3	1.50	0.76
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.96	0.75
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.95	0.74
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.70	0.73
1:A:339:GLU:O	1:A:343:ILE:HG13	1.90	0.72
1:C:152:MET:O	1:C:156:ILE:HG13	1.87	0.72
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.70	0.72
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.70	0.72
1:K:77:PRO:HG3	1:K:102:TYR:CZ	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.26	0.71
1:E:152:MET:O	1:E:156:ILE:HG13	1.90	0.71
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.05	0.70
2:B:39:ARG:HH11	2:B:39:ARG:CB	1.99	0.70
2:H:348:THR:O	2:H:352:GLU:HG2	1.92	0.69
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.55	0.69
1:I:333:ILE:HD13	1:I:336:LYS:HD2	1.75	0.69
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.74	0.69
1:A:91:ILE:O	1:A:91:ILE:HD12	1.93	0.68
1:I:91:ILE:HD12	1:I:91:ILE:O	1.93	0.68
2:F:339:LYS:O	2:F:348:THR:HG23	1.93	0.68
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.59	0.67
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.30	0.67
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.00	0.67
1:I:353:LYS:HG3	1:I:354:GLU:N	2.10	0.67
1:K:91:ILE:O	1:K:91:ILE:HD12	1.95	0.66
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.61	0.66
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.61	0.66
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.61	0.66
1:C:339:GLU:O	1:C:343:ILE:HG13	1.96	0.65
1:C:91:ILE:HD12	1:C:91:ILE:O	1.96	0.65
1:I:339:GLU:O	1:I:343:ILE:HG13	1.96	0.65
1:E:91:ILE:O	1:E:91:ILE:HD12	1.96	0.65
1:G:91:ILE:HD12	1:G:91:ILE:O	1.95	0.65
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.60	0.65
2:D:110:ASN:ND2	2:D:110:ASN:N	2.44	0.65
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.78	0.64
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.32	0.64
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.78	0.64
2:B:39:ARG:NH1	2:B:39:ARG:HB3	2.02	0.64
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.80	0.64
2:J:258:ASN:OD1	2:J:259:GLY:N	2.31	0.64
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.62	0.63
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.78	0.63
1:I:328:ASP:O	1:I:329:ASN:HB2	1.98	0.63
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.80	0.63
2:H:348:THR:O	2:H:351:SER:HB3	1.99	0.63
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.63	0.63
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.34	0.63
2:D:37:PRO:HB2	2:D:39:ARG:HG2	1.80	0.63
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:VAL:O	1:A:104:ARG:HD2	1.99	0.62
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.35	0.62
1:G:251:SER:HA	1:G:287:ARG:HH22	1.64	0.62
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.15	0.62
1:G:339:GLU:O	1:G:343:ILE:HG13	2.00	0.62
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.82	0.61
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.81	0.61
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.81	0.61
2:F:355:ARG:NH1	2:F:355:ARG:HB3	2.14	0.61
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.81	0.61
1:E:339:GLU:O	1:E:343:ILE:HG13	2.01	0.61
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.81	0.61
1:K:251:SER:HA	1:K:287:ARG:HH22	1.65	0.61
2:B:26:VAL:O	2:B:30:GLN:HG3	2.01	0.60
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.36	0.60
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.83	0.60
2:B:353:ARG:HH11	2:B:353:ARG:HG2	1.65	0.60
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.84	0.60
2:D:110:ASN:N	2:D:110:ASN:HD22	2.00	0.60
1:C:303:GLN:O	1:C:307:SER:HB2	2.02	0.60
1:A:332:ASP:O	1:A:336:LYS:HG3	2.01	0.59
2:H:245:LEU:O	2:H:249:LYS:HG3	2.02	0.59
1:G:334:LEU:O	1:G:338:LEU:HG	2.02	0.59
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.38	0.59
2:H:69:LYS:O	2:H:73:ILE:HG13	2.01	0.59
2:H:18:LEU:N	2:H:18:LEU:HD22	2.17	0.58
1:E:156:ILE:CG1	1:E:172:ARG:HH12	2.01	0.58
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.84	0.58
1:C:78:VAL:HG21	1:C:108:GLN:NE2	2.18	0.58
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.86	0.58
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.03	0.58
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.19	0.57
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.84	0.57
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.86	0.57
2:J:144:LYS:HG2	2:J:185:LEU:HD22	1.86	0.57
2:B:256:GLN:HG3	2:B:260:TYR:CZ	2.40	0.57
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.86	0.57
2:B:229:SER:O	2:B:233:MET:HG3	2.04	0.57
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.86	0.57
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.19	0.57
1:A:303:GLN:O	1:A:307:SER:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.85	0.57
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.40	0.57
1:I:303:GLN:N	1:I:304:PRO:HD2	2.20	0.57
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.35	0.57
1:A:287:ARG:O	1:A:291:ARG:HD3	2.05	0.57
1:C:214:ARG:HG2	1:C:214:ARG:O	2.03	0.57
1:G:334:LEU:HD22	1:G:367:HIS:O	2.04	0.57
2:H:133:ILE:HD13	2:H:354:LEU:HD13	1.87	0.57
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.05	0.56
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.87	0.56
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.86	0.56
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.87	0.56
1:I:334:LEU:HD22	1:I:367:HIS:O	2.06	0.56
2:H:210:LEU:HB2	2:H:223:THR:HA	1.87	0.56
1:E:303:GLN:N	1:E:304:PRO:HD2	2.21	0.56
1:K:303:GLN:O	1:K:307:SER:HB2	2.06	0.56
2:F:39:ARG:NH1	2:F:40:TYR:OH	2.39	0.56
2:D:69:LYS:O	2:D:73:ILE:HG13	2.05	0.55
2:L:37:PRO:HD2	2:L:40:TYR:CD1	2.41	0.55
2:D:37:PRO:HB2	2:D:39:ARG:HH11	1.72	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55
2:D:281:LYS:HE3	2:D:331:LEU:HD12	1.89	0.55
2:F:69:LYS:O	2:F:73:ILE:HG13	2.06	0.55
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.88	0.55
2:D:30:GLN:O	2:D:34:GLN:HG3	2.06	0.55
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.89	0.55
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.89	0.55
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.89	0.55
2:B:245:LEU:O	2:B:249:LYS:HG3	2.07	0.55
2:L:210:LEU:HB2	2:L:223:THR:HA	1.88	0.55
2:H:229:SER:O	2:H:233:MET:HG3	2.07	0.54
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.54
2:L:353:ARG:HD3	2:L:353:ARG:O	2.07	0.54
1:E:303:GLN:O	1:E:307:SER:HB2	2.06	0.54
2:F:210:LEU:HB2	2:F:223:THR:HA	1.89	0.54
2:F:245:LEU:O	2:F:249:LYS:HG3	2.07	0.54
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.54
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.90	0.54
1:A:284:LEU:O	1:A:287:ARG:HG2	2.08	0.54
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.22	0.54
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:334:LEU:HD22	1:K:367:HIS:O	2.08	0.53
2:B:333:GLU:OE1	2:J:23:ASP:HB2	2.08	0.53
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.43	0.53
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.89	0.53
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.90	0.53
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.42	0.53
2:J:210:LEU:HB2	2:J:223:THR:HA	1.88	0.53
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.44	0.53
1:G:59:ASP:N	1:G:59:ASP:OD1	2.41	0.53
1:I:323:LEU:HB3	1:I:367:HIS:CD2	2.44	0.53
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.90	0.53
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.73	0.53
2:B:210:LEU:HB2	2:B:223:THR:HA	1.90	0.53
1:G:303:GLN:O	1:G:307:SER:HB2	2.09	0.53
2:J:64:LEU:O	2:J:67:VAL:HG22	2.09	0.53
1:K:339:GLU:O	1:K:343:ILE:HG13	2.08	0.53
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.91	0.53
2:D:210:LEU:HB2	2:D:223:THR:HA	1.90	0.52
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.52
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.52
2:H:22:ARG:HG2	2:H:22:ARG:HH11	1.74	0.52
1:A:328:ASP:O	1:A:329:ASN:HB2	2.10	0.52
1:A:91:ILE:HD11	2:B:38:GLU:H	1.75	0.52
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.44	0.52
1:C:284:LEU:O	1:C:287:ARG:HG2	2.10	0.52
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.23	0.52
1:G:100:TYR:O	1:G:104:ARG:HG3	2.10	0.52
1:K:77:PRO:HG3	1:K:102:TYR:CE1	2.44	0.52
1:A:214:ARG:O	1:A:214:ARG:HG3	2.10	0.52
2:J:22:ARG:O	2:J:26:VAL:HG23	2.10	0.52
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.45	0.52
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.92	0.52
2:L:245:LEU:O	2:L:249:LYS:HG3	2.09	0.52
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.45	0.52
2:B:69:LYS:O	2:B:73:ILE:HG13	2.09	0.51
1:A:261:GLN:O	1:A:265:GLU:HG2	2.10	0.51
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.93	0.51
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.74	0.51
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.92	0.51
2:H:258:ASN:OD1	2:H:259:GLY:N	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:340:LEU:HD23	1:I:343:ILE:HD12	1.91	0.51
1:A:265:GLU:O	1:A:269:LEU:HD13	2.11	0.51
1:E:340:LEU:HD23	1:E:343:ILE:HD12	1.93	0.51
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.92	0.51
2:D:106:ASN:HD21	2:D:109:LYS:H	1.58	0.51
2:D:245:LEU:O	2:D:249:LYS:HG3	2.11	0.51
1:I:100:TYR:O	1:I:104:ARG:HG3	2.11	0.51
1:G:78:VAL:O	1:G:104:ARG:HD2	2.11	0.50
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.46	0.50
1:A:334:LEU:O	1:A:338:LEU:HG	2.11	0.50
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.76	0.50
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.41	0.50
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.93	0.50
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.72	0.50
2:H:133:ILE:HG22	2:H:350:THR:HG23	1.92	0.50
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.27	0.50
1:A:334:LEU:HD22	1:A:367:HIS:O	2.11	0.50
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.47	0.50
2:B:258:ASN:OD1	2:B:259:GLY:N	2.43	0.50
1:I:303:GLN:O	1:I:307:SER:HB2	2.12	0.50
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.84	0.50
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.47	0.49
1:C:334:LEU:HD22	1:C:367:HIS:O	2.12	0.49
1:G:82:ASP:HB2	1:G:86:PRO:HB3	1.94	0.49
1:A:71:GLU:CD	1:A:71:GLU:H	2.15	0.49
1:K:311:LEU:HD23	1:K:311:LEU:C	2.32	0.49
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.47	0.49
1:C:104:ARG:HG2	2:D:101:LEU:O	2.12	0.49
1:E:284:LEU:O	1:E:287:ARG:HG2	2.12	0.49
1:E:353:LYS:HE3	1:E:357:ARG:HH12	1.77	0.49
1:G:340:LEU:HD23	1:G:343:ILE:HD12	1.94	0.49
1:I:324:GLU:HA	1:I:324:GLU:OE1	2.13	0.49
1:K:251:SER:HA	1:K:287:ARG:NH2	2.28	0.49
1:K:265:GLU:O	1:K:269:LEU:HD13	2.13	0.49
1:I:311:LEU:C	1:I:311:LEU:HD23	2.33	0.49
1:I:78:VAL:O	1:I:104:ARG:HD2	2.13	0.49
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.12	0.49
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.95	0.49
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.77	0.48
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.28	0.48
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:88:VAL:O	1:K:88:VAL:HG12	2.13	0.48
2:D:39:ARG:HG2	2:D:39:ARG:HH11	1.78	0.48
2:J:351:SER:O	2:J:354:LEU:HB3	2.13	0.48
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.77	0.48
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.94	0.48
1:A:344:LEU:HA	1:A:348:LYS:HB2	1.96	0.48
2:H:130:SER:O	2:H:134:ILE:HG13	2.13	0.48
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.48
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.49	0.48
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.96	0.48
1:E:334:LEU:O	1:E:338:LEU:HG	2.13	0.48
1:G:328:ASP:O	1:G:329:ASN:HB2	2.14	0.48
1:I:144:LEU:HB2	1:I:146:LYS:HD3	1.96	0.48
2:B:250:ARG:O	2:B:254:MET:HG2	2.14	0.47
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.49	0.47
2:B:29:PHE:O	2:B:33:LEU:HD22	2.13	0.47
2:H:138:ASP:OD1	2:H:140:SER:HB3	2.15	0.47
2:H:64:LEU:O	2:H:67:VAL:HG22	2.14	0.47
2:J:229:SER:O	2:J:233:MET:HG3	2.14	0.47
2:F:130:SER:O	2:F:134:ILE:HG13	2.14	0.47
2:J:361:TRP:C	2:J:363:THR:H	2.18	0.47
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.28	0.47
1:E:334:LEU:HD22	1:E:367:HIS:O	2.14	0.47
1:C:91:ILE:HD11	2:D:38:GLU:H	1.80	0.47
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.96	0.47
1:E:265:GLU:O	1:E:269:LEU:HD13	2.15	0.47
1:G:261:GLN:O	1:G:265:GLU:HG2	2.15	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.14	0.47
2:J:33:LEU:CD2	2:J:54:ALA:HB1	2.45	0.47
1:E:91:ILE:HD11	2:F:38:GLU:H	1.79	0.47
1:A:191:ASP:O	1:A:194:ASN:HB2	2.15	0.47
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.50	0.47
2:J:207:ASP:O	2:J:208:ASN:HB2	2.15	0.47
2:J:245:LEU:O	2:J:249:LYS:HG3	2.15	0.47
1:K:114:GLU:OE2	1:K:146:LYS:NZ	2.41	0.47
1:C:265:GLU:O	1:C:269:LEU:HD13	2.14	0.46
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.79	0.46
1:A:332:ASP:OD1	1:A:336:LYS:HD2	2.15	0.46
2:J:138:ASP:OD1	2:J:140:SER:HB3	2.14	0.46
1:E:329:ASN:HB3	1:E:332:ASP:HB3	1.97	0.46
1:G:311:LEU:HD23	1:G:311:LEU:C	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:CG	1:A:214:ARG:O	2.64	0.46
1:E:331:GLU:O	1:E:335:ASN:ND2	2.48	0.46
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.50	0.46
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.97	0.46
1:I:325:ASN:O	1:I:326:GLN:C	2.53	0.46
1:K:334:LEU:O	1:K:338:LEU:HG	2.16	0.46
1:C:117:PHE:CE2	1:C:146:LYS:HE2	2.51	0.46
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.01	0.46
1:I:191:ASP:O	1:I:194:ASN:HB2	2.15	0.46
1:K:191:ASP:O	1:K:194:ASN:HB2	2.16	0.46
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.51	0.46
2:H:26:VAL:O	2:H:30:GLN:HG3	2.16	0.45
1:I:334:LEU:O	1:I:338:LEU:HG	2.16	0.45
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.15	0.45
2:J:21:LEU:HD11	2:J:304:ARG:NH2	2.30	0.45
2:L:133:ILE:HG22	2:L:350:THR:HG23	1.98	0.45
1:A:92:TYR:O	1:A:97:ARG:NH2	2.49	0.45
2:B:39:ARG:HG2	2:B:40:TYR:CE1	2.52	0.45
1:C:283:ILE:O	1:C:287:ARG:HD3	2.16	0.45
2:H:137:ASP:OD1	2:H:139:LEU:N	2.40	0.45
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.52	0.45
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.81	0.45
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.52	0.45
2:H:202:ARG:HG3	2:H:202:ARG:NH1	2.30	0.45
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.52	0.45
1:A:283:ILE:O	1:A:287:ARG:HD3	2.17	0.44
2:H:33:LEU:HD22	2:H:54:ALA:HB1	1.99	0.44
1:I:332:ASP:O	1:I:336:LYS:HG3	2.17	0.44
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.44
1:A:251:SER:HA	1:A:287:ARG:HH22	1.82	0.44
2:F:258:ASN:OD1	2:F:259:GLY:N	2.46	0.44
2:H:250:ARG:O	2:H:254:MET:HG2	2.18	0.44
2:D:130:SER:O	2:D:134:ILE:HG13	2.17	0.44
1:E:106:VAL:HG13	1:E:111:GLU:HB3	1.98	0.44
1:E:325:ASN:O	1:E:326:GLN:C	2.54	0.44
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.53	0.44
2:J:22:ARG:HG2	2:J:22:ARG:HH11	1.82	0.44
2:L:236:LEU:HD22	2:L:245:LEU:HD21	1.99	0.44
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.52	0.44
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.52	0.44
1:K:348:LYS:HD2	8:K:462:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:269:ASP:HB3	2:F:272:TYR:HD2	1.83	0.44
2:F:30:GLN:O	2:F:34:GLN:HG3	2.18	0.44
2:B:258:ASN:CG	2:B:259:GLY:H	2.20	0.44
1:I:173:ARG:HD2	8:I:403:HOH:O	2.17	0.44
2:J:138:ASP:OD1	2:J:140:SER:CB	2.66	0.44
2:F:92:ARG:HB3	2:F:119:SER:HB3	1.99	0.44
1:G:88:VAL:HG13	2:H:36:LEU:HD11	2.00	0.44
2:L:258:ASN:OD1	2:L:259:GLY:N	2.45	0.44
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.85	0.44
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.53	0.44
1:G:251:SER:HA	1:G:287:ARG:NH2	2.31	0.44
2:H:144:LYS:HD2	2:H:185:LEU:HD22	2.00	0.44
2:H:21:LEU:N	2:H:21:LEU:CD1	2.81	0.44
1:I:255:VAL:HG13	1:I:258:ARG:NH2	2.33	0.44
2:D:236:LEU:HD22	2:D:245:LEU:HD21	2.00	0.43
2:F:92:ARG:HB3	2:F:119:SER:CB	2.47	0.43
2:H:263:ARG:HB2	2:H:266:LYS:HG3	2.00	0.43
1:K:329:ASN:HB3	1:K:332:ASP:HB3	1.99	0.43
1:A:81:ASN:ND2	2:B:105:PHE:H	2.16	0.43
2:B:130:SER:O	2:B:134:ILE:HG13	2.17	0.43
1:G:65:LEU:HD12	1:G:67:ARG:NH1	2.33	0.43
2:D:106:ASN:ND2	2:D:109:LYS:H	2.16	0.43
2:D:29:PHE:O	2:D:33:LEU:HD22	2.18	0.43
2:H:236:LEU:HD22	2:H:245:LEU:HD21	2.00	0.43
2:H:235:LYS:O	2:H:239:VAL:HG23	2.17	0.43
2:H:357:LEU:O	2:H:360:SER:HB3	2.18	0.43
1:K:328:ASP:O	1:K:329:ASN:HB2	2.19	0.43
2:L:38:GLU:HG2	2:L:38:GLU:O	2.17	0.43
1:A:311:LEU:HD23	1:A:311:LEU:C	2.39	0.43
1:K:219:GLU:OE1	1:K:219:GLU:HA	2.19	0.43
2:L:263:ARG:HB2	2:L:266:LYS:HG3	2.00	0.43
1:C:78:VAL:HG21	1:C:108:GLN:HE22	1.82	0.43
1:K:184:GLN:HB2	8:K:379:HOH:O	2.18	0.43
1:K:311:LEU:HD23	1:K:311:LEU:O	2.19	0.43
2:B:357:LEU:HD22	2:B:361:TRP:NE1	2.34	0.43
1:E:65:LEU:HD12	1:E:67:ARG:NH1	2.32	0.43
2:H:207:ASP:O	2:H:208:ASN:HB2	2.19	0.43
1:I:344:LEU:HA	1:I:348:LYS:HB2	2.00	0.43
2:J:86:ASP:OD2	2:J:86:ASP:N	2.49	0.43
2:L:22:ARG:O	2:L:26:VAL:HG23	2.18	0.43
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:HD21	2:B:105:PHE:H	1.67	0.43
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.54	0.43
2:H:202:ARG:CG	2:H:202:ARG:HH11	2.31	0.43
2:J:232:LEU:HD13	2:J:343:ALA:HB1	2.00	0.43
1:C:105:ALA:O	1:C:109:ARG:HG3	2.18	0.43
1:E:239:GLN:OE1	1:E:239:GLN:HA	2.19	0.43
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.49	0.43
2:J:130:SER:O	2:J:134:ILE:HG13	2.19	0.43
2:L:103:ILE:HG23	2:L:104:PRO:HD2	2.00	0.43
2:L:22:ARG:HG2	2:L:22:ARG:NH1	2.33	0.43
2:F:29:PHE:O	2:F:33:LEU:HD22	2.19	0.43
1:G:252:ASP:OD1	1:G:255:VAL:HG23	2.19	0.43
2:L:22:ARG:HH11	2:L:22:ARG:HG2	1.82	0.43
1:C:311:LEU:HD23	1:C:311:LEU:C	2.40	0.42
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.54	0.42
1:G:287:ARG:O	1:G:291:ARG:HD3	2.19	0.42
1:G:325:ASN:O	1:G:326:GLN:C	2.57	0.42
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.82	0.42
2:D:36:LEU:HA	2:D:37:PRO:HD3	1.89	0.42
2:B:269:ASP:HB3	2:B:272:TYR:HD2	1.84	0.42
2:B:70:ASP:O	2:B:74:GLU:HG2	2.19	0.42
2:J:19:ASP:OD2	2:J:19:ASP:N	2.50	0.42
2:B:133:ILE:CD1	2:B:354:LEU:HD13	2.49	0.42
1:G:353:LYS:HB3	1:G:353:LYS:HE2	1.82	0.42
2:H:334:GLU:HB3	2:H:337:ILE:HD12	2.01	0.42
2:J:236:LEU:HD22	2:J:245:LEU:HD21	2.01	0.42
2:J:38:GLU:O	2:J:38:GLU:HG2	2.19	0.42
2:J:92:ARG:HB3	2:J:119:SER:HB3	2.00	0.42
2:B:92:ARG:HB3	2:B:119:SER:CB	2.50	0.42
2:D:22:ARG:HH11	2:D:22:ARG:HG2	1.83	0.42
2:D:250:ARG:O	2:D:254:MET:HG2	2.20	0.42
2:F:349:ARG:HH11	2:F:349:ARG:HG3	1.85	0.42
2:F:39:ARG:HG2	2:F:40:TYR:CE1	2.55	0.42
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.48	0.42
1:I:255:VAL:HG13	1:I:258:ARG:HH21	1.85	0.42
1:G:329:ASN:HB3	1:G:332:ASP:HB3	2.02	0.42
1:A:296:LEU:O	1:A:296:LEU:HD12	2.20	0.42
2:B:263:ARG:HB2	2:B:266:LYS:HG3	2.01	0.42
1:E:328:ASP:O	1:E:329:ASN:HB2	2.20	0.42
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.34	0.42
6:H:380:MGM:O1	6:H:380:MGM:HC41	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:92:ARG:HB3	2:J:119:SER:CB	2.49	0.42
1:A:184:GLN:HB2	8:A:379:HOH:O	2.20	0.42
2:D:22:ARG:O	2:D:26:VAL:HG23	2.19	0.42
2:F:266:LYS:HE3	2:F:266:LYS:HB3	1.91	0.42
2:F:360:SER:O	2:F:363:THR:HG23	2.20	0.42
2:F:36:LEU:HA	2:F:37:PRO:HD3	1.87	0.42
2:H:18:LEU:N	2:H:18:LEU:CD2	2.83	0.42
1:I:91:ILE:HG13	2:J:36:LEU:O	2.19	0.42
2:J:138:ASP:OD1	2:J:140:SER:N	2.53	0.42
2:J:269:ASP:HB3	2:J:272:TYR:HD2	1.85	0.42
1:K:325:ASN:O	1:K:326:GLN:C	2.58	0.42
2:B:207:ASP:O	2:B:208:ASN:HB2	2.19	0.42
2:D:258:ASN:CG	2:D:259:GLY:H	2.22	0.42
1:E:65:LEU:O	1:E:69:ARG:HG3	2.20	0.42
1:G:156:ILE:CG1	1:G:172:ARG:HH12	2.08	0.42
1:A:303:GLN:HB3	1:A:304:PRO:HD3	2.02	0.42
2:B:201:ARG:NH1	2:B:239:VAL:O	2.52	0.42
1:C:325:ASN:O	1:C:326:GLN:C	2.58	0.42
2:D:263:ARG:HB2	2:D:266:LYS:HG3	2.01	0.42
1:E:74:ASP:OD2	1:E:75:ILE:HG12	2.20	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.95	0.42
1:K:301:ASP:O	1:K:304:PRO:HD2	2.20	0.42
2:D:266:LYS:HB3	2:D:266:LYS:HE3	1.93	0.41
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.93	0.41
1:I:265:GLU:O	1:I:269:LEU:HD13	2.20	0.41
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.33	0.41
2:D:103:ILE:HG23	2:D:104:PRO:HD2	2.02	0.41
2:J:18:LEU:HB3	2:J:19:ASP:H	1.72	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.56	0.41
1:A:82:ASP:HB2	1:A:86:PRO:HB3	2.02	0.41
2:D:26:VAL:O	2:D:30:GLN:HG3	2.20	0.41
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.35	0.41
1:G:106:VAL:HG13	1:G:111:GLU:HB3	2.02	0.41
1:I:355:TYR:O	1:I:358:TYR:HB3	2.20	0.41
2:J:152:ARG:HD3	2:J:189:SER:O	2.21	0.41
1:K:330:LYS:HE2	1:K:367:HIS:HB3	2.01	0.41
2:L:269:ASP:HB3	2:L:272:TYR:HD2	1.85	0.41
2:D:39:ARG:H	2:D:39:ARG:NH1	2.18	0.41
2:F:357:LEU:HD23	2:F:357:LEU:HA	1.93	0.41
2:L:79:LEU:O	2:L:96:ARG:HG3	2.20	0.41
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:O	1:A:326:GLN:C	2.58	0.41
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.56	0.41
1:C:296:LEU:HD22	1:C:322:MET:HE3	2.03	0.41
1:E:308:SER:HB2	1:E:309:PRO:HD2	2.02	0.41
2:F:263:ARG:HB2	2:F:266:LYS:HG3	2.02	0.41
1:G:138:ARG:NH2	1:G:171:HIS:ND1	2.68	0.41
1:I:106:VAL:HG13	1:I:111:GLU:HB3	2.03	0.41
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.56	0.41
1:I:302:LEU:C	1:I:304:PRO:HD2	2.41	0.41
1:A:357:ARG:O	1:A:361:ARG:HG3	2.20	0.41
2:H:269:ASP:HB3	2:H:272:TYR:HD2	1.85	0.41
1:I:117:PHE:CE2	1:I:146:LYS:HE2	2.56	0.41
2:F:355:ARG:HH11	2:F:355:ARG:CB	2.24	0.41
1:K:107:LEU:HD11	2:L:117:TYR:HB2	2.03	0.41
1:C:329:ASN:HB3	1:C:332:ASP:HB3	2.03	0.41
2:F:236:LEU:HD22	2:F:245:LEU:HD21	2.03	0.41
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.86	0.41
2:J:22:ARG:HG2	2:J:22:ARG:NH1	2.36	0.41
2:J:64:LEU:HA	2:J:64:LEU:HD23	1.90	0.41
3:O:10:ILE:O	3:O:11:MET:HG3	2.20	0.41
1:C:173:ARG:HD2	8:C:400:HOH:O	2.20	0.41
1:C:286:ASP:HB2	8:C:405:HOH:O	2.19	0.41
1:G:91:ILE:HD12	2:H:38:GLU:HB2	2.03	0.41
1:I:86:PRO:HB2	1:I:89:GLN:NE2	2.35	0.41
2:L:250:ARG:O	2:L:254:MET:HG2	2.21	0.41
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.03	0.41
1:C:348:LYS:HD3	1:C:348:LYS:HA	1.93	0.41
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.03	0.41
2:H:37:PRO:HD2	2:H:40:TYR:CE1	2.56	0.41
2:J:263:ARG:HB2	2:J:266:LYS:HG3	2.02	0.41
2:B:256:GLN:HG3	2:B:260:TYR:CE1	2.55	0.40
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.37	0.40
1:G:252:ASP:C	1:G:252:ASP:OD2	2.57	0.40
1:G:287:ARG:H	1:G:287:ARG:HG2	1.60	0.40
2:J:266:LYS:HE3	2:J:266:LYS:HB3	1.94	0.40
1:K:287:ARG:HG2	1:K:287:ARG:H	1.63	0.40
2:L:207:ASP:O	2:L:208:ASN:HB2	2.21	0.40
2:L:340:VAL:HG22	2:L:341:HIS:N	2.35	0.40
1:A:333:ILE:HD13	1:A:336:LYS:HD3	2.03	0.40
1:A:81:ASN:HD21	2:B:104:PRO:HA	1.85	0.40
1:E:105:ALA:O	1:E:109:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:243:LYS:O	2:J:247:ARG:HG3	2.22	0.40
2:J:250:ARG:O	2:J:254:MET:HG2	2.21	0.40
2:B:33:LEU:CD2	2:B:54:ALA:HB1	2.52	0.40
1:C:106:VAL:HG13	1:C:111:GLU:HB3	2.03	0.40
1:C:88:VAL:HG13	2:D:36:LEU:HD11	2.03	0.40
1:E:78:VAL:O	1:E:104:ARG:HD2	2.21	0.40
1:E:283:ILE:O	1:E:287:ARG:HD3	2.22	0.40
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.57	0.40
2:D:173:ARG:HG2	6:D:380:MGM:H112	2.03	0.40
1:E:328:ASP:O	1:E:329:ASN:CB	2.70	0.40
2:H:201:ARG:NH1	2:H:239:VAL:O	2.54	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%)	289 (93%)	22 (7%)	1 (0%)	41	66
1	C	312/377 (83%)	293 (94%)	18 (6%)	1 (0%)	41	66
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	41	66
1	G	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	41	66
1	I	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	41	66
1	K	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
2	B	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	41	66
2	D	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	41	66
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	41	66
2	H	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	41	66
2	J	344/377 (91%)	329 (96%)	11 (3%)	4 (1%)	13	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	41	66
3	M	4/11 (36%)	4 (100%)	0	0	100	100
3	N	4/11 (36%)	4 (100%)	0	0	100	100
3	O	4/11 (36%)	4 (100%)	0	0	100	100
3	P	4/11 (36%)	4 (100%)	0	0	100	100
3	Q	4/11 (36%)	4 (100%)	0	0	100	100
3	R	4/11 (36%)	4 (100%)	0	0	100	100
All	All	3960/4590 (86%)	3761 (95%)	185 (5%)	14 (0%)	34	60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	258	ASN
1	E	326	GLN
1	G	326	GLN
2	J	333	GLU
2	J	362	LYS
1	C	326	GLN
2	D	258	ASN
2	F	258	ASN
2	H	258	ASN
1	I	326	GLN
2	J	258	ASN
2	L	258	ASN
1	A	326	GLN
2	J	34	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/338 (83%)	273 (98%)	7 (2%)	47	76
1	C	283/338 (84%)	275 (97%)	8 (3%)	43	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	284/338 (84%)	276 (97%)	8 (3%)	43	73
1	G	281/338 (83%)	277 (99%)	4 (1%)	67	86
1	I	287/338 (85%)	280 (98%)	7 (2%)	49	77
1	K	291/338 (86%)	286 (98%)	5 (2%)	60	84
2	B	289/326 (89%)	275 (95%)	14 (5%)	25	53
2	D	293/326 (90%)	279 (95%)	14 (5%)	25	53
2	F	294/326 (90%)	281 (96%)	13 (4%)	28	56
2	H	288/326 (88%)	278 (96%)	10 (4%)	36	65
2	J	292/326 (90%)	280 (96%)	12 (4%)	30	59
2	L	296/326 (91%)	283 (96%)	13 (4%)	28	56
3	M	6/11 (54%)	6 (100%)	0	100	100
3	N	6/11 (54%)	6 (100%)	0	100	100
3	O	6/11 (54%)	5 (83%)	1 (17%)	2	5
3	P	6/11 (54%)	6 (100%)	0	100	100
3	Q	6/11 (54%)	6 (100%)	0	100	100
3	R	6/11 (54%)	6 (100%)	0	100	100
All	All	3494/4050 (86%)	3378 (97%)	116 (3%)	38	67

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	107	LEU
1	A	182	PRO
1	A	194	ASN
1	A	214	ARG
1	A	287	ARG
1	A	332	ASP
2	B	21	LEU
2	B	33	LEU
2	B	39	ARG
2	B	113	THR
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU

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Mol	Chain	Res	Type
2	B	255	ARG
2	B	261	HIS
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	59	ASP
1	C	71	GLU
1	C	107	LEU
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	33	LEU
2	D	39	ARG
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	353	ARG
1	E	67	ARG
1	E	71	GLU
1	E	107	LEU
1	E	214	ARG
1	E	225	GLN
1	E	265	GLU
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	39	ARG
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU

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Mol	Chain	Res	Type
2	F	255	ARG
2	F	261	HIS
2	F	329	LEU
2	F	331	LEU
2	F	349	ARG
2	F	353	ARG
2	F	355	ARG
1	G	59	ASP
1	G	107	LEU
1	G	211	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	329	LEU
2	H	331	LEU
2	H	357	LEU
1	I	67	ARG
1	I	107	LEU
1	I	142	ARG
1	I	211	GLN
1	I	287	ARG
1	I	324	GLU
1	I	332	ASP
2	J	31	ARG
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	255	ARG
2	J	261	HIS
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	353	ARG
2	J	357	LEU
1	K	71	GLU
1	K	107	LEU

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Mol	Chain	Res	Type
1	K	142	ARG
1	K	287	ARG
1	K	301	ASP
2	L	21	LEU
2	L	33	LEU
2	L	65	ASP
2	L	151	LEU
2	L	216	LEU
2	L	232	LEU
2	L	236	LEU
2	L	255	ARG
2	L	258	ASN
2	L	261	HIS
2	L	329	LEU
2	L	331	LEU
2	L	353	ARG
3	O	7	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	89	GLN
1	A	194	ASN
1	A	201	HIS
1	A	278	ASN
1	A	329	ASN
1	A	335	ASN
1	C	81	ASN
1	C	108	GLN
1	C	201	HIS
1	C	218	ASN
1	C	298	GLN
1	C	364	GLN
2	D	106	ASN
2	D	110	ASN
2	D	246	ASN
1	E	81	ASN
1	E	145	GLN
1	E	184	GLN
1	E	225	GLN
1	E	325	ASN

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Mol	Chain	Res	Type
1	E	335	ASN
2	F	30	GLN
2	F	246	ASN
1	G	81	ASN
1	G	89	GLN
1	G	149	GLN
1	G	162	GLN
1	G	184	GLN
1	G	201	HIS
1	G	297	ASN
1	G	325	ASN
1	G	335	ASN
1	I	81	ASN
1	I	89	GLN
1	I	195	GLN
1	I	201	HIS
1	I	364	GLN
1	I	367	HIS
2	J	246	ASN
1	K	201	HIS
1	K	325	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 ⓘ

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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MGM	B	380	-	26,28,28	0.95	2 (7%)	33,37,37	2.03	5 (15%)
6	MGM	L	380	-	26,28,28	0.99	2 (7%)	33,37,37	2.03	5 (15%)
5	MES	F	380	-	12,12,12	9.13	8 (66%)	14,16,16	2.47	5 (35%)
6	MGM	H	380	-	26,28,28	0.91	2 (7%)	33,37,37	1.96	5 (15%)
6	MGM	J	379	-	26,28,28	0.98	2 (7%)	33,37,37	2.03	6 (18%)
5	MES	B	379	-	12,12,12	8.94	8 (66%)	14,16,16	2.44	5 (35%)
6	MGM	F	381	-	26,28,28	0.99	2 (7%)	33,37,37	2.03	6 (18%)
6	MGM	D	380	-	26,28,28	0.97	2 (7%)	33,37,37	2.05	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
6	MGM	B	380	-	-	9/31/31/31	-
6	MGM	L	380	-	-	8/31/31/31	-
5	MES	F	380	-	-	3/6/14/14	0/1/1/1
6	MGM	H	380	-	-	9/31/31/31	-
6	MGM	J	379	-	-	9/31/31/31	-
5	MES	B	379	-	-	1/6/14/14	0/1/1/1
6	MGM	F	381	-	-	9/31/31/31	-
6	MGM	D	380	-	-	8/31/31/31	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	380	MES	C8-S	-24.08	1.43	1.77
5	B	379	MES	C8-S	-22.34	1.45	1.77
5	B	379	MES	O2S-S	12.99	1.83	1.45
5	F	380	MES	O2S-S	12.46	1.81	1.45
5	B	379	MES	O1S-S	12.45	1.81	1.45
5	F	380	MES	O1S-S	11.49	1.78	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	379	MES	O3S-S	9.81	1.82	1.47
5	F	380	MES	O3S-S	9.28	1.80	1.47
5	F	380	MES	C7-C8	-4.80	1.39	1.52
5	B	379	MES	C7-C8	-4.42	1.40	1.52
5	F	380	MES	C3-C2	-2.67	1.40	1.50
5	F	380	MES	C7-N4	-2.51	1.41	1.47
6	L	380	MGM	C7-C8	2.47	1.38	1.33
5	B	379	MES	C3-C2	-2.40	1.41	1.50
6	F	381	MGM	C7-C8	2.36	1.38	1.33
5	F	380	MES	C5-C6	-2.36	1.41	1.50
6	D	380	MGM	C7-C8	2.21	1.38	1.33
6	B	380	MGM	C12-C13	2.19	1.38	1.33
6	J	379	MGM	C7-C8	2.19	1.38	1.33
6	B	380	MGM	C7-C8	2.17	1.38	1.33
5	B	379	MES	C5-C6	-2.16	1.42	1.50
5	B	379	MES	C7-N4	-2.15	1.42	1.47
6	L	380	MGM	C12-C13	2.13	1.38	1.33
6	J	379	MGM	C12-C13	2.10	1.38	1.33
6	D	380	MGM	C12-C13	2.08	1.38	1.33
6	F	381	MGM	C12-C13	2.06	1.37	1.33
6	H	380	MGM	C7-C8	2.03	1.37	1.33
6	H	380	MGM	C12-C13	2.00	1.37	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	380	MGM	C1-C2-N3	7.36	131.26	113.31
6	F	381	MGM	C1-C2-N3	7.27	131.04	113.31
6	D	380	MGM	C1-C2-N3	7.24	130.95	113.31
6	L	380	MGM	C1-C2-N3	7.15	130.73	113.31
6	J	379	MGM	C1-C2-N3	7.12	130.65	113.31
6	H	380	MGM	C1-C2-N3	6.85	130.00	113.31
5	B	379	MES	O1S-S-C8	5.87	113.98	106.92
6	J	379	MGM	C4-N3-C2	5.52	125.70	110.62
6	D	380	MGM	C4-N3-C2	5.46	125.53	110.62
6	F	381	MGM	C4-N3-C2	5.36	125.27	110.62
6	L	380	MGM	C4-N3-C2	5.33	125.17	110.62
6	B	380	MGM	C4-N3-C2	5.30	125.08	110.62
5	F	380	MES	O1S-S-C8	5.29	113.28	106.92
6	H	380	MGM	C4-N3-C2	5.21	124.85	110.62
5	F	380	MES	O3S-S-C8	4.62	113.24	105.77
5	B	379	MES	O3S-S-C8	4.53	113.10	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	380	MGM	O1-C1-C2	4.23	115.51	107.27
6	D	380	MGM	O1-C1-C2	4.11	115.26	107.27
6	B	380	MGM	O1-C1-C2	4.08	115.21	107.27
6	F	381	MGM	O1-C1-C2	4.04	115.14	107.27
6	H	380	MGM	O1-C1-C2	3.81	114.68	107.27
6	J	379	MGM	O1-C1-C2	3.73	114.53	107.27
5	F	380	MES	O2S-S-C8	3.67	111.33	106.92
6	L	380	MGM	O1B-PB-O3A	2.76	113.88	104.64
5	F	380	MES	O3S-S-O2S	-2.71	104.64	111.27
5	B	379	MES	O2S-S-C8	2.71	110.18	106.92
6	J	379	MGM	O1B-PB-O3A	2.70	113.70	104.64
6	H	380	MGM	C2-N3-C5	2.68	122.72	111.92
6	B	380	MGM	C2-N3-C5	2.64	122.55	111.92
6	F	381	MGM	C2-N3-C5	2.61	122.44	111.92
6	L	380	MGM	C2-N3-C5	2.61	122.43	111.92
6	D	380	MGM	O1B-PB-O3A	2.59	113.33	104.64
6	B	380	MGM	O1B-PB-O3A	2.56	113.21	104.64
6	F	381	MGM	O1B-PB-O3A	2.55	113.19	104.64
6	D	380	MGM	C2-N3-C5	2.53	122.13	111.92
6	J	379	MGM	C2-N3-C5	2.48	121.91	111.92
6	H	380	MGM	O1B-PB-O3A	2.43	112.78	104.64
5	B	379	MES	O3S-S-O2S	-2.42	105.37	111.27
5	F	380	MES	O2S-S-O1S	-2.17	106.43	113.95
5	B	379	MES	O2S-S-O1S	-2.17	106.43	113.95
6	J	379	MGM	C10-C8-C9	-2.10	111.74	115.27
6	F	381	MGM	C10-C8-C9	-2.04	111.83	115.27

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	380	MGM	C1-C2-N3-C4
6	B	380	MGM	O1-C1-C2-N3
6	B	380	MGM	PA-O3A-PB-O1B
6	L	380	MGM	C1-C2-N3-C4
6	L	380	MGM	O1-C1-C2-N3
6	L	380	MGM	PA-O3A-PB-O1B
5	F	380	MES	C7-C8-S-O2S
5	F	380	MES	C7-C8-S-O3S
6	H	380	MGM	C1-C2-N3-C4
6	H	380	MGM	O1-C1-C2-N3
6	H	380	MGM	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	B	379	MES	N4-C7-C8-S
6	J	379	MGM	C1-C2-N3-C4
6	J	379	MGM	O1-C1-C2-N3
6	J	379	MGM	PA-O3A-PB-O1B
6	F	381	MGM	C1-C2-N3-C4
6	F	381	MGM	O1-C1-C2-N3
6	F	381	MGM	PA-O3A-PB-O1B
6	D	380	MGM	C1-C2-N3-C4
6	D	380	MGM	O1-C1-C2-N3
6	D	380	MGM	PA-O3A-PB-O1B
6	B	380	MGM	C6-C5-N3-C4
6	L	380	MGM	C6-C5-N3-C4
6	H	380	MGM	C6-C5-N3-C4
6	J	379	MGM	C6-C5-N3-C4
6	F	381	MGM	C6-C5-N3-C4
6	D	380	MGM	C6-C5-N3-C4
6	B	380	MGM	C10-C8-C9-C11
5	F	380	MES	C7-C8-S-O1S
6	D	380	MGM	C10-C8-C9-C11
6	H	380	MGM	C10-C8-C9-C11
6	L	380	MGM	C10-C8-C9-C11
6	J	379	MGM	C10-C8-C9-C11
6	F	381	MGM	C10-C8-C9-C11
6	B	380	MGM	C7-C8-C9-C11
6	H	380	MGM	C7-C8-C9-C11
6	L	380	MGM	C7-C8-C9-C11
6	J	379	MGM	C7-C8-C9-C11
6	F	381	MGM	C7-C8-C9-C11
6	D	380	MGM	C7-C8-C9-C11
6	J	379	MGM	PA-O3A-PB-O3B
6	F	381	MGM	PA-O3A-PB-O3B
6	B	380	MGM	PA-O3A-PB-O2B
6	L	380	MGM	PA-O3A-PB-O2B
6	H	380	MGM	PA-O3A-PB-O2B
6	J	379	MGM	PA-O3A-PB-O2B
6	F	381	MGM	PA-O3A-PB-O2B
6	D	380	MGM	PA-O3A-PB-O2B
6	B	380	MGM	C9-C11-C12-C13
6	L	380	MGM	C9-C11-C12-C13
6	H	380	MGM	C9-C11-C12-C13
6	J	379	MGM	C9-C11-C12-C13
6	F	381	MGM	C9-C11-C12-C13

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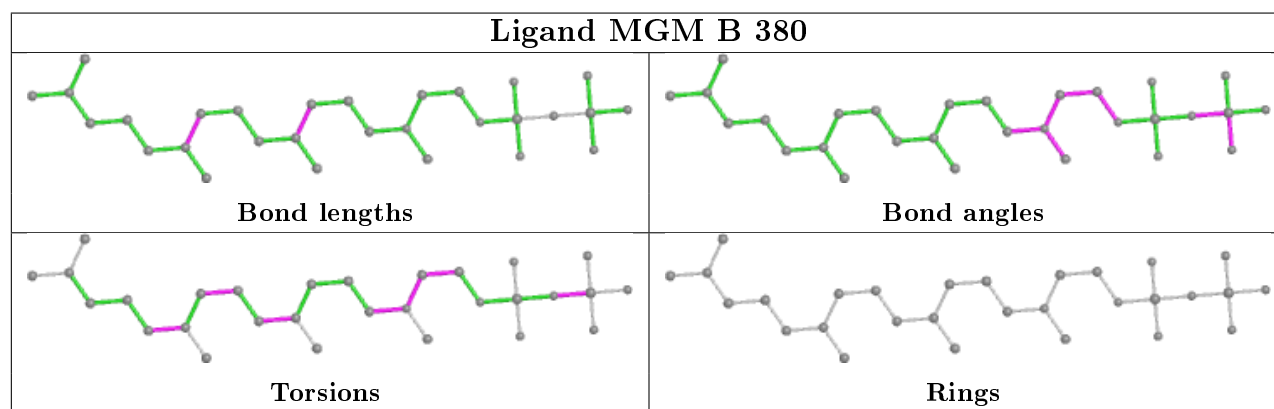
Mol	Chain	Res	Type	Atoms
6	D	380	MGM	C9-C11-C12-C13
6	B	380	MGM	C14-C13-C15-C16
6	H	380	MGM	C14-C13-C15-C16

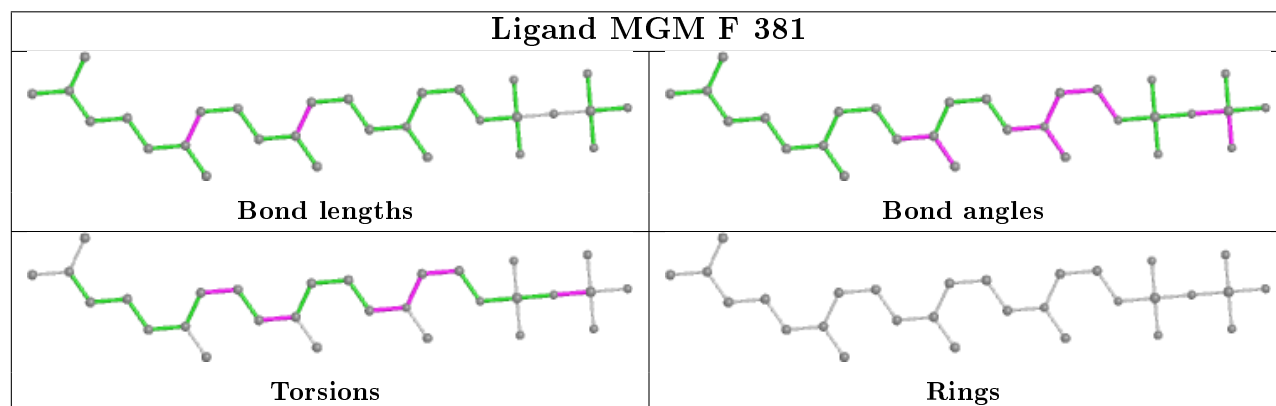
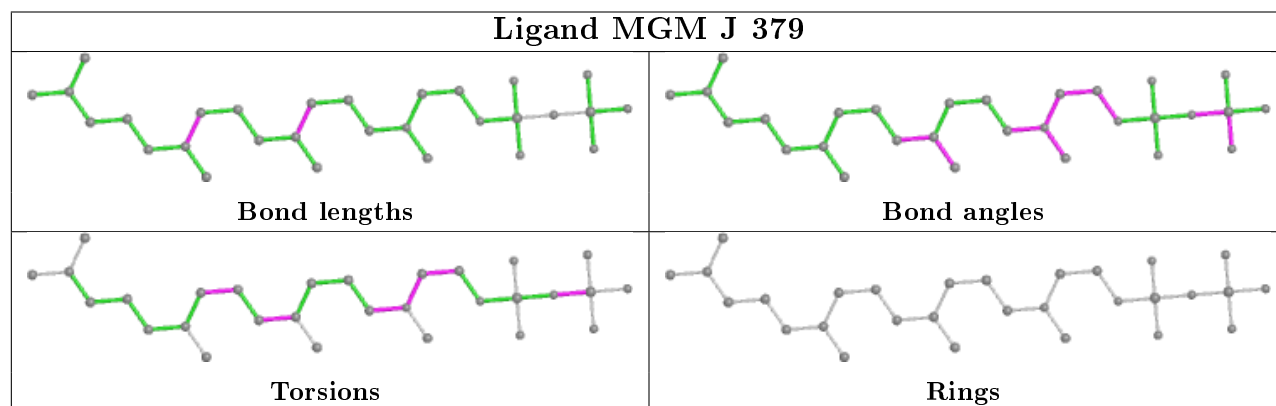
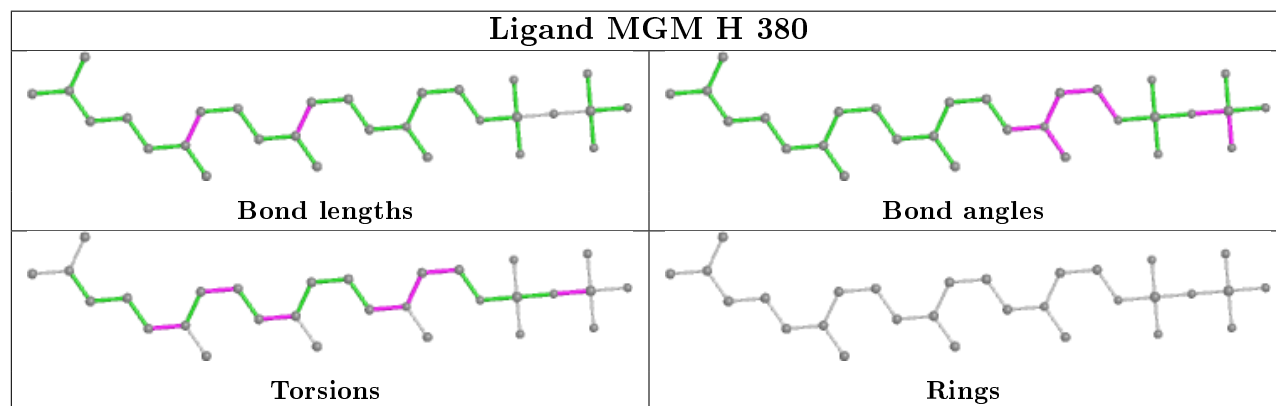
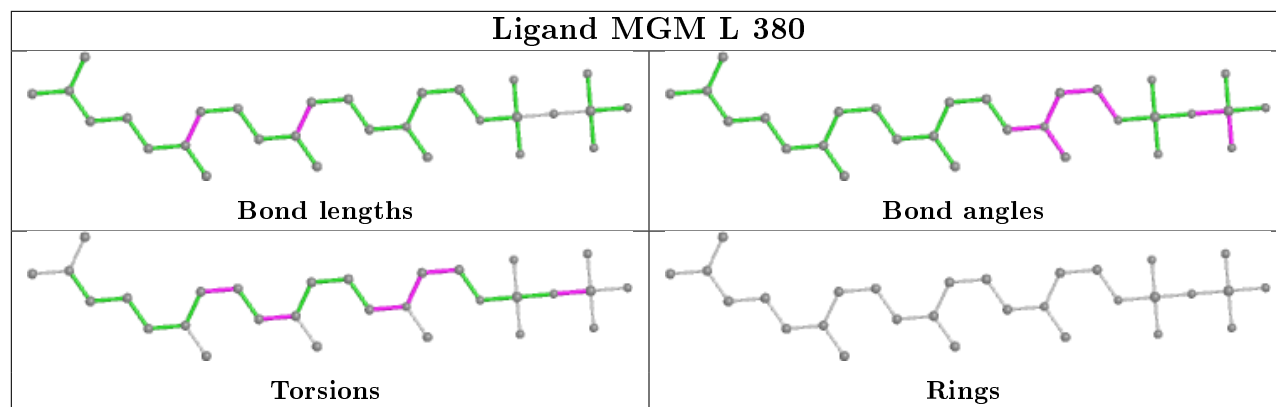
There are no ring outliers.

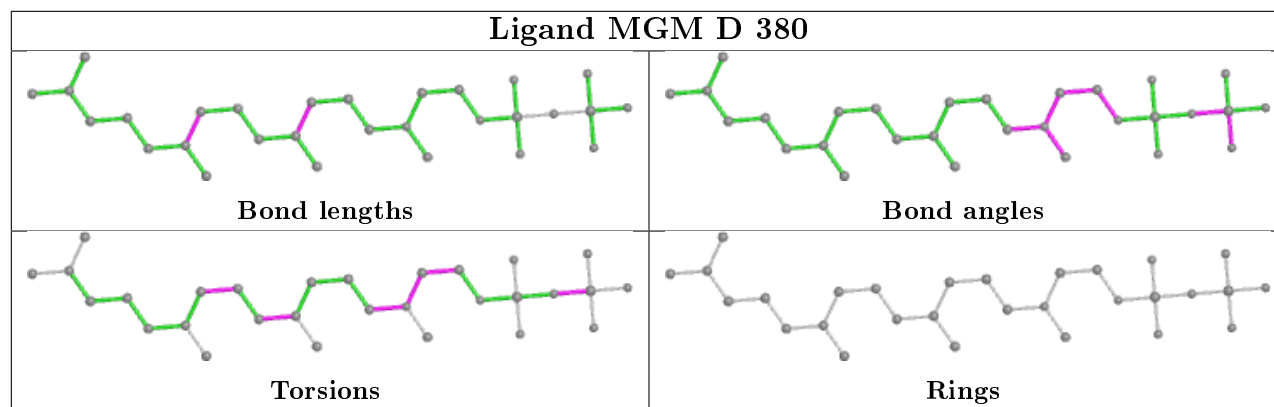
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	380	MGM	1	0
6	D	380	MGM	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	314/377 (83%)	-0.06	13 (4%) 37 36	47, 69, 103, 119	0
1	C	314/377 (83%)	-0.16	7 (2%) 62 63	44, 66, 94, 111	0
1	E	314/377 (83%)	-0.09	6 (1%) 66 69	42, 67, 96, 113	0
1	G	314/377 (83%)	-0.16	9 (2%) 51 52	43, 65, 96, 109	0
1	I	314/377 (83%)	-0.06	15 (4%) 30 28	43, 68, 98, 109	0
1	K	314/377 (83%)	-0.32	5 (1%) 72 74	35, 55, 80, 94	0
2	B	346/377 (91%)	-0.07	8 (2%) 60 62	48, 63, 89, 112	0
2	D	346/377 (91%)	-0.05	15 (4%) 35 33	43, 59, 86, 103	0
2	F	346/377 (91%)	-0.12	10 (2%) 51 52	42, 56, 84, 108	0
2	H	346/377 (91%)	0.11	21 (6%) 21 20	44, 72, 102, 119	0
2	J	346/377 (91%)	-0.03	11 (3%) 47 48	45, 65, 92, 117	0
2	L	346/377 (91%)	-0.14	4 (1%) 79 80	39, 53, 77, 106	0
3	M	6/11 (54%)	0.03	1 (16%) 1 1	53, 57, 78, 88	0
3	N	6/11 (54%)	0.00	0 100 100	53, 59, 78, 83	0
3	O	6/11 (54%)	0.23	1 (16%) 1 1	50, 58, 77, 85	0
3	P	6/11 (54%)	0.37	1 (16%) 1 1	60, 69, 86, 92	0
3	Q	6/11 (54%)	0.42	1 (16%) 1 1	51, 63, 82, 91	0
3	R	6/11 (54%)	0.35	1 (16%) 1 1	47, 58, 76, 84	0
All	All	3996/4590 (87%)	-0.09	129 (3%) 47 48	35, 63, 93, 119	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	5.3
2	B	363	THR	5.0
1	C	55	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
3	P	6	THR	4.0
1	C	306	HIS	4.0
1	I	328	ASP	3.9
1	E	306	HIS	3.9
2	D	363	THR	3.9
2	H	363	THR	3.8
1	A	329	ASN	3.8
2	L	363	THR	3.7
1	E	55	PHE	3.7
2	J	363	THR	3.6
2	H	65	ASP	3.5
1	A	328	ASP	3.5
1	I	306	HIS	3.5
1	A	368	SER	3.5
1	A	304	PRO	3.4
1	E	91	ILE	3.4
2	F	39	ARG	3.4
2	H	111	PRO	3.3
2	B	362	LYS	3.3
2	F	363	THR	3.2
2	H	126	TYR	3.1
1	G	326	GLN	3.1
2	H	53	PHE	3.0
2	D	39	ARG	3.0
3	Q	6	THR	3.0
1	I	368	SER	3.0
2	H	112	GLY	3.0
1	G	306	HIS	3.0
1	I	327	CYS	3.0
2	F	305	LEU	3.0
1	I	326	GLN	3.0
2	J	108	SER	3.0
2	H	362	LYS	2.9
1	G	305	SER	2.9
2	F	40	TYR	2.9
1	A	330	LYS	2.9
1	I	305	SER	2.9
2	H	127	THR	2.9
1	E	328	ASP	2.9
1	K	328	ASP	2.9
1	I	329	ASN	2.9
2	H	305	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	111	PRO	2.8
2	H	45	THR	2.8
2	B	305	LEU	2.8
2	J	85	GLU	2.7
2	B	86	ASP	2.7
1	K	55	PHE	2.7
1	C	304	PRO	2.7
2	D	127	THR	2.7
2	D	110	ASN	2.7
2	H	361	TRP	2.7
2	B	39	ARG	2.7
2	H	38	GLU	2.6
2	B	37	PRO	2.6
1	I	367	HIS	2.6
1	C	305	SER	2.6
1	G	327	CYS	2.6
1	K	305	SER	2.6
2	D	126	TYR	2.6
1	G	304	PRO	2.5
1	I	304	PRO	2.5
2	H	37	PRO	2.5
1	A	91	ILE	2.5
1	G	56	LEU	2.5
1	I	251	SER	2.5
3	R	6	THR	2.4
1	A	314	PHE	2.4
1	C	327	CYS	2.4
2	D	90	LEU	2.4
2	H	49	THR	2.4
2	J	361	TRP	2.4
1	G	367	HIS	2.4
1	A	305	SER	2.4
2	D	305	LEU	2.4
3	M	6	THR	2.4
2	J	86	ASP	2.3
1	A	281	LYS	2.3
1	C	328	ASP	2.3
1	I	364	GLN	2.3
2	H	157	GLU	2.3
2	D	38	GLU	2.3
2	D	361	TRP	2.3
2	D	362	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	345	ASN	2.3
2	F	84	THR	2.3
1	I	84	PRO	2.3
1	I	85	SER	2.3
1	K	84	PRO	2.3
2	D	37	PRO	2.3
2	J	88	SER	2.3
1	A	278	ASN	2.3
1	E	278	ASN	2.3
2	F	49	THR	2.3
2	J	345	ASN	2.2
2	J	127	THR	2.2
2	J	39	ARG	2.2
2	H	52	PHE	2.2
2	J	111	PRO	2.2
1	I	91	ILE	2.2
2	F	316	HIS	2.2
2	H	316	HIS	2.2
3	O	6	THR	2.2
2	D	113	THR	2.2
2	H	125	THR	2.2
2	F	37	PRO	2.2
1	E	305	SER	2.1
1	A	326	GLN	2.1
2	L	113	THR	2.1
2	L	127	THR	2.1
1	C	329	ASN	2.1
2	J	52	PHE	2.1
2	F	314	ASP	2.1
2	H	324	PHE	2.1
2	D	314	ASP	2.1
1	I	330	LYS	2.1
2	D	316	HIS	2.1
1	G	368	SER	2.1
2	F	38	GLU	2.1
1	K	85	SER	2.1
2	H	323	TYR	2.1
2	B	40	TYR	2.0
1	A	313	ALA	2.0
1	A	306	HIS	2.0
2	L	112	GLY	2.0
2	B	87	ARG	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](#)

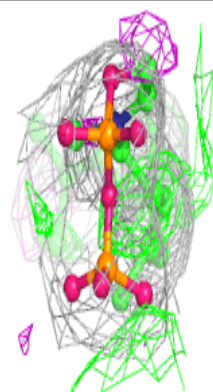
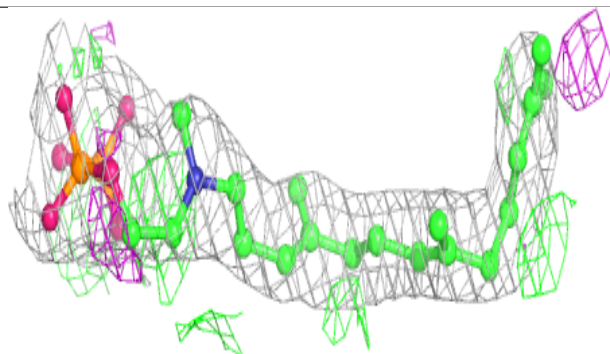
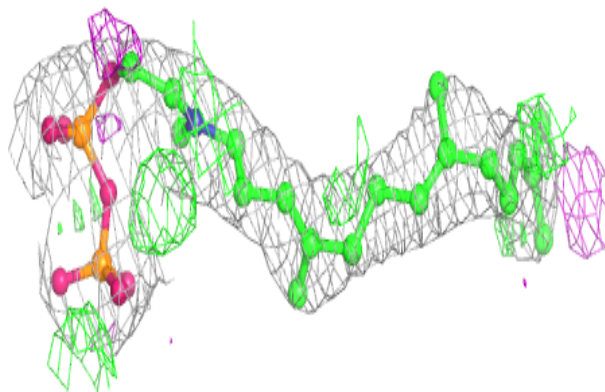
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MES	B	379	12/12	0.88	0.25	99,108,110,110	0
6	MGM	H	380	29/29	0.95	0.19	56,65,74,75	0
6	MGM	J	379	29/29	0.95	0.23	50,58,70,71	0
5	MES	F	380	12/12	0.96	0.22	86,94,97,97	0
6	MGM	L	380	29/29	0.96	0.22	41,54,65,67	0
7	CL	D	379	1/1	0.96	0.08	62,62,62,62	0
6	MGM	F	381	29/29	0.96	0.19	49,56,66,69	0
6	MGM	D	380	29/29	0.96	0.17	50,59,67,69	0
6	MGM	B	380	29/29	0.97	0.19	52,59,69,72	0
7	CL	L	379	1/1	0.98	0.04	59,59,59,59	0
7	CL	H	379	1/1	0.98	0.07	69,69,69,69	0
4	ZN	L	378	1/1	0.99	0.09	46,46,46,46	0
4	ZN	F	378	1/1	0.99	0.08	48,48,48,48	0
4	ZN	H	378	1/1	0.99	0.09	60,60,60,60	0
7	CL	F	379	1/1	0.99	0.10	55,55,55,55	0
4	ZN	B	378	1/1	0.99	0.08	51,51,51,51	0
4	ZN	J	378	1/1	0.99	0.08	53,53,53,53	0
4	ZN	D	378	1/1	1.00	0.09	53,53,53,53	0

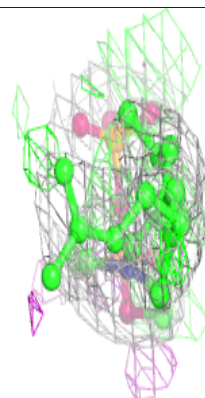
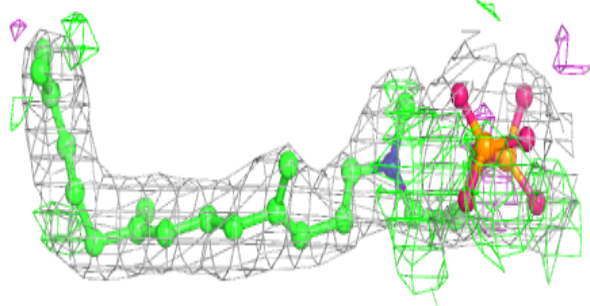
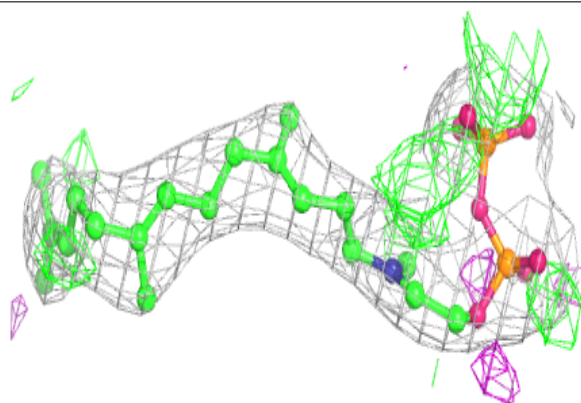
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

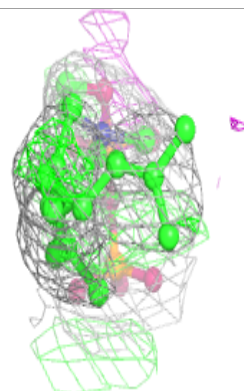
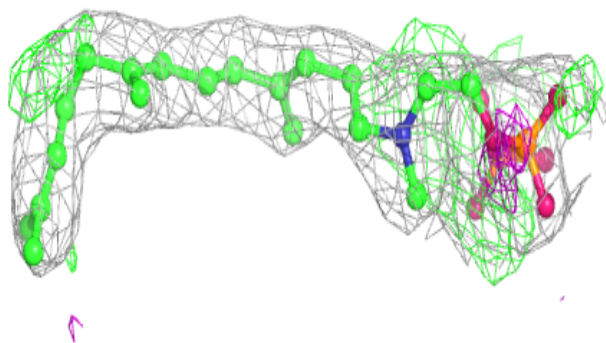
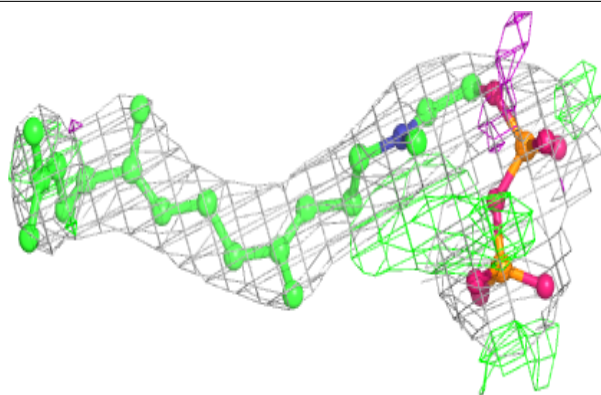
**Electron density around MGM J 379:**

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

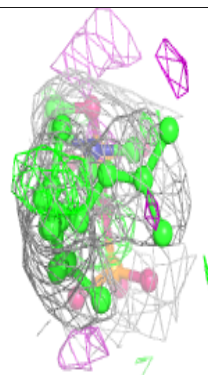
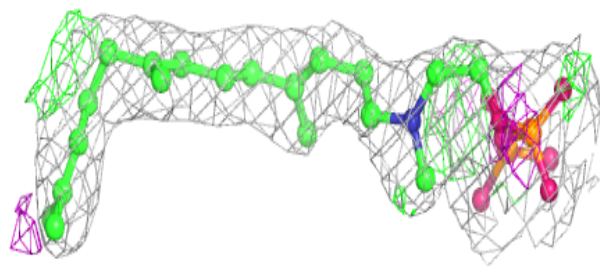
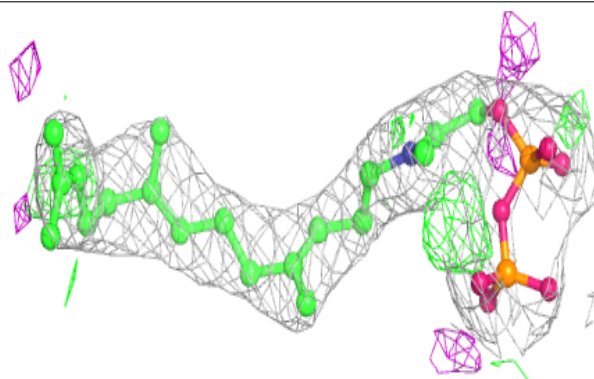


Electron density around MGM L 380:

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

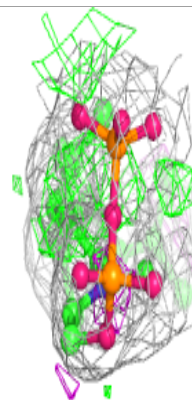
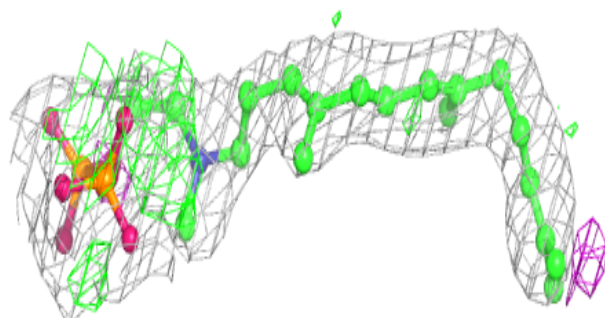
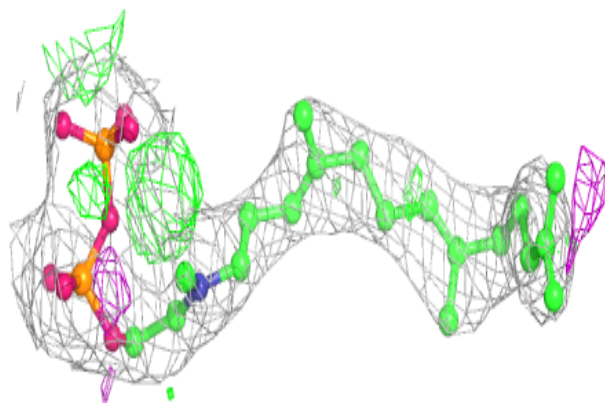
**Electron density around MGM F 381:**

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

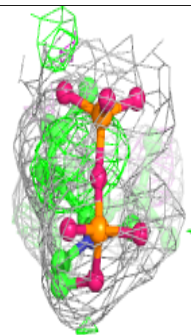
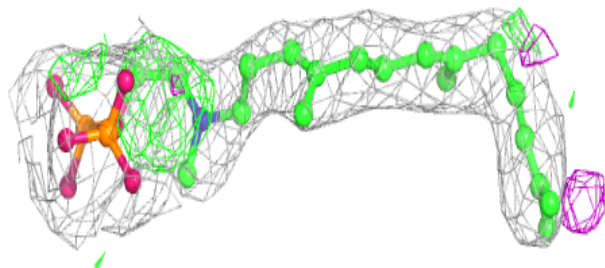
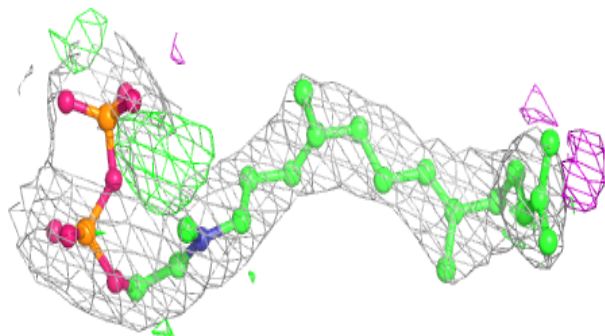


Electron density around MGM D 380:

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

**Electron density around MGM B 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.