



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:13 AM UTC

PDB ID : 1TNU / pdb_00001tnu
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 types of validation reports are described at

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

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

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

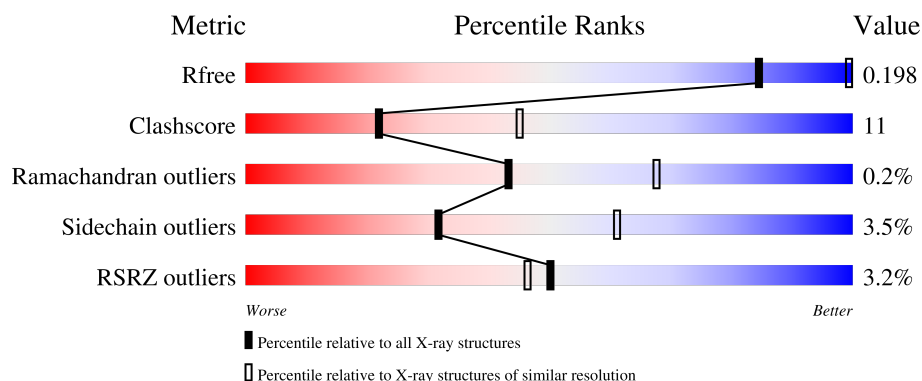
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	3% 59% 22% • 17%
1	C	377	2% 62% 20% • 17%
1	E	377	2% 59% 24% • 17%
1	G	377	4% 59% 23% • 17%
1	I	377	4% 64% 18% • 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	377	 2% 64% 19% 17%
2	B	377	 2% 68% 21% 8%
2	D	377	 2% 67% 23% 8%
2	F	377	 2% 71% 18% 8%
2	H	377	 4% 67% 22% 8%
2	J	377	 4% 67% 23% 8%
2	L	377	 2% 73% 18% 8%
3	M	9	 11% 67% 33%
3	N	9	 11% 67% 33%
3	O	9	 11% 56% 11% 33%
3	P	9	 11% 56% 11% 33%
3	Q	9	 67% 33%
3	R	9	 56% 11% 33%

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			

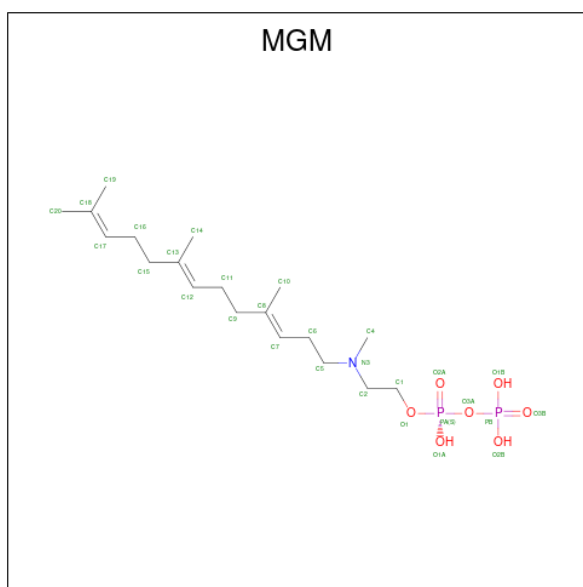
- Molecule 3 is a protein called Transforming protein RhoB.

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: 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		

Continued on next page...

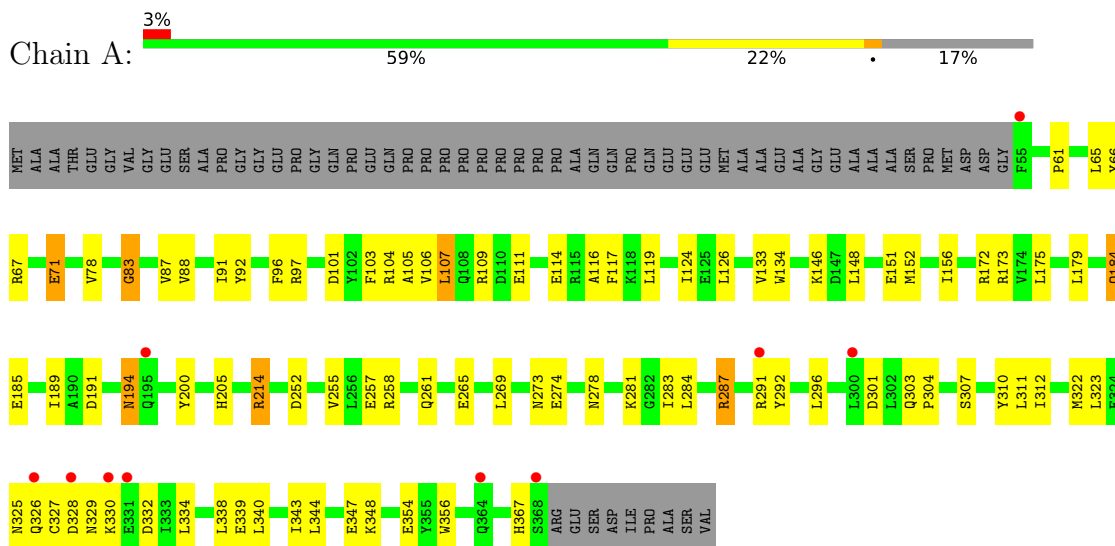
Continued from previous page...

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

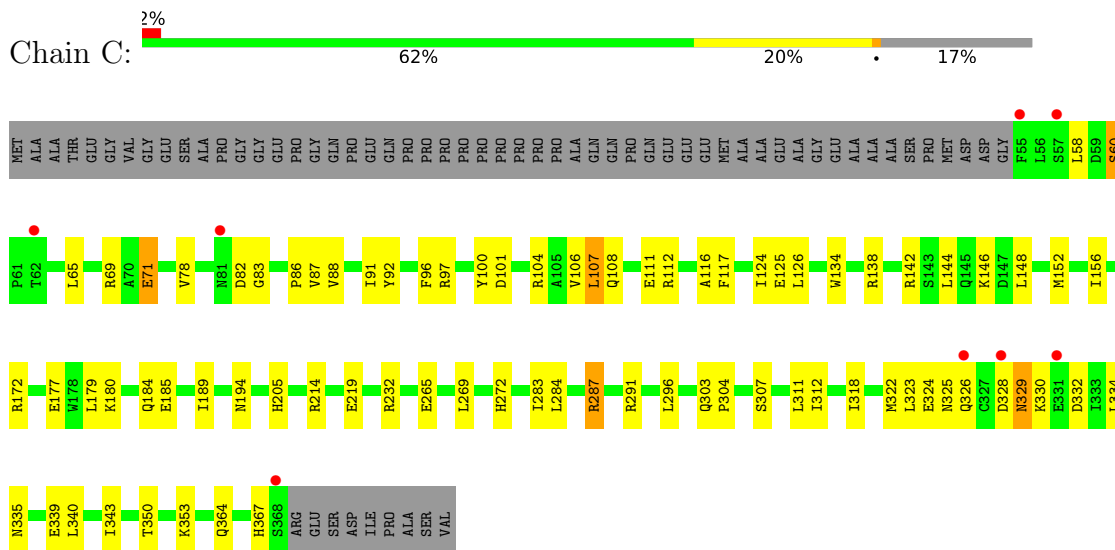
3 Residue-property plots

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

- Molecule 1: geranylgeranyltransferase type I alpha subunit

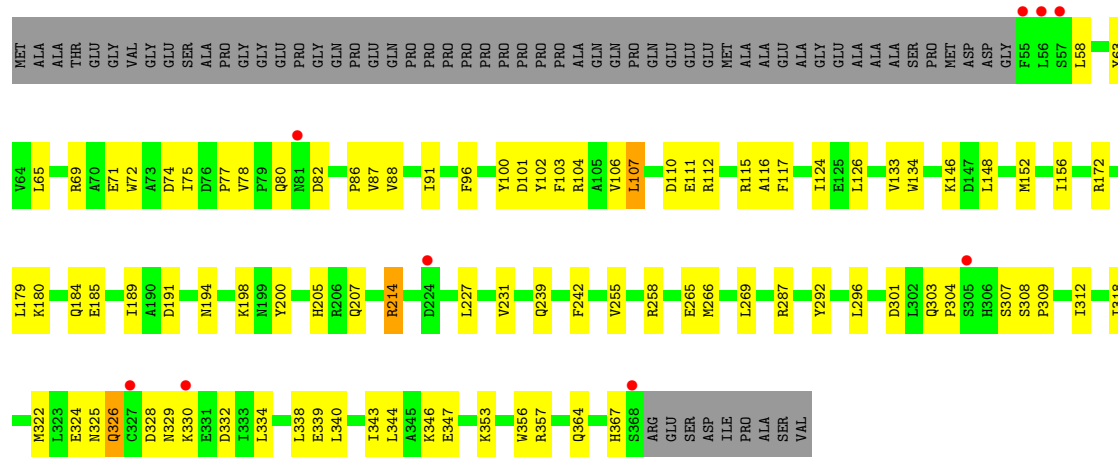


- Molecule 1: geranylgeranyltransferase type I alpha subunit

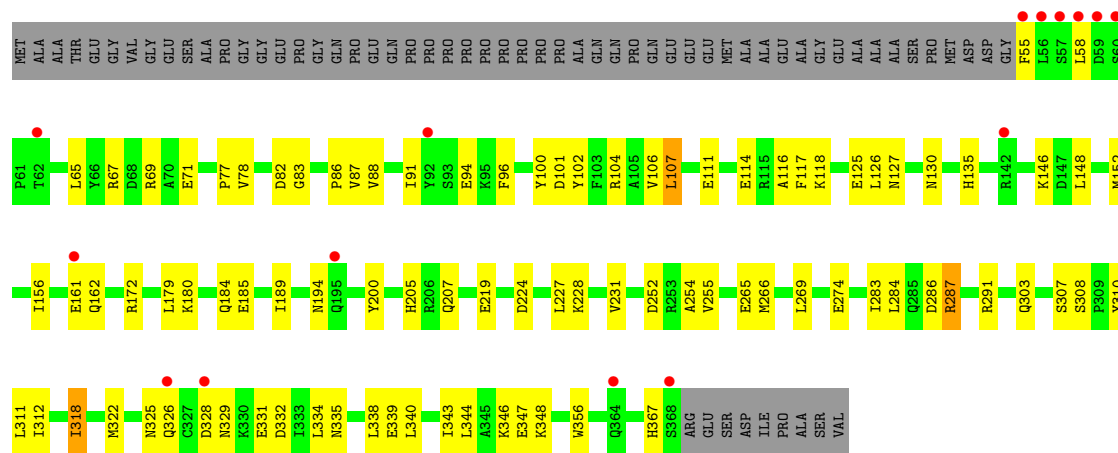


- Molecule 1: geranylgeranyltransferase type I alpha subunit

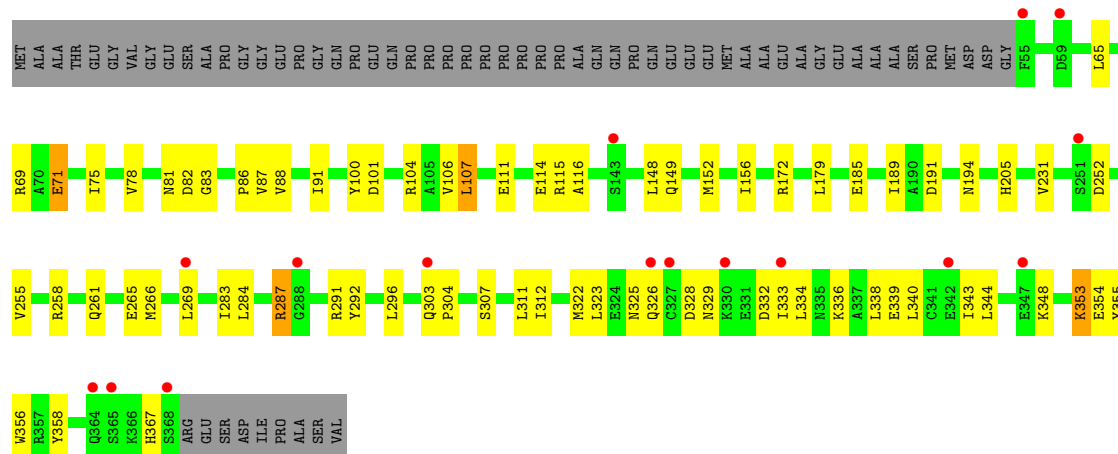




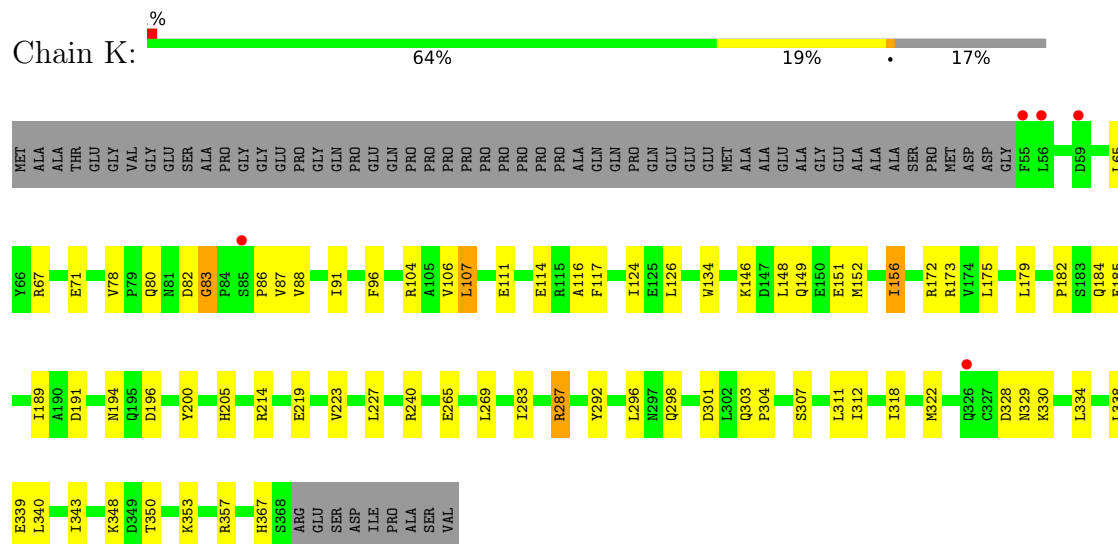
• Molecule 1: geranylgeranyltransferase type I alpha subunit



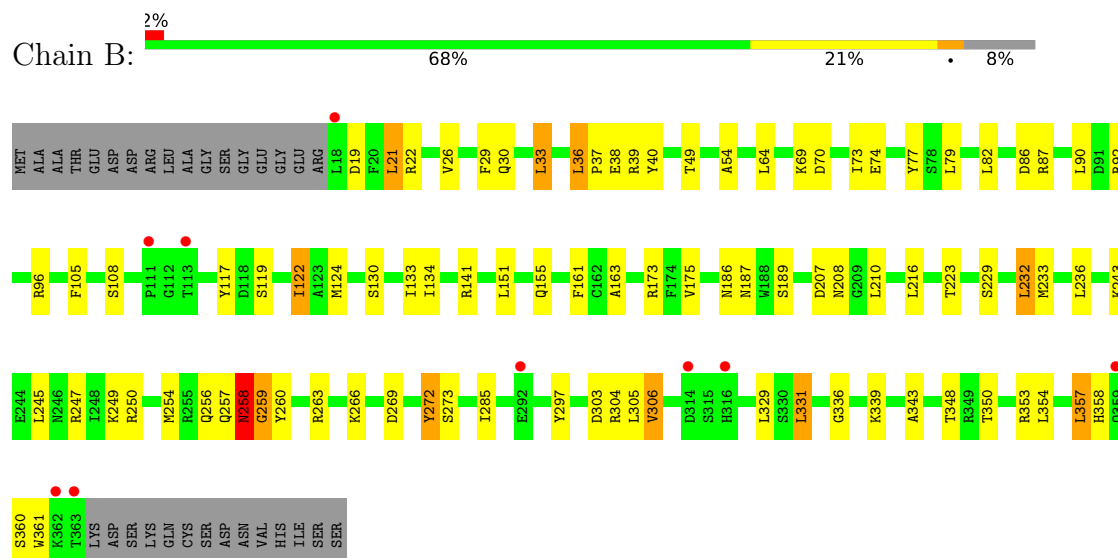
• Molecule 1: geranylgeranyltransferase type I alpha subunit



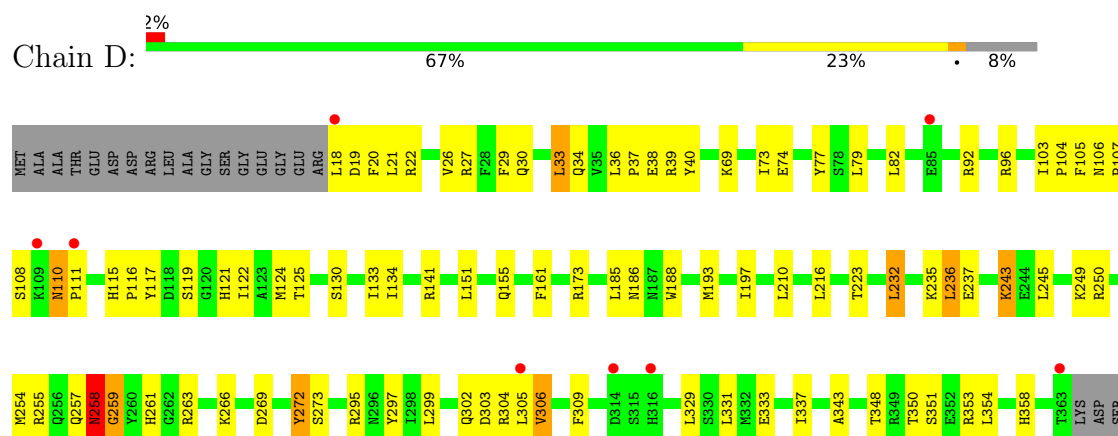
- Molecule 1: geranylgeranyltransferase type I alpha subunit



- Molecule 2: Geranylgeranyl transferase type I beta subunit



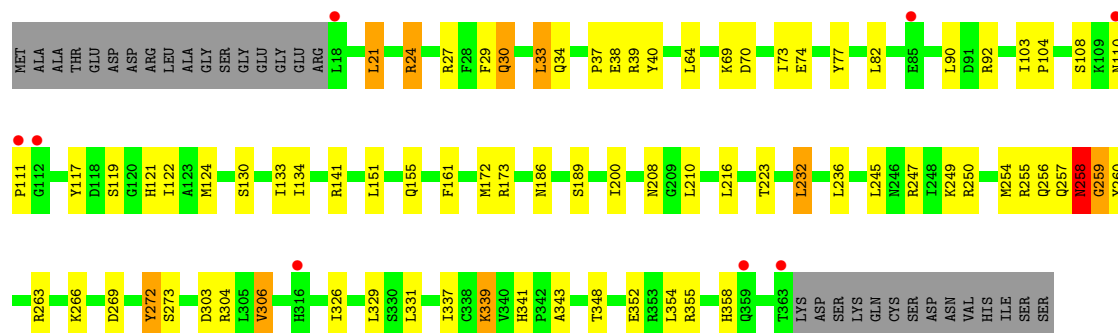
- Molecule 2: Geranylgeranyl transferase type I beta subunit



LYS
GLN
CYS
SER
ASP
ASN
VAL
HIS
ILE
SER
SER

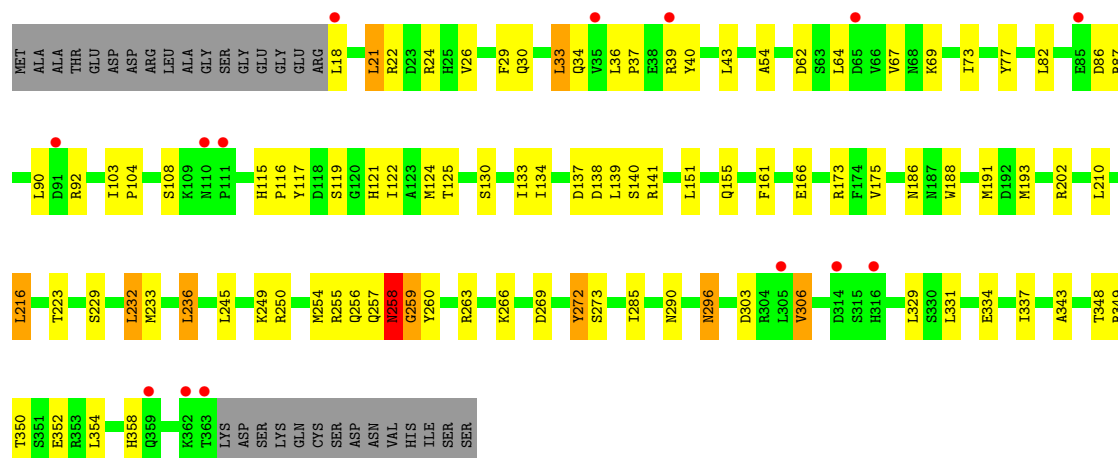
• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain F:  2% 71% 18% 8%



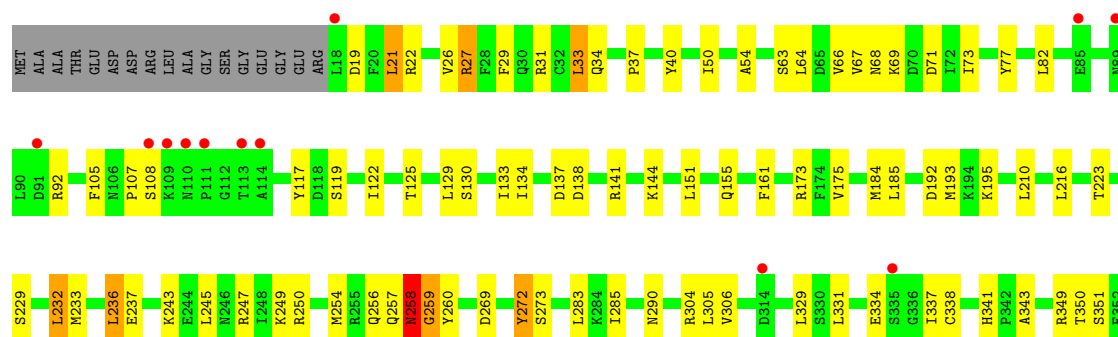
• Molecule 2: Geranylgeranyl transferase type I beta subunit

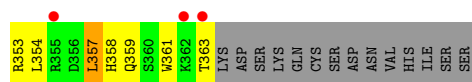
Chain H:  4% 67% 22% 8%



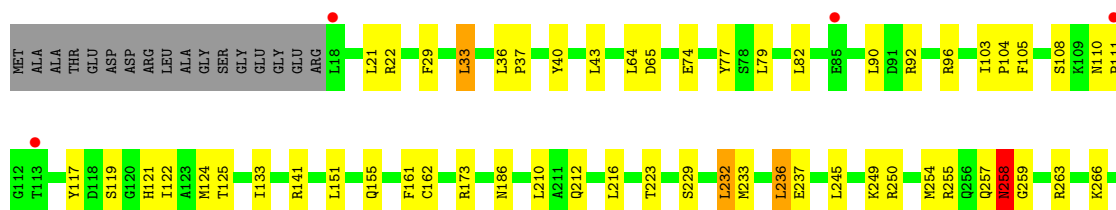
• Molecule 2: Geranylgeranyl transferase type I beta subunit

Chain J:  4% 67% 23% 8%

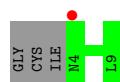




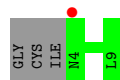
- Molecule 2: Geranylgeranyl transferase type I beta subunit



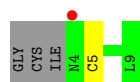
- Molecule 3: Transforming protein RhoB



- Molecule 3: Transforming protein RhoB



- Molecule 3: Transforming protein RhoB



- Molecule 3: Transforming protein RhoB



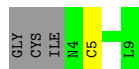
- Molecule 3: Transforming protein RhoB

Chain Q:  67% 33%



- Molecule 3: Transforming protein RhoB

Chain R:  56% 11% 33%



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 29.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.94-2.70) 90.8 (29.94-2.70)	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 0.179 , 0.198	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 , 53.4	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: CL, MGM, ZN, MES

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	0.41	0/2702	0.85	4/3677 (0.1%)
1	C	0.42	0/2721	0.84	4/3698 (0.1%)
1	E	0.42	0/2730	0.84	5/3710 (0.1%)
1	G	0.43	0/2717	0.86	7/3692 (0.2%)
1	I	0.43	0/2714	0.83	5/3690 (0.1%)
1	K	0.47	0/2741	0.84	7/3722 (0.2%)
2	B	0.42	0/2765	0.91	9/3741 (0.2%)
2	D	0.44	0/2768	0.90	7/3743 (0.2%)
2	F	0.43	0/2779	0.91	8/3757 (0.2%)
2	H	0.40	0/2755	0.90	7/3727 (0.2%)
2	J	0.42	0/2769	0.92	9/3744 (0.2%)
2	L	0.46	0/2781	0.93	7/3759 (0.2%)
3	M	0.46	0/44	0.79	0/56
3	N	0.42	0/44	0.74	0/56
3	O	0.49	0/44	0.78	0/56
3	P	0.43	0/44	0.84	0/56
3	Q	0.52	0/44	0.76	0/56
3	R	0.38	0/44	0.66	0/56
All	All	0.43	0/33206	0.88	79/44996 (0.2%)

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

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

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-9.57	98.92	112.60
2	H	259	GLY	N-CA-C	-9.57	98.92	112.60
2	D	259	GLY	N-CA-C	-9.54	98.96	112.60
2	L	259	GLY	N-CA-C	-9.51	99.01	112.60
2	B	259	GLY	N-CA-C	-9.38	99.18	112.60
2	F	259	GLY	N-CA-C	-9.37	99.20	112.60
1	K	348	LYS	N-CA-C	8.19	122.55	112.23
1	A	83	GLY	CA-C-N	8.14	127.71	119.24
1	A	83	GLY	C-N-CA	8.14	127.71	119.24
2	D	258	ASN	N-CA-C	-7.13	95.62	110.80
2	B	258	ASN	N-CA-C	-6.89	96.11	110.80
2	F	258	ASN	N-CA-C	-6.89	96.12	110.80
2	L	258	ASN	N-CA-C	-6.89	96.12	110.80
2	H	258	ASN	N-CA-C	-6.87	96.18	110.80
2	J	258	ASN	N-CA-C	-6.84	96.22	110.80
1	K	83	GLY	CA-C-N	6.43	125.93	119.24
1	K	83	GLY	C-N-CA	6.43	125.93	119.24
1	C	83	GLY	CA-C-N	6.32	125.81	119.24
1	C	83	GLY	C-N-CA	6.32	125.81	119.24
2	F	257	GLN	N-CA-C	-6.14	105.81	113.55
2	H	257	GLN	N-CA-C	-6.06	105.92	113.55
2	L	257	GLN	N-CA-C	-6.06	105.92	113.55
2	J	257	GLN	N-CA-C	-6.03	105.96	113.55
2	D	257	GLN	N-CA-C	-5.96	106.05	113.55
1	G	83	GLY	CA-C-N	5.94	126.09	119.32
1	G	83	GLY	C-N-CA	5.94	126.09	119.32
1	K	185	GLU	N-CA-C	5.89	117.50	111.14
1	I	185	GLU	N-CA-C	5.76	117.25	110.97
2	J	273	SER	N-CA-C	-5.75	105.36	112.38
2	H	273	SER	N-CA-C	-5.71	105.41	112.38
2	D	273	SER	N-CA-C	-5.69	105.44	112.38
2	B	257	GLN	N-CA-C	-5.68	106.39	113.55
1	I	83	GLY	CA-C-N	5.62	124.81	118.97
1	I	83	GLY	C-N-CA	5.62	124.81	118.97
2	L	273	SER	N-CA-C	-5.61	105.53	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	273	SER	N-CA-C	-5.59	105.56	112.38
1	C	350	THR	N-CA-C	5.58	118.08	111.33
1	C	185	GLU	N-CA-C	5.54	117.18	111.03
2	B	273	SER	N-CA-C	-5.53	105.64	112.38
1	E	185	GLU	N-CA-C	5.52	117.16	111.03
2	L	122	ILE	N-CA-C	5.48	116.87	110.62
2	F	189	SER	N-CA-C	-5.46	106.59	113.20
1	G	318	ILE	N-CA-C	-5.43	105.42	110.53
1	E	347	GLU	N-CA-C	5.43	120.81	114.62
2	J	122	ILE	N-CA-C	5.42	116.80	110.62
2	H	122	ILE	N-CA-C	5.40	116.78	110.62
1	A	347	GLU	N-CA-C	5.39	120.77	114.62
2	F	122	ILE	N-CA-C	5.39	116.77	110.62
2	B	175	VAL	N-CA-C	-5.38	105.28	110.72
1	G	347	GLU	N-CA-C	5.38	120.76	114.62
1	I	292	TYR	CA-C-N	5.37	125.44	119.32
1	I	292	TYR	C-N-CA	5.37	125.44	119.32
1	K	292	TYR	CA-C-N	5.32	126.49	119.84
1	K	292	TYR	C-N-CA	5.32	126.49	119.84
2	F	341	HIS	CA-C-N	5.31	125.63	119.47
2	F	341	HIS	C-N-CA	5.31	125.63	119.47
2	J	125	THR	N-CA-C	-5.31	105.49	111.28
2	D	125	THR	N-CA-C	-5.30	105.50	111.28
2	B	122	ILE	N-CA-C	5.30	116.66	110.62
1	E	346	LYS	N-CA-C	5.27	118.17	111.69
1	E	292	TYR	CA-C-N	5.26	125.31	119.32
1	E	292	TYR	C-N-CA	5.26	125.31	119.32
2	L	162	CYS	N-CA-C	-5.26	102.67	110.46
2	H	175	VAL	N-CA-C	-5.25	105.41	110.72
1	G	346	LYS	N-CA-C	5.24	118.83	112.23
2	L	125	THR	N-CA-C	-5.23	105.58	111.28
2	H	125	THR	N-CA-C	-5.23	105.58	111.28
2	J	353	ARG	N-CA-C	-5.22	106.01	112.38
2	B	189	SER	N-CA-C	-5.21	106.90	113.20
1	G	308	SER	N-CA-C	-5.18	103.47	108.13
1	A	185	GLU	N-CA-C	5.16	116.76	111.03
2	D	122	ILE	N-CA-C	5.16	116.50	110.62
1	G	185	GLU	N-CA-C	5.11	116.70	111.03
2	J	50	ILE	N-CA-C	-5.09	105.58	110.72
2	J	175	VAL	N-CA-C	-5.07	105.60	110.72
1	K	350	THR	N-CA-C	5.06	118.23	111.75
2	D	185	LEU	N-CA-C	-5.05	107.14	113.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	LEU	CA-C-N	5.01	124.91	119.85
2	B	36	LEU	C-N-CA	5.01	124.91	119.85

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	77	1
1	C	2655	0	2562	57	1
1	E	2664	0	2570	68	0
1	G	2651	0	2563	61	0
1	I	2648	0	2547	54	0
1	K	2675	0	2594	57	0
2	B	2703	0	2606	63	0
2	D	2706	0	2616	55	0
2	F	2717	0	2635	50	0
2	H	2694	0	2589	67	0
2	J	2708	0	2613	61	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	686	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 11.

All (686) 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:E:318:ILE:HG22	1:E:322:MET:HE3	1.66	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
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:I:231:VAL:HG23	1:I:266:MET:HE3	1.72	0.71
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.70	0.71
1:E:296:LEU:HD22	1:E:322:MET:HE1	1.71	0.71
1:K:91:ILE:HD12	1:K:91:ILE:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:91:ILE:O	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
2:H:296:ASN:HD22	2:H:296:ASN:C	2.03	0.66
1:K:107:LEU:HD22	2:L:117:TYR:CD2	2.31	0.65
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:O	1:C:91:ILE:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:229:SER:O	2:H:233:MET:HG3	1.99	0.62
1:A:296:LEU:CD2	1:A:322:MET:HE1	2.28	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:G:231:VAL:HG23	1:G:266:MET:HE3	1.81	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
1:A:296:LEU:HD22	1:A:322:MET:HE1	1.82	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:HD22	2:H:18:LEU:N	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:A:258:ARG:NH1	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:HG2	2:B:353:ARG:HH11	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:HG3	1:A:214:ARG:O	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
1:I:100:TYR:O	1:I:104:ARG:HG3	2.04	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:CD	1:A:71:GLU:H	2.13	0.56
2:H:133:ILE:HG22	2:H:350:THR:HG23	1.87	0.56
1:I:340:LEU:HD23	1:I:343:ILE:HD12	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:I:231:VAL:CG2	1:I:266:MET:HE3	2.36	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: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
1:A:328:ASP:O	1:A:329:ASN:HB2	2.07	0.54
1:E:296:LEU:CD2	1:E:322:MET:HE1	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.43	0.54
1:G:311:LEU:HD23	1:G:311:LEU:C	2.33	0.54
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:HE21	2:J:359:GLN:CA	2.17	0.53
1:A:303:GLN:HB3	1:A:304:PRO:HD3	1.89	0.53
1:C:214:ARG:O	1:C:214:ARG:HG2	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
2:H:296:ASN:C	2:H:296:ASN:ND2	2.67	0.53
1:I:78:VAL:O	1:I:104:ARG:HD2	2.08	0.53
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.44	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:83:GLY:HA3	2:L:105:PHE:CD1	2.44	0.53
1:K:303:GLN:O	1:K:307:SER:HB2	2.09	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
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:HD2	2:D:353:ARG:O	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:E:107:LEU:HD22	2:F:117:TYR:CD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:258:ASN:CG	2:B:259:GLY:H	2.18	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:I:325:ASN:O	1:I:326:GLN:C	2.54	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:HH11	2:F:24:ARG:HB2	1.76	0.51
1:G:106:VAL:HG13	1:G:111:GLU:HB3	1.93	0.51
1:I:100:TYR:C	1:I:104:ARG:NH1	2.69	0.51
1:I:311:LEU:HD23	1:I:311:LEU:C	2.36	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
1:C:311:LEU:C	1:C:311:LEU:HD23	2.36	0.50
1:E:100:TYR:C	1:E:104:ARG:NH1	2.69	0.50
2:B:22:ARG:HG2	2:B:22:ARG:NH1	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
1:G:318:ILE:HG22	1:G:322:MET:HE2	1.92	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
1:E:326:GLN:HE21	1:E:326:GLN:CA	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
2:H:188:TRP:CE3	2:H:193:MET:HE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:311:LEU:C	1:A:311:LEU:HD23	2.37	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
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
2:D:188:TRP:CE3	2:D:193:MET:HE2	2.48	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:HG3	2:J:27:ARG:HH11	1.78	0.48
2:J:359:GLN:C	2:J:361:TRP:H	2.20	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:J:359:GLN:C	2:J:361:TRP:N	2.70	0.48
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	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:K:311:LEU:C	1:K:311:LEU:HD23	2.38	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
2:H:82:LEU:HD11	2:H:108:SER:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:LEU:CD2	1:I:322:MET:HE1	2.44	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
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.44	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
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:B:130:SER:O	2:B:134:ILE:HG13	2.14	0.47
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.96	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:HG3	2:J:27:ARG:NH1	2.29	0.47
2:J:361:TRP:C	2:J:363:THR:H	2.23	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
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.23	0.46
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.50	0.46
1:A:296:LEU:O	1:A:296:LEU:HD12	2.16	0.46
2:B:303:ASP:OD1	2:B:306:VAL:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:86:ASP:OD2	2:H:86:ASP:N	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:64:LEU:O	2:H:67:VAL:HG22	2.16	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
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
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: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
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:G:325:ASN:O	1:G:326:GLN:C	2.59	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
2:H:133:ILE:HD13	2:H:354:LEU:HD13	1.97	0.46
2:H:250:ARG:O	2:H:254:MET:HG2	2.17	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
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:81:ASN:HD21	2:J:105:PHE:H	1.64	0.45
1:I:333:ILE:HA	1:I:336:LYS:HG3	1.98	0.45
2:J:133:ILE:HG22	2:J:350:THR:CG2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:258:ASN:CG	2:D:259:GLY:H	2.23	0.45
1:E:318:ILE:HG22	1:E:322:MET:CE	2.42	0.45
2:F:103:ILE:HG23	2:F:104:PRO:HD2	1.98	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:E:231:VAL:HG23	1:E:266:MET:HE3	1.99	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:J:193:MET:HG3	2:J:233:MET:HE2	1.99	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
1:A:344:LEU:HA	1:A:348:LYS:HB2	2.00	0.44
1:C:296:LEU:CD2	1:C:322:MET:HE1	2.48	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:HH11	1:A:258:ARG:CB	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:129:LEU:HB2	2:J:184:MET:HE1	1.99	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:C:87:VAL:O	1:C:88:VAL:C	2.61	0.44
1:C:329:ASN:O	1:C:330:LYS:C	2.60	0.44
1:E:328:ASP:O	1:E:329:ASN:HB2	2.18	0.44
2:F:64:LEU:HA	2:F:64:LEU:HD23	1.86	0.44
1:G:88:VAL:HG13	2:H:36:LEU:HD11	2.00	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: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:K:296:LEU:CD2	1:K:322:MET:HE1	2.47	0.44
1:G:100:TYR:C	1:G:104:ARG:NH1	2.76	0.43
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:E:200:TYR:HB3	5:F:380:MGM:HC12	1.99	0.43
1:E:329:ASN:O	1:E:330:LYS:C	2.61	0.43
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.00	0.43
1:C:318:ILE:HG22	1:C:322:MET:HE3	1.99	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:40:TYR:HB3	2:L:43:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:245:LEU:O	2:L:249:LYS:HG3	2.17	0.43
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
1:A:329:ASN:O	1:A:330:LYS:C	2.61	0.43
2:F:258:ASN:CG	2:F:259:GLY:H	2.26	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
1:K:318:ILE:HG22	1:K:322:MET:HE3	2.01	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
1:K:329:ASN:O	1:K:330:LYS:C	2.61	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
2:F:37:PRO:C	2:F:39:ARG:H	2.26	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
1:C:325:ASN:O	1:C:326:GLN:C	2.62	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:HD23	1:G:227:LEU:HA	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
1:G:55:PHE:HD2	1:G:118:LYS:HZ3	1.61	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
1:A:214:ARG:O	1:A:214:ARG:CG	2.62	0.42
2:B:29:PHE:CD2	2:B:54:ALA:HA	2.54	0.42
2:B:33:LEU:CD2	2:B:54:ALA:HB1	2.50	0.42
2:B:37:PRO:C	2:B:39:ARG:N	2.74	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:F:37:PRO:C	2:F:39:ARG:N	2.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:TYR:HB3	2:H:43:LEU:HD12	2.01	0.42
2:H:258:ASN:CG	2:H:259:GLY:H	2.25	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:OE1	1:E:239:GLN:HA	2.19	0.42
1:G:331:GLU:O	1:G:335:ASN:ND2	2.53	0.42
1:A:83:GLY:HA3	2:B:105:PHE:CE1	2.54	0.42
1:A:124:ILE:HD13	1:A:134:TRP:CH2	2.55	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
2:D:263:ARG:HB2	2:D:266:LYS:HG3	2.01	0.42
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.55	0.42
1:E:326:GLN:HE21	1:E:326:GLN:H	1.66	0.42
1:G:284:LEU:O	1:G:287:ARG:HG2	2.19	0.42
2:H:37:PRO:C	2:H:39:ARG:N	2.77	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:91:ILE:HD11	2:F:38:GLU:H	1.83	0.42
1:E:180:LYS:HD3	1:E:180:LYS:HA	1.86	0.42
1:E:325:ASN:O	1:E:326:GLN:C	2.61	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
1:C:91:ILE:HD11	2:D:38:GLU:H	1.85	0.42
2:D:255:ARG:HD3	2:D:261:HIS:CD2	2.54	0.42
2:F:90:LEU:HD23	2:F:90:LEU:HA	1.90	0.42
1:G:318:ILE:HG22	1:G:322:MET:CE	2.50	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
2:D:74:GLU:CD	2:D:141:ARG:HH22	2.28	0.42
1:E:65:LEU:O	1:E:69:ARG:HG3	2.19	0.42
1:E:124:ILE:HD13	1:E:134:TRP:CH2	2.54	0.42
2:F:339:LYS:HB3	2:F:339:LYS:HZ3	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:PRO:C	2:D:39:ARG:N	2.77	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
2:H:37:PRO:C	2:H:39:ARG:H	2.28	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:B:122:ILE:HG22	2:B:163:ALA:HA	2.02	0.41
1:C:58:LEU:HB2	1:C:125:GLU:OE2	2.20	0.41
1:I:258:ARG:HE	1:I:258:ARG:HB3	1.64	0.41
2:J:258:ASN:CG	2:J:259:GLY:H	2.25	0.41
2:J:269:ASP:HB3	2:J:272:TYR:CD2	2.52	0.41
2:L:212:GLN:HA	2:L:212:GLN:NE2	2.35	0.41
1:A:325:ASN:O	1:A:326:GLN:C	2.63	0.41
2:D:243:LYS:HB3	2:D:243:LYS:NZ	2.35	0.41
2:H:24:ARG:HG2	2:H:24:ARG:NH1	2.35	0.41
2:H:26:VAL:O	2:H:30:GLN:HG3	2.20	0.41
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.34	0.41
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.51	0.41
1:K:196:ASP:HB3	8:K:493:HOH:O	2.20	0.41
2:B:208:ASN:CG	2:B:247:ARG:HB3	2.45	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
1:I:252:ASP:OD2	1:I:252:ASP:C	2.64	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:B:86:ASP:OD2	2:B:86:ASP:N	2.53	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:E:296:LEU:HD22	1:E:322:MET:CE	2.46	0.41
1:G:219:GLU:HA	1:G:219:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:ARG:HH11	2:H:22:ARG:HG2	1.86	0.41
1:K:91:ILE:HG13	2:L:36:LEU:O	2.21	0.41
2:L:229:SER:O	2:L:233:MET:HG3	2.20	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
2:H:290:ASN:OD1	2:H:290:ASN:C	2.63	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:296:LEU:HD22	1:C:322:MET:HE1	2.03	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:290:ASN:OD1	2:J:290:ASN:C	2.63	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
2:B:263:ARG:HB2	2:B:266:LYS:HG3	2.01	0.41
1:C:284:LEU:O	1:C:287:ARG:HG2	2.21	0.41
2:D:121:HIS:HB3	2:D:124:MET:HG2	2.03	0.41
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
1:I:81:ASN:ND2	2:J:105:PHE:H	2.18	0.41
1:K:296:LEU:HD22	1:K:322:MET:HE1	2.02	0.41
2:L:121:HIS:HB3	2:L:124:MET:HG2	2.03	0.41
3:P:7:LYS:HD3	8:P:65:HOH:O	2.21	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:F:208:ASN:CG	2:F:247:ARG:HB3	2.46	0.41
2:H:21:LEU:N	2:H:21:LEU:CD1	2.84	0.41
2:H:115:HIS:HA	2:H:116:PRO:HD3	1.89	0.41
2:H:188:TRP:CZ3	2:H:191:MET:HE3	2.56	0.41
1:K:149:GLN:HG3	8:K:492:HOH:O	2.20	0.41
2:B:187:ASN:OD1	2:B:187:ASN:C	2.64	0.40
1:C:106:VAL:HG11	1:C:116:ALA:CB	2.51	0.40
2:F:172:MET:HE1	2:F:200:ILE:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:N	2:H:18:LEU:CD2	2.83	0.40
2:H:121:HIS:HB3	2:H:124:MET:HG2	2.03	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:37:PRO:HD2	2:F:40:TYR:HE1	1.81	0.40
2:F:266:LYS:HE3	2:F:266:LYS:HB3	1.93	0.40
2:H:62:ASP:OD1	2:H:349:ARG:NH2	2.54	0.40
2:H:103:ILE:HG23	2:H:104:PRO:HD2	2.02	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:90:LEU:HD23	2:L:90:LEU:HA	1.87	0.40
2:L:269:ASP:HB3	2:L:272:TYR:CD2	2.54	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
1:G:200:TYR:CB	5:H:380:MGM:HC12	2.52	0.40
2:H:173:ARG:HG2	5:H:380:MGM:H112	2.04	0.40
1:K:156:ILE:CD1	1:K:172:ARG:HH22	2.33	0.40
2:L:64:LEU:HA	2:L:64:LEU:HD23	1.83	0.40
1:A:273:ASN:OD1	1:A:273:ASN:C	2.65	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:135:HIS:CD2	2:H:166:GLU:HG2	2.56	0.40
1:G:161:GLU:HG2	1:G:162:GLN:HG3	2.03	0.40
2:H:22:ARG:HG2	2:H:22:ARG:NH1	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/377 (83%)	287 (92%)	25 (8%)	0	100	100
1	C	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	36	60
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%)	36	60
2	D	344/377 (91%)	331 (96%)	11 (3%)	2 (1%)	21	44
2	F	344/377 (91%)	330 (96%)	13 (4%)	1 (0%)	36	60
2	H	344/377 (91%)	328 (95%)	15 (4%)	1 (0%)	36	60
2	J	344/377 (91%)	328 (95%)	14 (4%)	2 (1%)	21	44
2	L	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	36	60
3	M	4/9 (44%)	4 (100%)	0	0	100	100
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%)	43	68

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	274 (97%)	8 (3%)	38	68
1	C	286/338 (85%)	277 (97%)	9 (3%)	35	65
1	E	289/338 (86%)	280 (97%)	9 (3%)	35	65
1	G	285/338 (84%)	280 (98%)	5 (2%)	51	78
1	I	285/338 (84%)	279 (98%)	6 (2%)	47	75
1	K	292/338 (86%)	285 (98%)	7 (2%)	43	72
2	B	291/326 (89%)	280 (96%)	11 (4%)	29	58
2	D	291/326 (89%)	276 (95%)	15 (5%)	21	47
2	F	295/326 (90%)	282 (96%)	13 (4%)	25	53
2	H	288/326 (88%)	277 (96%)	11 (4%)	29	58
2	J	291/326 (89%)	277 (95%)	14 (5%)	23	50
2	L	295/326 (90%)	281 (95%)	14 (5%)	23	51
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%)	3384 (96%)	122 (4%)	32	61

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	107	LEU
1	A	114	GLU
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	305	LEU
2	B	306	VAL
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	177	GLU
1	C	184	GLN
1	C	194	ASN
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	243	LYS
2	D	258	ASN
2	D	305	LEU
2	D	306	VAL
2	D	329	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	30	GLN
2	F	33	LEU
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	255	ARG
2	F	306	VAL
2	F	329	LEU
2	F	331	LEU
2	F	339	LYS
1	G	107	LEU
1	G	114	GLU
1	G	184	GLN
1	G	194	ASN
1	G	287	ARG
2	H	21	LEU
2	H	33	LEU
2	H	151	LEU
2	H	216	LEU
2	H	232	LEU
2	H	236	LEU
2	H	255	ARG
2	H	296	ASN
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
1	I	71	GLU
1	I	107	LEU
1	I	114	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	261	GLN
1	I	287	ARG
1	I	353	LYS
2	J	21	LEU
2	J	27	ARG
2	J	31	ARG
2	J	33	LEU
2	J	151	LEU
2	J	216	LEU
2	J	232	LEU
2	J	236	LEU
2	J	237	GLU
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	341	HIS
2	J	357	LEU
1	K	71	GLU
1	K	80	GLN
1	K	107	LEU
1	K	114	GLU
1	K	156	ILE
1	K	182	PRO
1	K	287	ARG
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	237	GLU
2	L	255	ARG
2	L	258	ASN
2	L	284	LYS
2	L	306	VAL
2	L	329	LEU
2	L	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	135	HIS
1	A	149	GLN
1	A	184	GLN
1	A	194	ASN
1	A	225	GLN
1	A	272	HIS
1	A	278	ASN
1	A	285	GLN
1	A	335	ASN
1	A	367	HIS
2	B	208	ASN
2	B	257	GLN
1	C	108	GLN
1	C	135	HIS
1	C	149	GLN
1	C	153	ASN
1	C	184	GLN
1	C	218	ASN
1	C	285	GLN
1	C	298	GLN
1	C	364	GLN
1	C	367	HIS
2	D	34	GLN
2	D	208	ASN
2	D	246	ASN
1	E	135	HIS
1	E	149	GLN
1	E	184	GLN
1	E	204	GLN
1	E	272	HIS
1	E	285	GLN
1	E	297	ASN
1	E	325	ASN
1	E	326	GLN
1	E	335	ASN
1	E	364	GLN
1	E	367	HIS
2	F	30	GLN
2	F	34	GLN
2	F	208	ASN
2	F	246	ASN
1	G	81	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	149	GLN
1	G	184	GLN
1	G	225	GLN
1	G	272	HIS
1	G	297	ASN
1	G	303	GLN
1	G	335	ASN
1	G	367	HIS
2	H	34	GLN
2	H	296	ASN
1	I	81	ASN
1	I	89	GLN
1	I	135	HIS
1	I	149	GLN
1	I	184	GLN
1	I	234	ASN
1	I	261	GLN
1	I	367	HIS
2	J	212	GLN
2	J	246	ASN
2	J	257	GLN
2	J	287	GLN
2	J	296	ASN
2	J	359	GLN
1	K	89	GLN
1	K	108	GLN
1	K	135	HIS
1	K	149	GLN
1	K	184	GLN
1	K	205	HIS
1	K	285	GLN
1	K	298	GLN
1	K	325	ASN
1	K	367	HIS
2	L	208	ASN
2	L	212	GLN
2	L	257	GLN
3	M	4	ASN
3	N	4	ASN
3	O	4	ASN
3	P	4	ASN
3	Q	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	R	4	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	J	379	-	27,28,28	0.99	2 (7%)	34,37,37	1.99	6 (17%)
5	MGM	B	379	-	27,28,28	0.93	2 (7%)	34,37,37	2.04	6 (17%)
5	MGM	F	380	-	27,28,28	0.96	1 (3%)	34,37,37	2.05	6 (17%)
5	MGM	L	379	-	27,28,28	1.01	2 (7%)	34,37,37	2.02	7 (20%)
5	MGM	H	380	-	27,28,28	0.88	1 (3%)	34,37,37	2.00	6 (17%)
5	MGM	D	380	-	27,28,28	0.97	2 (7%)	34,37,37	2.02	6 (17%)
7	MES	F	381	-	12,12,12	9.30	8 (66%)	15,16,16	2.11	5 (33%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	381	MES	C8-S	-24.53	1.43	1.77
7	F	381	MES	O2S-S	12.76	1.81	1.45
7	F	381	MES	O1S-S	12.16	1.79	1.45
7	F	381	MES	O3S-S	8.61	1.79	1.47
7	F	381	MES	C7-C8	-4.79	1.39	1.52
7	F	381	MES	C3-C2	-2.88	1.39	1.50
7	F	381	MES	C5-C6	-2.61	1.40	1.50
7	F	381	MES	C7-N4	-2.59	1.41	1.47
5	L	379	MGM	C7-C8	2.43	1.38	1.33
5	D	380	MGM	C7-C8	2.37	1.38	1.33
5	L	379	MGM	C12-C13	2.29	1.38	1.33
5	H	380	MGM	C7-C8	2.28	1.38	1.33
5	F	380	MGM	C7-C8	2.23	1.38	1.33
5	J	379	MGM	C12-C13	2.17	1.38	1.33
5	B	379	MGM	C7-C8	2.16	1.38	1.33
5	B	379	MGM	C12-C13	2.14	1.38	1.33
5	D	380	MGM	C12-C13	2.13	1.38	1.33
5	J	379	MGM	C7-C8	2.09	1.37	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	379	MGM	C1-C2-N3	7.38	131.02	113.30
5	F	380	MGM	C1-C2-N3	7.33	130.91	113.30
5	D	380	MGM	C1-C2-N3	7.09	130.33	113.30
5	L	379	MGM	C1-C2-N3	7.04	130.20	113.30
5	H	380	MGM	C1-C2-N3	7.01	130.14	113.30
5	J	379	MGM	C1-C2-N3	7.00	130.10	113.30
5	J	379	MGM	C4-N3-C2	5.24	125.58	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	379	MGM	C4-N3-C2	5.19	125.44	110.55
5	D	380	MGM	C4-N3-C2	5.16	125.36	110.55
5	B	379	MGM	C4-N3-C2	5.16	125.36	110.55
5	H	380	MGM	C4-N3-C2	5.12	125.25	110.55
5	F	380	MGM	C4-N3-C2	5.11	125.22	110.55
7	F	381	MES	O3S-S-C8	4.22	114.27	106.00
5	F	380	MGM	O1-C1-C2	4.04	115.46	107.38
5	B	379	MGM	O1-C1-C2	3.97	115.31	107.38
5	L	379	MGM	O1-C1-C2	3.80	114.97	107.38
7	F	381	MES	O1S-S-C8	3.74	112.37	106.73
5	D	380	MGM	O1-C1-C2	3.73	114.84	107.38
5	H	380	MGM	O1-C1-C2	3.67	114.71	107.38
5	J	379	MGM	O1-C1-C2	3.44	114.26	107.38
7	F	381	MES	O2S-S-C8	3.14	111.48	106.73
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
5	L	379	MGM	O1A-PA-O3A	3.06	115.53	107.27
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	F	380	MGM	O1A-PA-O3A	2.91	115.15	107.27
5	D	380	MGM	O1A-PA-O3A	2.89	115.09	107.27
5	H	380	MGM	O1A-PA-O3A	2.84	114.94	107.27
5	J	379	MGM	O1A-PA-O3A	2.81	114.86	107.27
5	B	379	MGM	O1A-PA-O3A	2.78	114.78	107.27
5	B	379	MGM	O1B-PB-O3A	2.72	113.76	104.64
7	F	381	MES	O2S-S-O1S	-2.59	105.41	113.82
7	F	381	MES	O3S-S-O2S	-2.53	105.06	111.40
5	D	380	MGM	C2-N3-C5	2.27	122.62	112.03
5	L	379	MGM	C2-N3-C5	2.26	122.57	112.03
5	H	380	MGM	C2-N3-C5	2.25	122.50	112.03
5	B	379	MGM	C2-N3-C5	2.25	122.49	112.03
5	F	380	MGM	C2-N3-C5	2.24	122.49	112.03
5	J	379	MGM	C2-N3-C5	2.15	122.04	112.03
5	L	379	MGM	O3A-PA-O2A	-2.06	104.51	110.70

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	379	MGM	C1-C2-N3-C4
5	B	379	MGM	O1-C1-C2-N3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	379	MGM	PA-O3A-PB-O1B
5	D	380	MGM	C1-C2-N3-C4
5	D	380	MGM	O1-C1-C2-N3
5	D	380	MGM	PA-O3A-PB-O1B
5	F	380	MGM	C1-C2-N3-C4
5	F	380	MGM	O1-C1-C2-N3
5	F	380	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
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	L	379	MGM	C1-C2-N3-C4
5	L	379	MGM	O1-C1-C2-N3
5	L	379	MGM	PA-O3A-PB-O1B
7	F	381	MES	C7-C8-S-O3S
5	B	379	MGM	C6-C5-N3-C4
5	D	380	MGM	C6-C5-N3-C4
5	F	380	MGM	C6-C5-N3-C4
5	H	380	MGM	C6-C5-N3-C4
5	J	379	MGM	C6-C5-N3-C4
5	L	379	MGM	C6-C5-N3-C4
7	F	381	MES	C7-C8-S-O1S
7	F	381	MES	C7-C8-S-O2S
5	L	379	MGM	C6-C5-N3-C2
5	H	380	MGM	C10-C8-C9-C11
5	B	379	MGM	C10-C8-C9-C11
5	F	380	MGM	C10-C8-C9-C11
5	H	380	MGM	C7-C8-C9-C11
5	D	380	MGM	C10-C8-C9-C11
5	J	379	MGM	C10-C8-C9-C11
5	L	379	MGM	C10-C8-C9-C11
5	B	379	MGM	C7-C8-C9-C11
5	F	380	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	L	379	MGM	C7-C8-C9-C11
5	F	380	MGM	C6-C5-N3-C2
5	H	380	MGM	C6-C5-N3-C2
5	J	379	MGM	C6-C5-N3-C2

Continued on next page...

Continued from previous page...

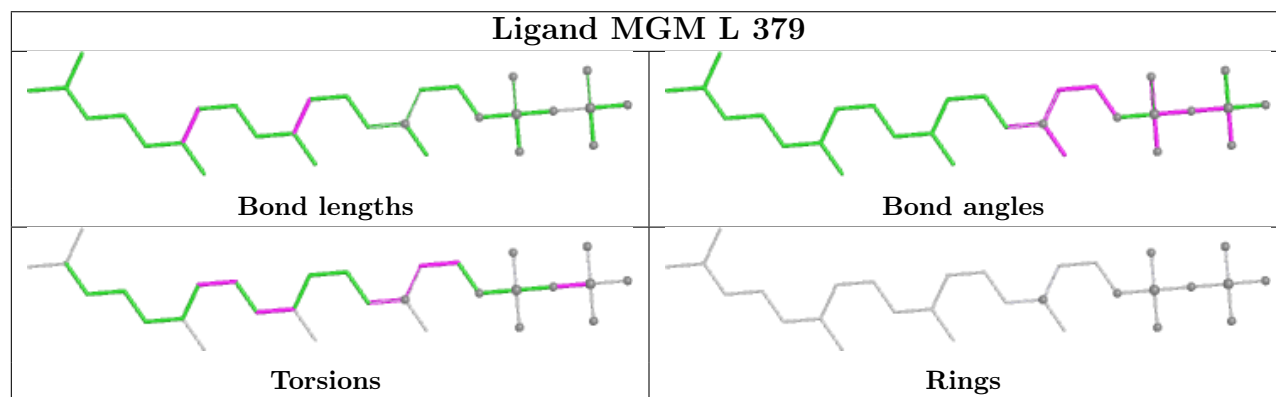
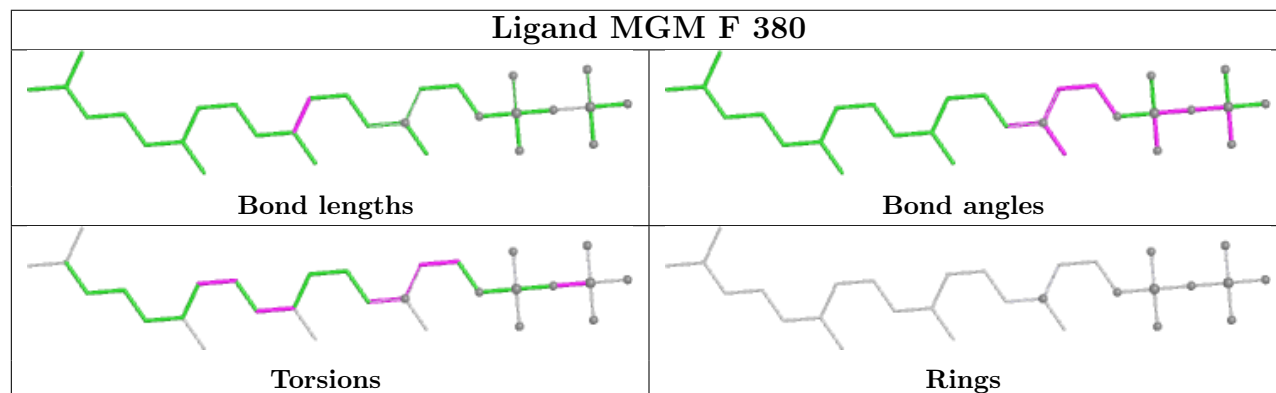
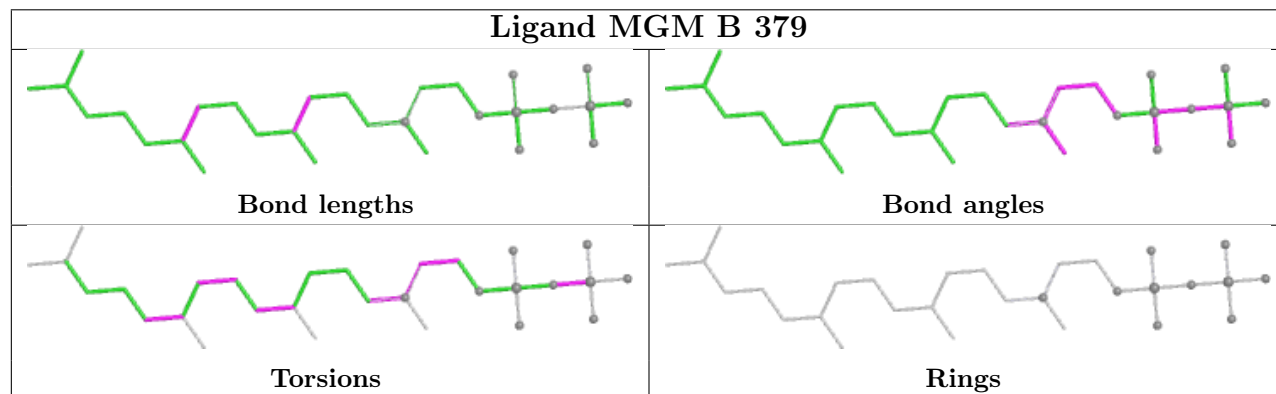
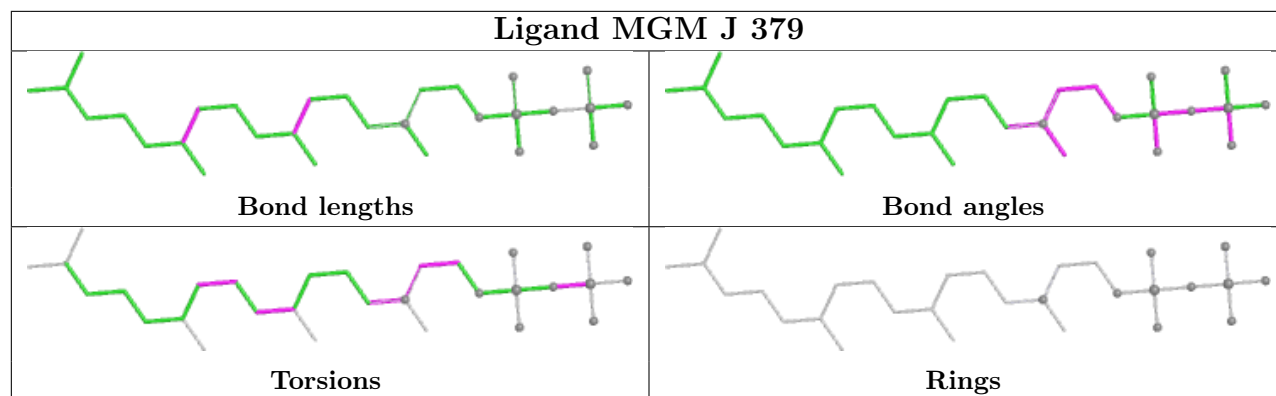
Mol	Chain	Res	Type	Atoms
5	B	379	MGM	PA-O3A-PB-O2B
5	D	380	MGM	PA-O3A-PB-O2B
5	F	380	MGM	PA-O3A-PB-O2B
5	H	380	MGM	PA-O3A-PB-O2B
5	J	379	MGM	PA-O3A-PB-O2B
5	L	379	MGM	PA-O3A-PB-O2B
5	B	379	MGM	C6-C5-N3-C2
5	B	379	MGM	C14-C13-C15-C16
5	H	380	MGM	C14-C13-C15-C16
5	H	380	MGM	C9-C11-C12-C13
5	L	379	MGM	C9-C11-C12-C13
5	J	379	MGM	C9-C11-C12-C13
5	B	379	MGM	C9-C11-C12-C13
5	D	380	MGM	C9-C11-C12-C13
5	F	380	MGM	C9-C11-C12-C13
5	D	380	MGM	C14-C13-C15-C16

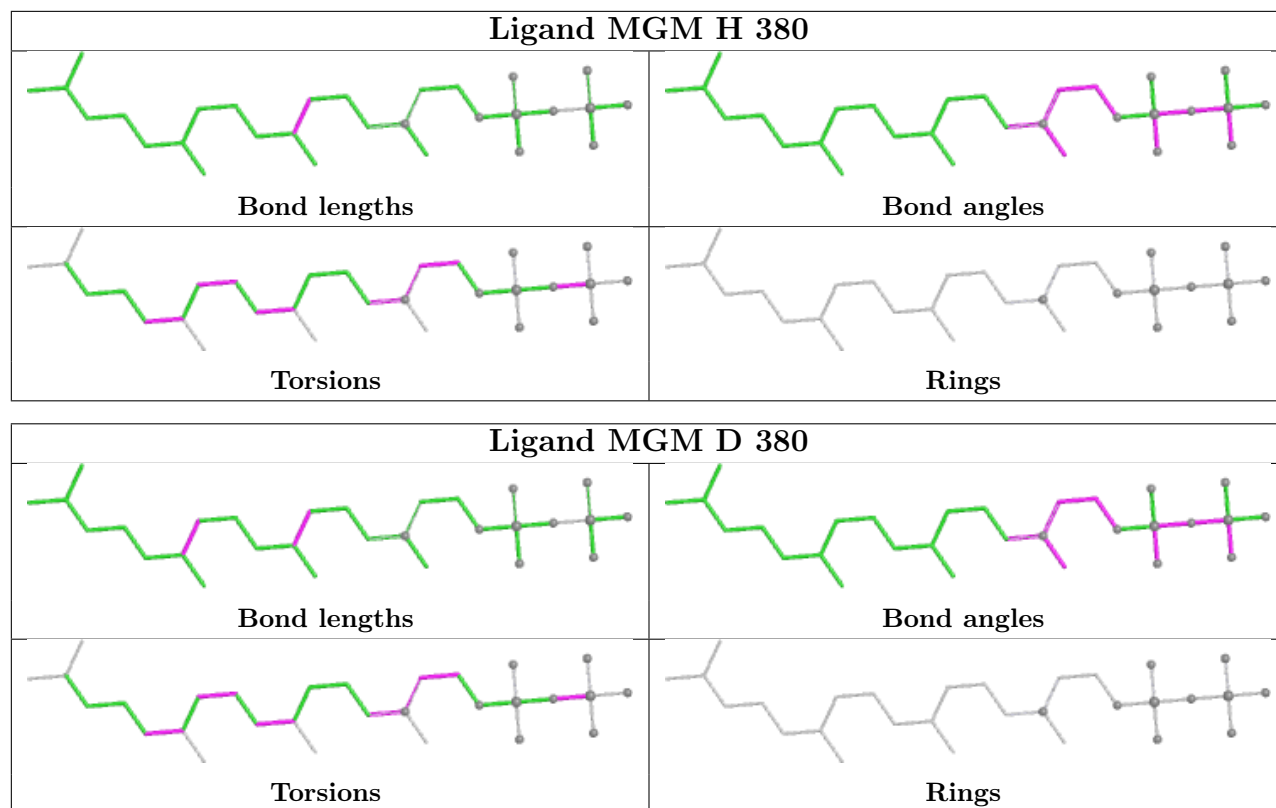
There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	379	MGM	1	0
5	B	379	MGM	2	0
5	F	380	MGM	3	0
5	L	379	MGM	2	0
5	H	380	MGM	2	0
5	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%)	0.24	10 (3%) 50 46	45, 67, 100, 113	0
1	C	314/377 (83%)	0.32	8 (2%) 58 55	44, 64, 93, 114	0
1	E	314/377 (83%)	0.33	9 (2%) 53 50	42, 65, 92, 110	0
1	G	314/377 (83%)	0.30	15 (4%) 35 32	43, 63, 90, 112	0
1	I	314/377 (83%)	0.51	16 (5%) 33 29	42, 67, 97, 111	0
1	K	314/377 (83%)	-0.20	5 (1%) 70 68	35, 51, 77, 89	0
2	B	346/377 (91%)	0.01	9 (2%) 57 54	43, 59, 80, 105	0
2	D	346/377 (91%)	-0.12	8 (2%) 61 58	42, 55, 78, 92	0
2	F	346/377 (91%)	-0.19	8 (2%) 61 58	38, 52, 78, 100	0
2	H	346/377 (91%)	0.22	14 (4%) 42 38	44, 64, 88, 110	0
2	J	346/377 (91%)	0.28	15 (4%) 40 36	43, 63, 89, 109	0
2	L	346/377 (91%)	-0.33	5 (1%) 73 72	35, 48, 68, 91	0
3	M	6/9 (66%)	0.36	1 (16%) 4 3	48, 65, 80, 94	0
3	N	6/9 (66%)	0.36	1 (16%) 4 3	52, 65, 82, 94	0
3	O	6/9 (66%)	0.40	1 (16%) 4 3	52, 63, 79, 92	0
3	P	6/9 (66%)	0.33	1 (16%) 4 3	53, 70, 85, 97	0
3	Q	6/9 (66%)	0.22	0 100 100	46, 63, 79, 88	0
3	R	6/9 (66%)	0.10	0 100 100	43, 65, 78, 88	0
All	All	3996/4578 (87%)	0.11	126 (3%) 50 46	35, 59, 88, 114	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	PHE	7.6
1	E	55	PHE	7.2
1	G	55	PHE	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	55	PHE	6.4
2	H	18	LEU	6.4
2	F	18	LEU	6.3
2	B	18	LEU	5.9
2	J	18	LEU	5.3
1	C	368	SER	5.1
2	J	363	THR	4.8
1	K	55	PHE	4.8
2	J	110	ASN	4.7
1	A	55	PHE	4.7
2	D	18	LEU	4.5
2	B	363	THR	4.4
2	H	363	THR	4.3
1	A	368	SER	4.2
1	I	368	SER	4.2
1	E	56	LEU	4.1
1	G	59	ASP	4.0
1	I	364	GLN	4.0
2	J	85	GLU	4.0
2	D	314	ASP	4.0
2	J	111	PRO	3.7
2	H	111	PRO	3.7
1	A	331	GLU	3.6
1	G	57	SER	3.5
2	L	363	THR	3.5
1	I	330	LYS	3.5
2	J	108	SER	3.5
2	F	363	THR	3.5
2	L	18	LEU	3.5
1	C	328	ASP	3.4
2	F	111	PRO	3.4
1	G	368	SER	3.4
2	B	362	LYS	3.3
1	C	57	SER	3.3
2	H	85	GLU	3.3
3	O	4	ASN	3.2
1	I	327	CYS	3.2
1	I	326	GLN	3.1
2	D	111	PRO	3.1
1	G	364	GLN	3.1
1	G	56	LEU	3.1
2	B	292	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	363	THR	3.0
1	E	368	SER	3.0
2	H	362	LYS	3.0
1	K	56	LEU	2.9
2	B	111	PRO	2.9
1	C	331	GLU	2.9
3	N	4	ASN	2.9
3	M	4	ASN	2.8
1	G	62	THR	2.8
2	L	85	GLU	2.8
2	H	359	GLN	2.7
3	P	4	ASN	2.7
2	H	314	ASP	2.7
2	J	314	ASP	2.7
1	A	291	ARG	2.7
2	J	114	ALA	2.7
2	J	91	ASP	2.7
2	D	85	GLU	2.7
2	J	89	ASN	2.7
1	A	330	LYS	2.6
2	J	109	LYS	2.6
1	A	328	ASP	2.6
1	E	81	ASN	2.6
2	H	39	ARG	2.6
1	E	330	LYS	2.6
1	A	326	GLN	2.6
2	F	316	HIS	2.6
1	I	347	GLU	2.5
2	H	91	ASP	2.5
1	G	58	LEU	2.5
2	F	112	GLY	2.5
2	L	111	PRO	2.5
2	J	335	SER	2.5
2	J	362	LYS	2.5
1	G	326	GLN	2.5
1	C	326	GLN	2.5
1	C	81	ASN	2.4
1	I	251	SER	2.4
1	G	142	ARG	2.4
2	F	110	ASN	2.4
1	K	326	GLN	2.4
2	H	110	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	60	SER	2.4
1	G	328	ASP	2.4
1	K	59	ASP	2.4
2	F	359	GLN	2.4
2	L	113	THR	2.3
1	E	57	SER	2.3
1	G	92	TYR	2.3
1	K	85	SER	2.3
2	H	65	ASP	2.3
2	H	316	HIS	2.2
2	J	113	THR	2.2
2	J	355	ARG	2.2
2	B	314	ASP	2.2
1	A	195	GLN	2.2
1	I	288	GLY	2.2
1	A	364	GLN	2.2
2	B	359	GLN	2.2
1	I	365	SER	2.2
1	A	300	LEU	2.2
2	H	305	LEU	2.2
1	I	143	SER	2.2
2	B	316	HIS	2.2
2	F	85	GLU	2.1
2	B	113	THR	2.1
2	D	305	LEU	2.1
1	E	224	ASP	2.1
1	I	333	ILE	2.1
2	H	35	VAL	2.1
2	D	109	LYS	2.1
1	E	327	CYS	2.1
1	I	342	GLU	2.1
1	I	303	GLN	2.1
1	I	59	ASP	2.1
1	G	161	GLU	2.0
1	E	305	SER	2.0
1	C	62	THR	2.0
1	G	195	GLN	2.0
2	D	316	HIS	2.0
1	I	269	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

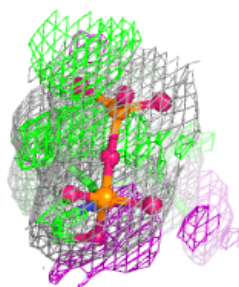
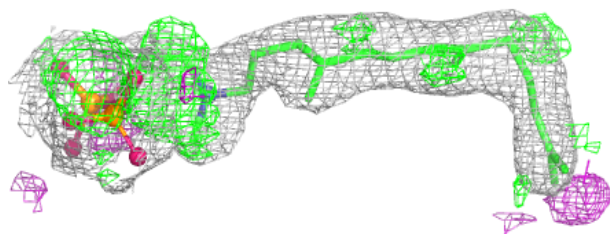
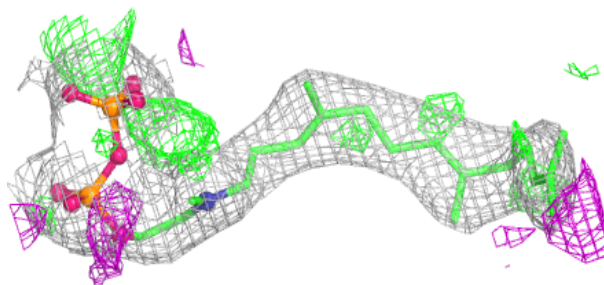
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MES	F	381	12/12	0.89	0.18	89,95,99,99	0
5	MGM	J	379	29/29	0.94	0.14	43,52,65,66	0
5	MGM	L	379	29/29	0.94	0.14	34,50,63,64	0
5	MGM	H	380	29/29	0.94	0.14	45,58,70,72	0
5	MGM	B	379	29/29	0.95	0.13	48,56,68,70	0
5	MGM	D	380	29/29	0.96	0.12	45,55,67,67	0
5	MGM	F	380	29/29	0.96	0.12	44,55,67,70	0
6	CL	F	379	1/1	0.98	0.06	55,55,55,55	0
6	CL	H	379	1/1	0.99	0.06	62,62,62,62	0
6	CL	D	379	1/1	0.99	0.05	59,59,59,59	0
4	ZN	J	378	1/1	1.00	0.02	58,58,58,58	0
4	ZN	L	378	1/1	1.00	0.02	50,50,50,50	0
4	ZN	B	378	1/1	1.00	0.01	54,54,54,54	0
4	ZN	D	378	1/1	1.00	0.02	53,53,53,53	0
4	ZN	F	378	1/1	1.00	0.02	51,51,51,51	0
4	ZN	H	378	1/1	1.00	0.01	59,59,59,59	0

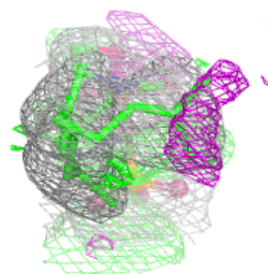
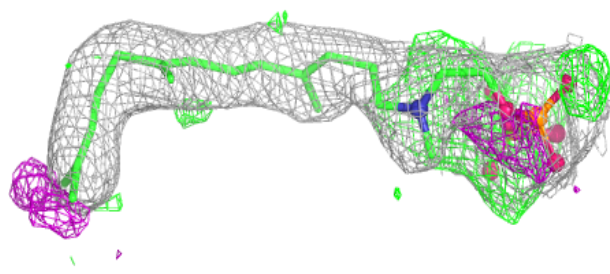
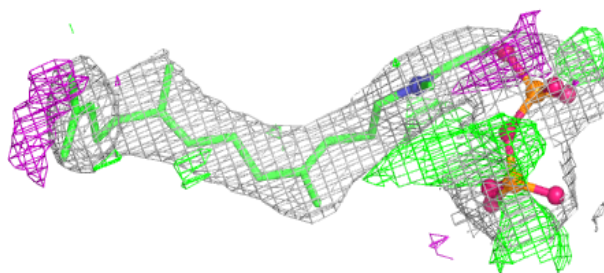
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGM 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)

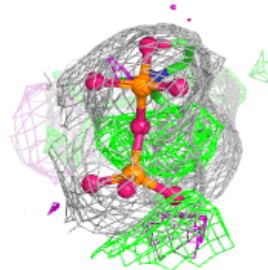
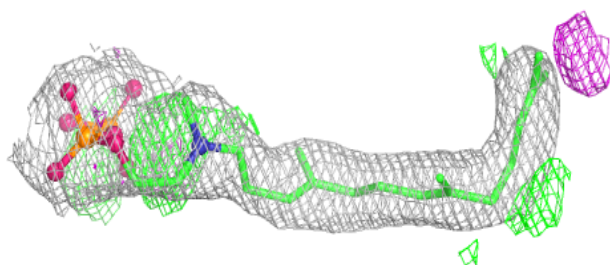
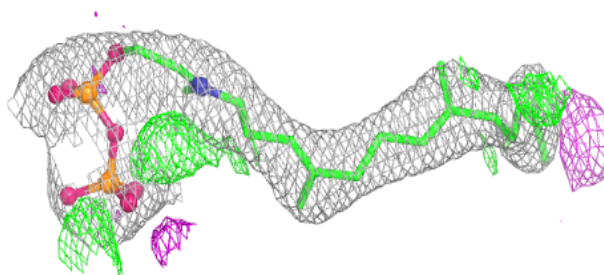
**Electron density around MGM L 379:**

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

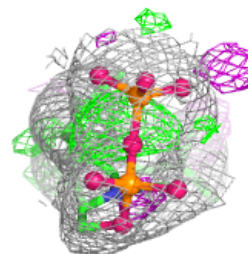
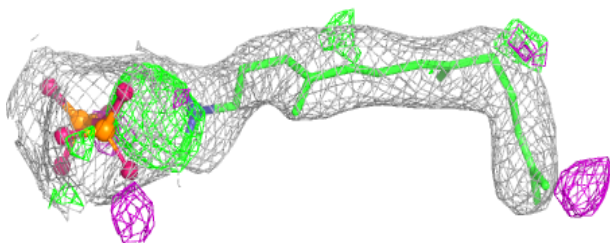
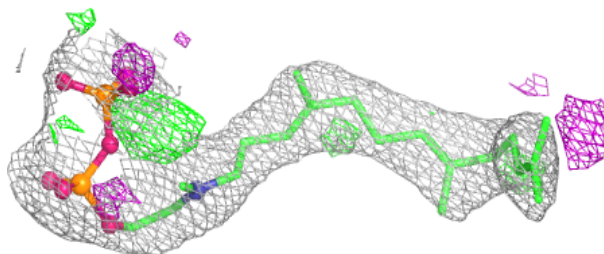


Electron density around MGM H 380:

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

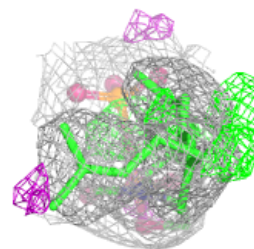
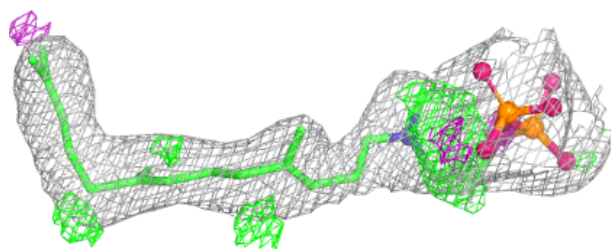
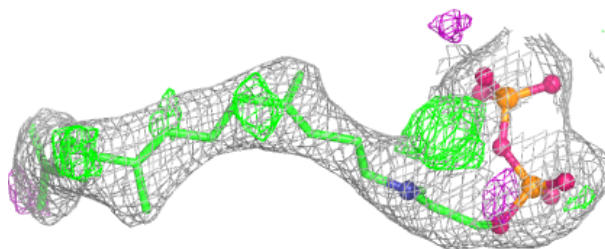
**Electron density around MGM B 379:**

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

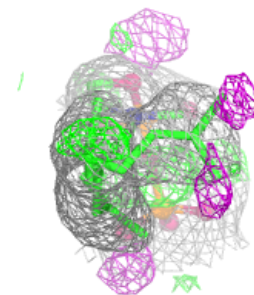
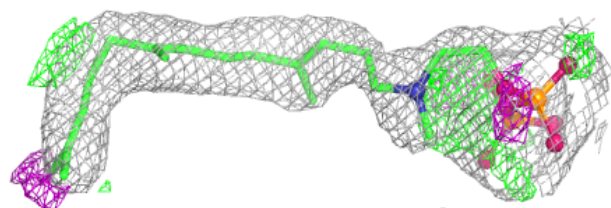
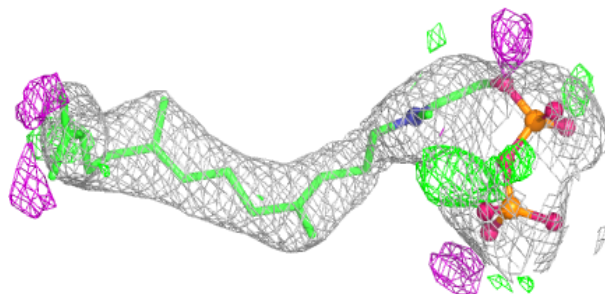


Electron density around MGM D 380:

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

**Electron density around MGM 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 [i](#)

There are no such residues in this entry.