



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:31 AM UTC

PDB ID : 1TNB / pdb_00001tnb
Title : Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a substrate KKSKTKCVIF Peptide Derived from TC21
Authors : Reid, T.S.; Terry, K.L.; Casey, P.J.; Beese, L.S.
Deposited on : 2004-06-11
Resolution : 2.85 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

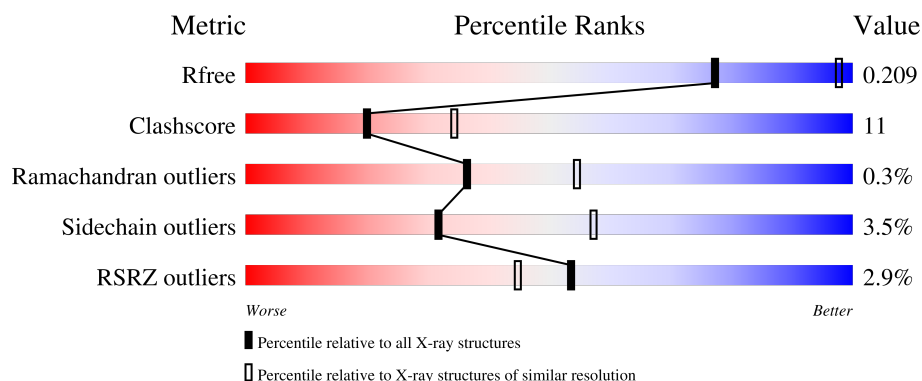
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	2% 58% 23% • 17%
1	C	377	3% 62% 21% • 17%
1	E	377	2% 59% 23% • 17%
1	G	377	3% 62% 20% • 17%
1	I	377	4% 62% 20% • 17%

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Mol	Chain	Length	Quality of chain
1	K	377	
2	B	377	
2	D	377	
2	F	377	
2	H	377	
2	J	377	
2	L	377	
3	M	10	
3	N	10	
3	O	10	
3	P	10	
3	Q	10	
3	R	10	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33504 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			

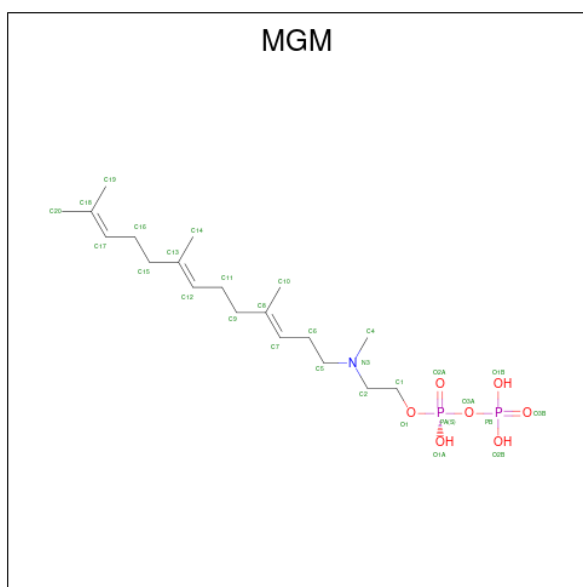
- Molecule 3 is a protein called Fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	N	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	O	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	P	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	Q	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			
3	R	5	Total	C	N	O	S	0	0	0
			42	29	6	6	1			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (CCD ID: MGM) (formula: C₁₉H₃₇NO₇P₂).

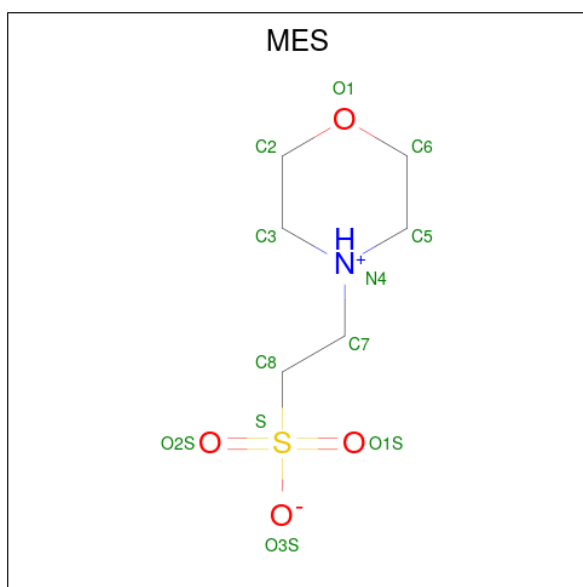


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	D	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	F	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	H	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	J	1	Total	C	N	O	P	0	0
			29	19	1	7	2		
5	L	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

- 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	56	Total	O	0	0
			56	56		
8	B	55	Total	O	0	0
			55	55		
8	C	64	Total	O	0	0
			64	64		
8	D	70	Total	O	0	0
			70	70		
8	E	60	Total	O	0	0
			60	60		
8	F	77	Total	O	0	0
			77	77		
8	G	57	Total	O	0	0
			57	57		
8	H	49	Total	O	0	0
			49	49		
8	I	62	Total	O	0	0
			62	62		
8	J	59	Total	O	0	0
			59	59		
8	K	128	Total	O	0	0
			128	128		

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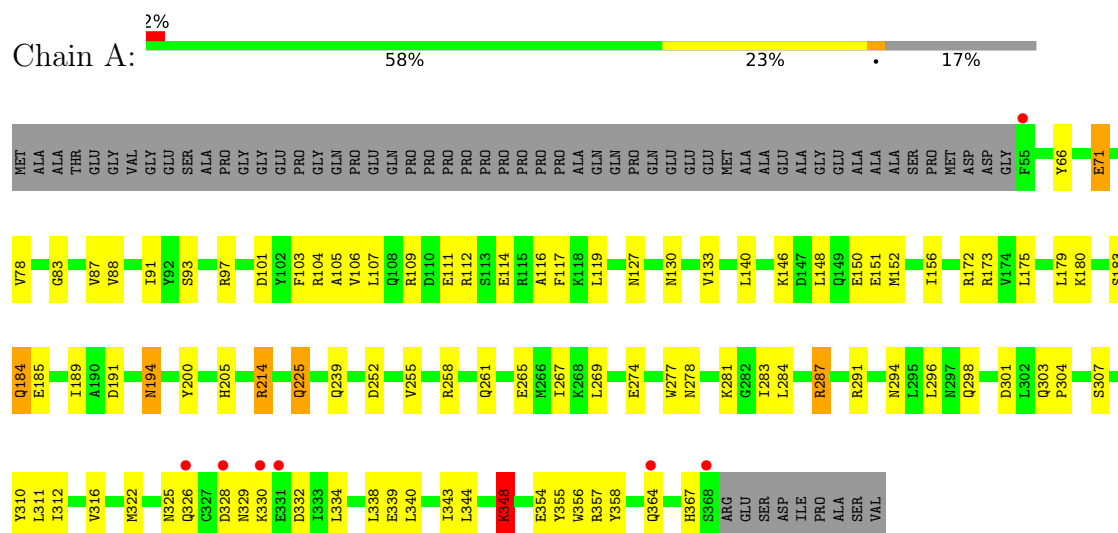
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	110	Total 110	O 110	0	0
8	M	9	Total 9	O 9	0	0
8	N	7	Total 7	O 7	0	0
8	O	2	Total 2	O 2	0	0
8	P	4	Total 4	O 4	0	0
8	Q	6	Total 6	O 6	0	0
8	R	6	Total 6	O 6	0	0

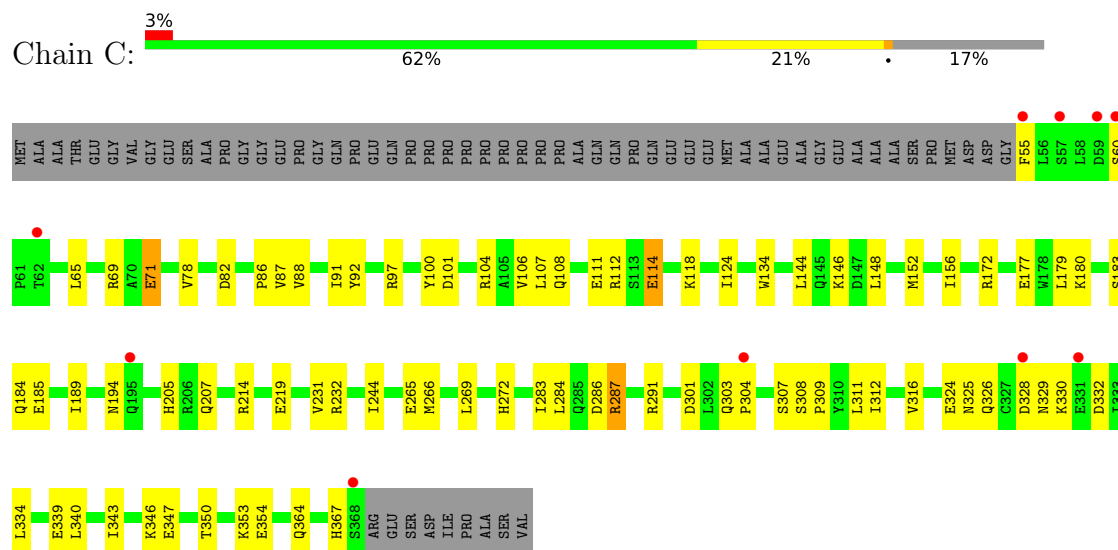
3 Residue-property plots

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

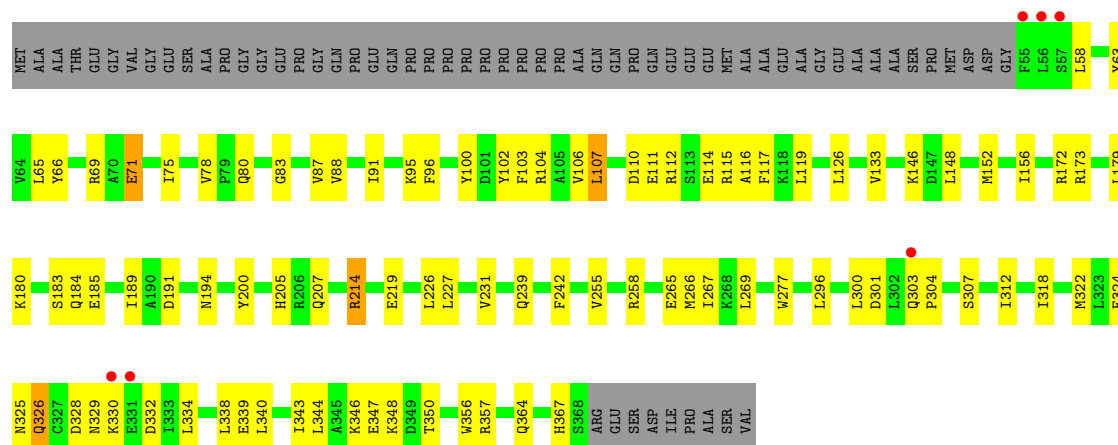


- Molecule 1: geranylgeranyltransferase type I alpha subunit

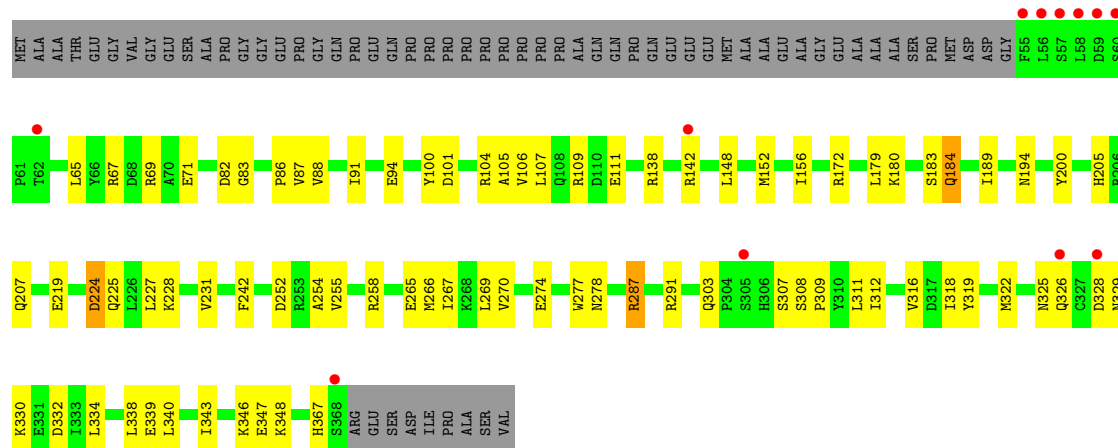


- Molecule 1: geranylgeranyltransferase type I alpha subunit

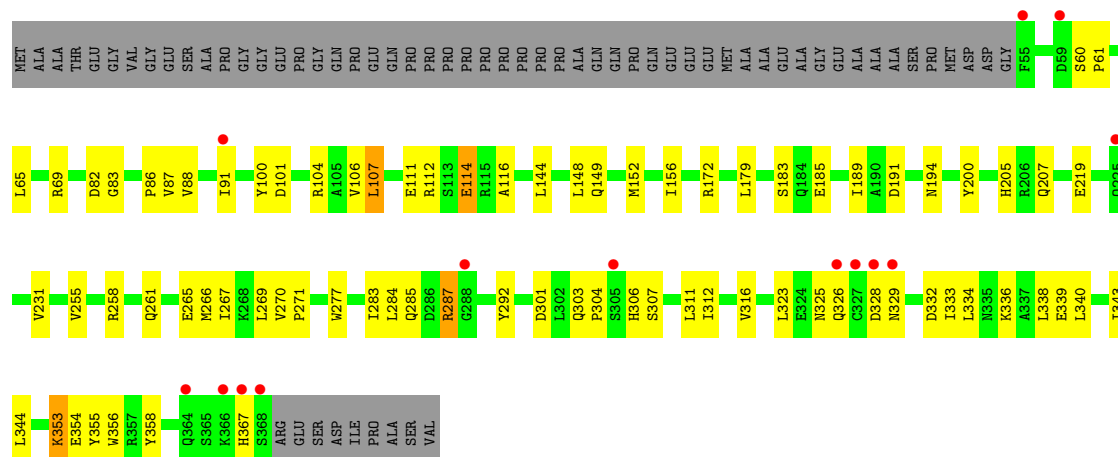




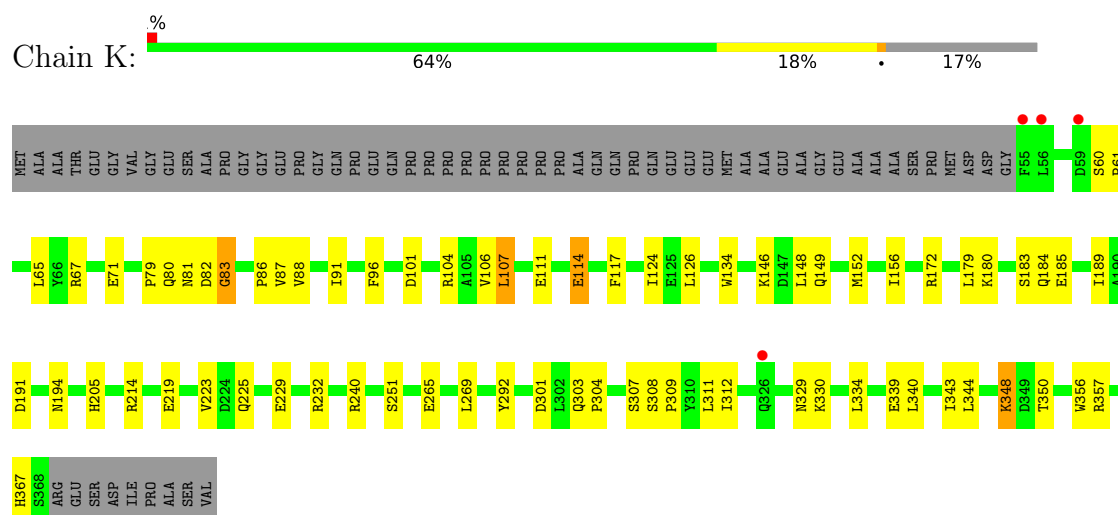
- Molecule 1: geranylgeranyltransferase type I alpha subunit



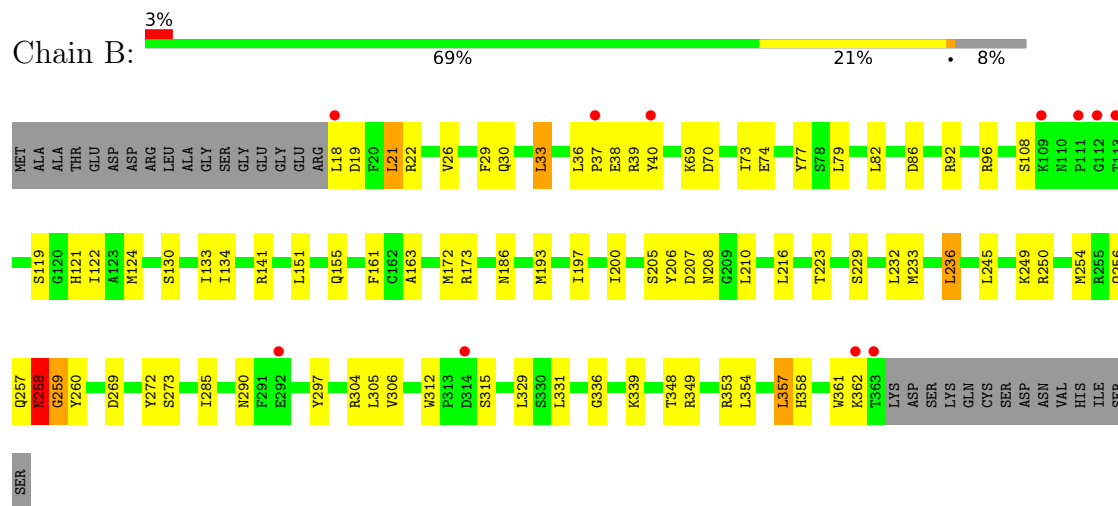
- Molecule 1: geranylgeranyltransferase type I alpha subunit



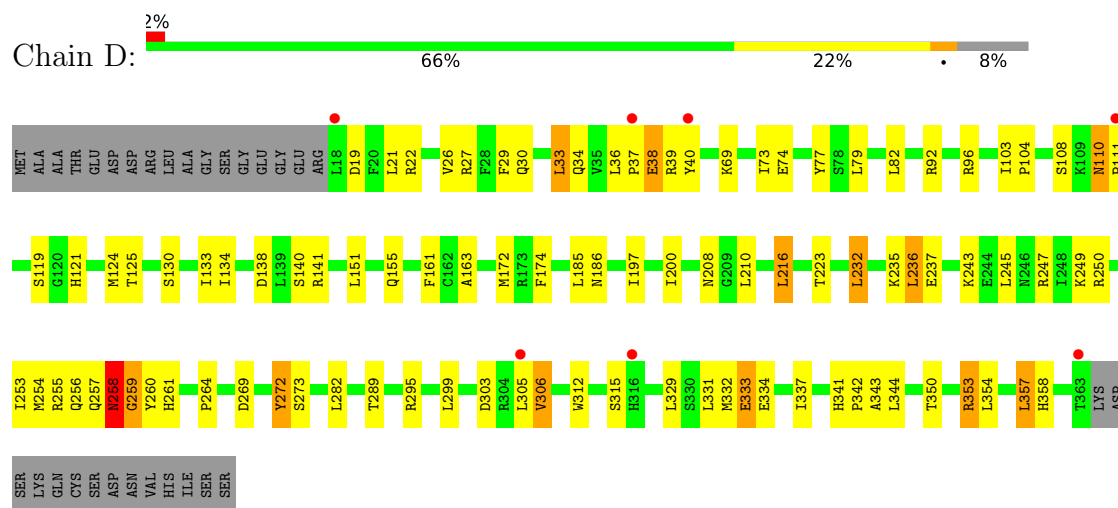
- Molecule 1: geranylgeranyltransferase type I alpha subunit



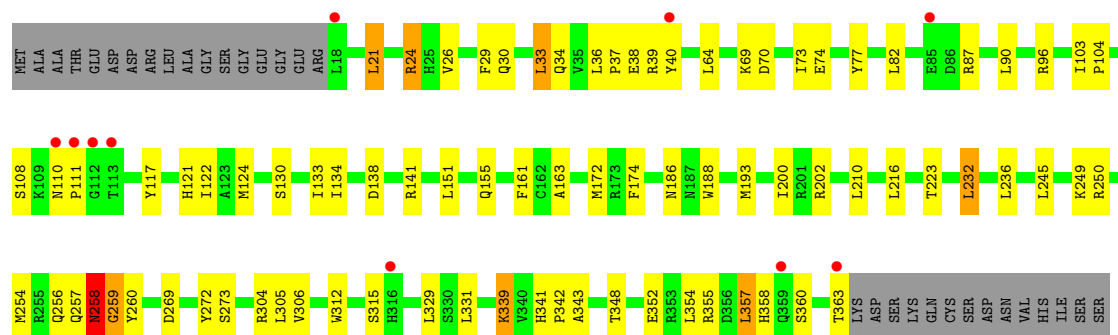
- Molecule 2: Geranylgeranyl transferase type I beta subunit



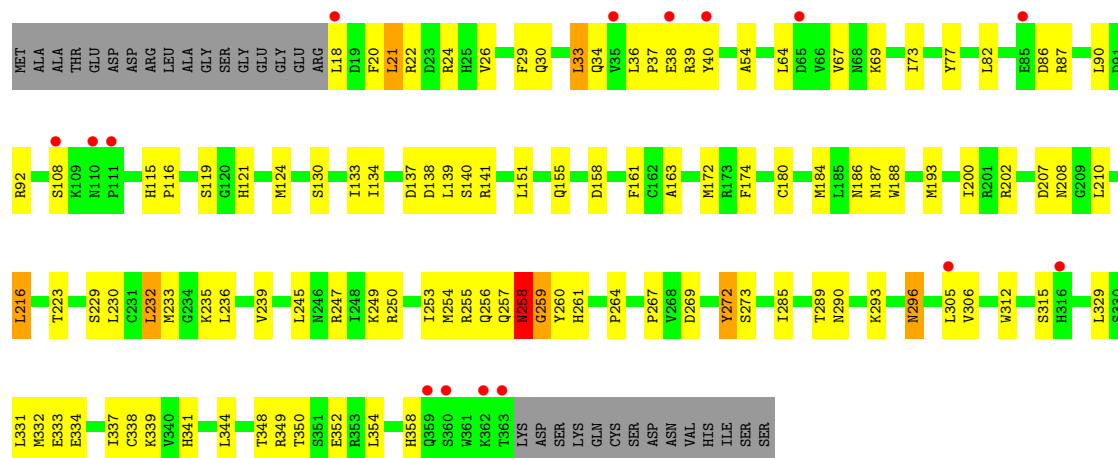
- Molecule 2: Geranylgeranyl transferase type I beta subunit



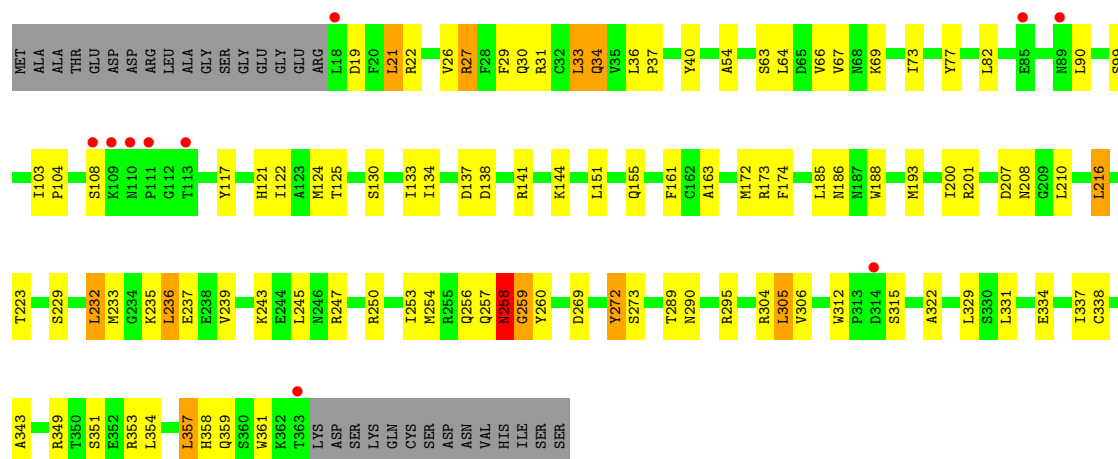
- Molecule 2: Geranylgeranyl transferase type I beta subunit



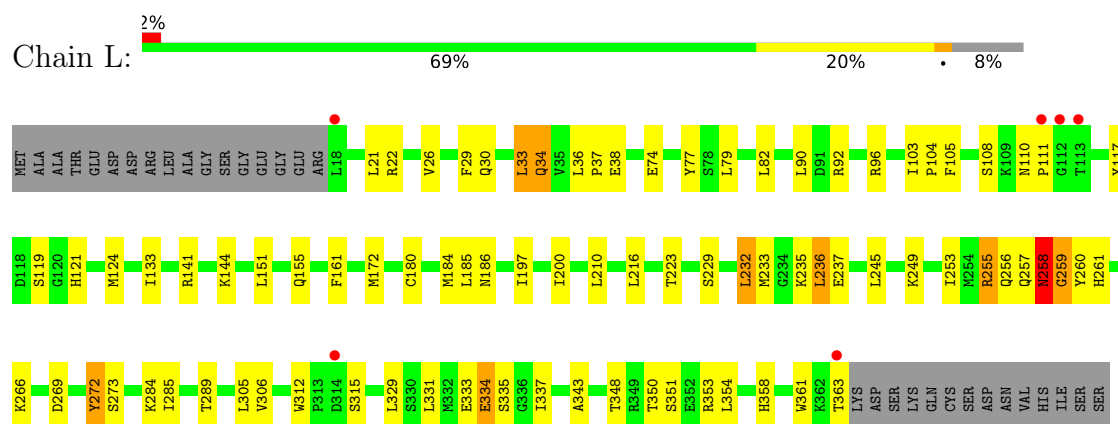
• Molecule 2: Geranylgeranyl transferase type I beta subunit



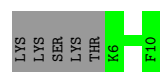
• Molecule 2: Geranylgeranyl transferase type I beta subunit



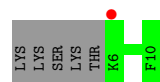
• Molecule 2: Geranylgeranyl transferase type I beta subunit



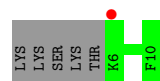
- Molecule 3: Fusion protein



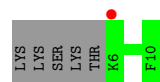
- Molecule 3: Fusion protein



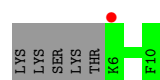
- Molecule 3: Fusion protein



- Molecule 3: Fusion protein



- Molecule 3: Fusion protein



- Molecule 3: Fusion protein



LYS	LYS	LYS	SER	LYS	THR	R6	R10
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	271.13Å 266.72Å 185.14Å 90.00° 131.68° 90.00°	Depositor
Resolution (Å)	27.66 – 2.85 27.66 – 2.85	Depositor EDS
% Data completeness (in resolution range)	93.6 (27.66-2.85) 93.6 (27.66-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.210 0.188 , 0.209	Depositor DCC
R_{free} test set	10767 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.087 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33504	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: MGM, CL, 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	0.87	6/3677 (0.2%)
1	C	0.41	0/2721	0.86	6/3698 (0.2%)
1	E	0.42	0/2730	0.87	8/3710 (0.2%)
1	G	0.43	0/2717	0.88	7/3692 (0.2%)
1	I	0.42	0/2714	0.85	8/3690 (0.2%)
1	K	0.46	0/2741	0.87	8/3722 (0.2%)
2	B	0.41	0/2765	0.90	4/3741 (0.1%)
2	D	0.43	0/2768	0.90	9/3743 (0.2%)
2	F	0.44	0/2779	0.91	7/3757 (0.2%)
2	H	0.41	0/2755	0.90	6/3727 (0.2%)
2	J	0.41	0/2769	0.90	6/3744 (0.2%)
2	L	0.45	0/2781	0.91	5/3759 (0.1%)
3	M	0.55	0/42	0.75	0/53
3	N	0.57	0/42	0.74	0/53
3	O	0.59	0/42	0.84	0/53
3	P	0.61	0/42	0.78	0/53
3	Q	0.58	0/42	0.83	0/53
3	R	0.64	0/42	0.77	0/53
All	All	0.43	0/33194	0.89	80/44978 (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
1	E	0	1
2	B	0	1
2	D	0	1
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
All	All	0	6

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-10.58	97.48	112.60
2	D	259	GLY	N-CA-C	-10.38	97.75	112.60
2	H	259	GLY	N-CA-C	-10.27	97.92	112.60
2	L	259	GLY	N-CA-C	-10.22	97.98	112.60
2	F	259	GLY	N-CA-C	-10.18	98.04	112.60
2	B	259	GLY	N-CA-C	-10.11	98.14	112.60
1	A	83	GLY	CA-C-N	8.69	128.28	119.24
1	A	83	GLY	C-N-CA	8.69	128.28	119.24
1	K	348	LYS	N-CA-C	8.08	122.41	112.23
1	K	83	GLY	CA-C-N	6.78	126.29	119.24
1	K	83	GLY	C-N-CA	6.78	126.29	119.24
2	D	258	ASN	N-CA-C	-6.77	96.38	110.80
2	H	257	GLN	N-CA-C	-6.68	105.13	113.55
2	B	257	GLN	N-CA-C	-6.65	105.17	113.55
2	D	257	GLN	N-CA-C	-6.62	105.20	113.55
2	L	257	GLN	N-CA-C	-6.62	105.21	113.55
2	J	257	GLN	N-CA-C	-6.61	105.22	113.55
2	H	258	ASN	N-CA-C	-6.59	96.77	110.80
1	I	83	GLY	CA-C-N	6.51	125.74	118.97
1	I	83	GLY	C-N-CA	6.51	125.74	118.97
2	J	258	ASN	N-CA-C	-6.50	96.96	110.80
2	L	258	ASN	N-CA-C	-6.48	96.99	110.80
2	F	257	GLN	N-CA-C	-6.45	105.43	113.55
1	E	183	SER	N-CA-C	6.44	119.12	111.33
1	C	350	THR	N-CA-C	6.42	119.10	111.33
2	F	258	ASN	N-CA-C	-6.41	97.16	110.80
2	D	353	ARG	N-CA-C	-6.39	104.32	111.28
1	E	348	LYS	N-CA-C	6.36	119.51	111.69
2	B	258	ASN	N-CA-C	-6.34	97.28	110.80
1	E	83	GLY	CA-C-N	6.32	125.82	119.24
1	E	83	GLY	C-N-CA	6.32	125.82	119.24
1	G	183	SER	N-CA-C	6.29	118.94	111.33
1	I	185	GLU	N-CA-C	6.25	117.78	110.97
1	C	183	SER	N-CA-C	6.21	118.84	111.33
2	D	341	HIS	CA-C-N	6.15	125.64	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	341	HIS	C-N-CA	6.15	125.64	119.24
1	E	346	LYS	N-CA-C	6.13	118.04	111.36
1	A	183	SER	N-CA-C	6.11	118.72	111.33
1	C	346	LYS	N-CA-C	6.04	117.95	111.36
1	A	348	LYS	N-CA-C	5.98	119.04	111.69
1	C	185	GLU	N-CA-C	5.96	117.47	110.97
1	K	185	GLU	N-CA-C	5.93	117.61	111.03
1	A	185	GLU	N-CA-C	5.90	117.40	110.97
1	I	292	TYR	CA-C-N	5.89	126.03	119.32
1	I	292	TYR	C-N-CA	5.89	126.03	119.32
1	E	185	GLU	N-CA-C	5.86	117.54	111.03
2	J	273	SER	N-CA-C	-5.85	105.40	112.54
2	L	273	SER	N-CA-C	-5.85	105.40	112.54
1	C	347	GLU	N-CA-C	5.84	121.28	114.62
1	I	183	SER	N-CA-C	5.83	118.38	111.33
2	D	273	SER	N-CA-C	-5.61	105.70	112.54
1	G	346	LYS	N-CA-C	5.60	118.32	111.82
2	F	341	HIS	CA-C-N	5.58	125.25	119.56
2	F	341	HIS	C-N-CA	5.58	125.25	119.56
2	H	273	SER	N-CA-C	-5.57	105.75	112.54
2	F	273	SER	N-CA-C	-5.56	105.75	112.54
2	B	273	SER	N-CA-C	-5.56	105.76	112.54
1	G	347	GLU	N-CA-C	5.51	120.90	114.62
1	I	270	VAL	CA-C-N	5.43	125.77	119.47
1	I	270	VAL	C-N-CA	5.43	125.77	119.47
1	K	292	TYR	CA-C-N	5.42	125.50	119.32
1	K	292	TYR	C-N-CA	5.42	125.50	119.32
1	K	350	THR	N-CA-C	5.40	117.86	111.33
1	K	183	SER	N-CA-C	5.35	118.60	111.75
1	G	83	GLY	CA-C-N	5.34	125.41	119.32
1	G	83	GLY	C-N-CA	5.34	125.41	119.32
2	D	185	LEU	N-CA-C	-5.32	106.77	113.20
1	E	347	GLU	N-CA-C	5.31	120.68	114.62
1	E	350	THR	N-CA-C	5.29	117.73	111.33
2	L	334	GLU	N-CA-C	-5.24	102.53	110.28
2	D	125	THR	N-CA-C	-5.21	105.68	111.36
1	G	270	VAL	CA-C-N	5.15	125.45	119.47
1	G	270	VAL	C-N-CA	5.15	125.45	119.47
2	H	341	HIS	CA-C-N	5.10	126.22	119.84
2	H	341	HIS	C-N-CA	5.10	126.22	119.84
1	A	180	LYS	N-CA-C	-5.10	105.71	112.24
2	J	322	ALA	N-CA-C	-5.09	105.64	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	342	PRO	N-CA-C	5.09	120.45	113.84
2	J	125	THR	N-CA-C	-5.06	105.84	111.36
1	C	244	ILE	N-CA-C	5.06	115.28	110.42

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	TYR	Sidechain
2	D	272	TYR	Sidechain
1	E	102	TYR	Sidechain
2	H	272	TYR	Sidechain
2	J	272	TYR	Sidechain
2	L	272	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2636	0	2526	79	0
1	C	2655	0	2562	58	0
1	E	2664	0	2570	70	0
1	G	2651	0	2563	59	0
1	I	2648	0	2547	52	0
1	K	2675	0	2594	57	0
2	B	2703	0	2606	58	0
2	D	2706	0	2616	70	0
2	F	2717	0	2635	52	0
2	H	2694	0	2589	81	0
2	J	2708	0	2613	73	0
2	L	2719	0	2639	57	0
3	M	42	0	45	0	0
3	N	42	0	45	0	0
3	O	42	0	45	0	0
3	P	42	0	45	0	0
3	Q	42	0	45	0	0
3	R	42	0	45	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
5	F	29	0	34	2	0
5	H	29	0	34	1	0
5	J	29	0	34	2	0
5	L	29	0	34	0	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	56	0	0	4	0
8	B	55	0	0	0	0
8	C	64	0	0	2	0
8	D	70	0	0	1	0
8	E	60	0	0	1	0
8	F	77	0	0	3	0
8	G	57	0	0	1	0
8	H	49	0	0	2	0
8	I	62	0	0	2	0
8	J	59	0	0	0	0
8	K	128	0	0	5	0
8	L	110	0	0	3	0
8	M	9	0	0	0	0
8	N	7	0	0	0	0
8	O	2	0	0	0	0
8	P	4	0	0	0	0
8	Q	6	0	0	0	0
8	R	6	0	0	0	0
All	All	33504	0	31547	731	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 11.

All (731) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.12	1.14
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.15	1.08
1:K:156:ILE:HG12	1:K:172:ARG:HH12	0.98	1.08
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.12	1.07
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.17	1.04
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.21	1.02
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.84	0.92
1:A:348:LYS:NZ	1:A:348:LYS:HA	1.84	0.91
1:E:255:VAL:HG13	1:E:258:ARG:NH2	1.89	0.86
2:D:37:PRO:HG2	2:D:40:TYR:CE1	2.12	0.83
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.94	0.82
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.59	0.81
1:A:255:VAL:HG13	1:A:258:ARG:HH12	1.44	0.81
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.60	0.81
2:D:353:ARG:NH1	2:D:357:LEU:HG	1.97	0.80
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.63	0.79
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.63	0.78
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.63	0.78
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.66	0.77
1:A:348:LYS:HA	1:A:348:LYS:HZ3	1.48	0.77
1:G:152:MET:O	1:G:156:ILE:HG13	1.86	0.76
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.67	0.76
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.99	0.76
1:C:353:LYS:HE3	1:K:339:GLU:HG3	1.68	0.75
1:K:152:MET:O	1:K:156:ILE:HG13	1.85	0.75
1:G:231:VAL:HG23	1:G:266:MET:HE3	1.67	0.74
1:A:152:MET:O	1:A:156:ILE:HG13	1.87	0.74
1:K:156:ILE:CG1	1:K:172:ARG:HH12	1.91	0.74
1:E:152:MET:O	1:E:156:ILE:HG13	1.87	0.74
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.53	0.74
1:I:152:MET:O	1:I:156:ILE:HG13	1.86	0.74
2:H:348:THR:O	2:H:352:GLU:HG2	1.88	0.74
1:E:231:VAL:HG23	1:E:266:MET:HE3	1.70	0.73
1:I:231:VAL:HG23	1:I:266:MET:HE3	1.68	0.73
1:C:329:ASN:HB3	1:C:332:ASP:HB3	1.69	0.73
1:G:252:ASP:OD2	1:G:255:VAL:HG23	1.89	0.73
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.70	0.72
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.24	0.72
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.70	0.71
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.97	0.71
2:D:37:PRO:HG2	2:D:40:TYR:HE1	1.54	0.71
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.72	0.71
1:I:340:LEU:HD23	1:I:343:ILE:HD12	1.72	0.71
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.54	0.70
1:C:152:MET:O	1:C:156:ILE:HG13	1.90	0.70
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.26	0.70
1:E:296:LEU:HD22	1:E:322:MET:HE1	1.72	0.70
2:F:110:ASN:HB3	2:F:111:PRO:HD2	1.70	0.70
1:C:231:VAL:HG23	1:C:266:MET:HE3	1.73	0.70
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.72	0.70
1:A:348:LYS:HA	1:A:348:LYS:HZ2	1.57	0.69
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.74	0.69
1:E:156:ILE:CG1	1:E:172:ARG:HH12	1.98	0.69
2:F:339:LYS:O	2:F:348:THR:HG23	1.92	0.69
1:A:344:LEU:HA	1:A:348:LYS:HB2	1.76	0.68
2:L:348:THR:HA	2:L:351:SER:HB3	1.74	0.68
1:E:301:ASP:O	1:E:304:PRO:HD2	1.94	0.68
1:A:339:GLU:O	1:A:343:ILE:HG13	1.94	0.68
1:I:114:GLU:HG2	8:I:436:HOH:O	1.94	0.68
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.28	0.67
1:K:91:ILE:HD12	1:K:91:ILE:O	1.94	0.67
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.77	0.67
1:A:303:GLN:O	1:A:307:SER:HB2	1.94	0.67
1:G:105:ALA:O	1:G:109:ARG:HG3	1.95	0.67
1:E:339:GLU:O	1:E:343:ILE:HG13	1.95	0.67
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.76	0.66
1:E:340:LEU:HD23	1:E:343:ILE:HD12	1.76	0.66
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.77	0.66
1:C:303:GLN:O	1:C:307:SER:HB2	1.96	0.66
2:D:69:LYS:O	2:D:73:ILE:HG13	1.94	0.66
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.78	0.66
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.78	0.66
2:H:30:GLN:O	2:H:34:GLN:HG3	1.95	0.66
1:I:91:ILE:HD12	1:I:91:ILE:O	1.94	0.66
1:A:91:ILE:HD12	1:A:91:ILE:O	1.96	0.65
1:I:303:GLN:HB3	1:I:304:PRO:HD3	1.78	0.65
2:F:24:ARG:HH11	2:F:24:ARG:HB2	1.60	0.65
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.79	0.65
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.77	0.65
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.31	0.65
1:I:353:LYS:HG2	1:I:354:GLU:N	2.10	0.65
2:F:363:THR:HG22	8:F:451:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.78	0.65
2:H:290:ASN:CG	2:H:293:LYS:HG3	2.22	0.65
1:G:91:ILE:HD12	1:G:91:ILE:O	1.97	0.64
1:G:339:GLU:O	1:G:343:ILE:HG13	1.97	0.64
2:J:144:LYS:HG2	2:J:185:LEU:HD22	1.79	0.64
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.78	0.64
2:H:69:LYS:O	2:H:73:ILE:HG13	1.96	0.64
2:H:290:ASN:OD1	2:H:293:LYS:HG3	1.96	0.64
1:A:93:SER:N	2:B:38:GLU:OE1	2.30	0.64
1:I:339:GLU:O	1:I:343:ILE:HG13	1.99	0.63
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.32	0.63
1:E:91:ILE:O	1:E:91:ILE:HD12	1.97	0.63
2:H:18:LEU:HD22	2:H:18:LEU:N	2.14	0.63
2:J:359:GLN:HA	2:J:359:GLN:NE2	2.12	0.63
2:H:229:SER:O	2:H:233:MET:HG3	1.98	0.63
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.79	0.62
1:K:330:LYS:HE3	1:K:367:HIS:HB3	1.80	0.62
1:C:91:ILE:O	1:C:91:ILE:HD12	1.99	0.62
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.81	0.62
1:K:303:GLN:O	1:K:307:SER:HB2	2.00	0.62
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.81	0.62
1:G:340:LEU:HD23	1:G:343:ILE:HD12	1.82	0.61
2:D:30:GLN:O	2:D:34:GLN:HG3	2.00	0.61
2:H:296:ASN:HD22	2:H:296:ASN:C	2.08	0.61
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.82	0.61
1:G:329:ASN:HB3	1:G:332:ASP:HB3	1.82	0.61
2:B:258:ASN:OD1	2:B:259:GLY:N	2.33	0.61
2:B:26:VAL:O	2:B:30:GLN:HG3	2.00	0.60
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.82	0.60
1:E:78:VAL:O	1:E:104:ARG:HD2	2.00	0.60
2:B:69:LYS:O	2:B:73:ILE:HG13	2.01	0.60
2:H:92:ARG:HD2	2:H:119:SER:OG	2.01	0.60
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.67	0.60
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.37	0.60
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.66	0.60
2:F:352:GLU:HG2	2:F:355:ARG:HH12	1.67	0.60
1:G:252:ASP:OD2	1:G:254:ALA:HB3	2.02	0.60
2:B:245:LEU:O	2:B:249:LYS:HG3	2.02	0.59
1:A:287:ARG:O	1:A:291:ARG:HD3	2.03	0.59
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.84	0.59
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:O	1:A:287:ARG:HG2	2.03	0.59
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.05	0.59
1:I:100:TYR:O	1:I:104:ARG:HG3	2.03	0.59
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.85	0.59
1:A:312:ILE:O	1:A:316:VAL:HG23	2.02	0.59
1:E:329:ASN:HB3	1:E:332:ASP:HB3	1.83	0.59
1:G:334:LEU:HD22	1:G:367:HIS:O	2.02	0.59
1:A:104:ARG:NH2	8:A:390:HOH:O	2.36	0.58
1:I:231:VAL:CG2	1:I:266:MET:HE3	2.34	0.58
1:K:156:ILE:HD11	1:K:184:GLN:HE21	1.67	0.58
1:A:91:ILE:HD11	2:B:38:GLU:H	1.67	0.58
2:F:30:GLN:O	2:F:34:GLN:HG3	2.03	0.58
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.69	0.58
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.39	0.57
2:J:359:GLN:HA	2:J:359:GLN:HE21	1.69	0.57
1:C:88:VAL:CG1	2:D:36:LEU:HD11	2.34	0.57
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.04	0.57
1:C:339:GLU:O	1:C:343:ILE:HG13	2.05	0.57
1:I:333:ILE:HA	1:I:336:LYS:HG3	1.86	0.57
2:F:69:LYS:O	2:F:73:ILE:HG13	2.04	0.57
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.00	0.57
2:D:37:PRO:HG2	2:D:40:TYR:CD1	2.40	0.57
2:F:245:LEU:O	2:F:249:LYS:HG3	2.04	0.57
1:A:301:ASP:O	1:A:304:PRO:HD2	2.05	0.56
1:A:184:GLN:HG3	8:A:380:HOH:O	2.04	0.56
1:A:283:ILE:O	1:A:287:ARG:HD3	2.06	0.56
1:G:65:LEU:HD12	1:G:67:ARG:NH1	2.20	0.56
1:G:318:ILE:HG22	1:G:322:MET:HE2	1.86	0.56
2:H:258:ASN:OD1	2:H:259:GLY:N	2.37	0.56
1:K:184:GLN:HG2	8:K:382:HOH:O	2.04	0.56
2:B:353:ARG:HG2	2:B:353:ARG:HH11	1.70	0.56
1:E:303:GLN:O	1:E:307:SER:HB2	2.05	0.56
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.70	0.56
1:I:82:ASP:HB2	1:I:86:PRO:HB3	1.87	0.56
1:I:328:ASP:O	1:I:329:ASN:HB2	2.06	0.56
1:K:339:GLU:O	1:K:343:ILE:HG13	2.04	0.56
1:A:296:LEU:CD2	1:A:322:MET:HE1	2.35	0.56
1:C:91:ILE:HD11	2:D:38:GLU:H	1.71	0.56
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.70	0.56
1:E:326:GLN:N	1:E:326:GLN:HE21	2.04	0.56
1:A:265:GLU:O	1:A:269:LEU:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.35	0.56
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.87	0.56
1:I:334:LEU:HD22	1:I:367:HIS:O	2.06	0.56
1:C:78:VAL:HG21	1:C:108:GLN:NE2	2.20	0.56
1:I:312:ILE:O	1:I:316:VAL:HG23	2.06	0.56
2:L:30:GLN:O	2:L:34:GLN:HG3	2.06	0.56
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.88	0.55
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.07	0.55
1:G:274:GLU:HG2	1:G:278:ASN:HD21	1.71	0.55
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.88	0.55
1:C:328:ASP:O	1:C:329:ASN:HB2	2.06	0.55
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.41	0.55
2:J:269:ASP:HB3	2:J:272:TYR:HD2	1.72	0.55
2:L:22:ARG:HG2	2:L:22:ARG:HH11	1.69	0.55
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.72	0.55
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.41	0.55
1:G:100:TYR:O	1:G:104:ARG:HG3	2.07	0.55
2:J:210:LEU:HB2	2:J:223:THR:HA	1.88	0.55
2:L:79:LEU:O	2:L:96:ARG:HG3	2.06	0.55
2:B:269:ASP:HB3	2:B:272:TYR:HD2	1.72	0.55
2:D:19:ASP:OD2	2:D:19:ASP:N	2.39	0.55
2:F:269:ASP:HB3	2:F:272:TYR:HD2	1.72	0.55
2:H:37:PRO:C	2:H:39:ARG:H	2.15	0.55
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.41	0.55
1:K:107:LEU:HD11	2:L:117:TYR:HB2	1.88	0.55
2:L:269:ASP:HB3	2:L:272:TYR:HD2	1.71	0.55
1:G:303:GLN:O	1:G:307:SER:HB2	2.07	0.55
1:I:303:GLN:O	1:I:307:SER:HB2	2.08	0.54
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.88	0.54
2:J:359:GLN:C	2:J:361:TRP:H	2.14	0.54
2:L:210:LEU:HB2	2:L:223:THR:HA	1.90	0.54
2:L:245:LEU:O	2:L:249:LYS:HG3	2.07	0.54
2:H:210:LEU:HB2	2:H:223:THR:HA	1.89	0.54
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.22	0.54
2:B:210:LEU:HB2	2:B:223:THR:HA	1.88	0.54
2:B:229:SER:O	2:B:233:MET:HG3	2.07	0.54
2:D:92:ARG:HD2	2:D:119:SER:OG	2.08	0.54
1:G:274:GLU:HG2	1:G:278:ASN:ND2	2.22	0.54
2:H:133:ILE:HD13	2:H:354:LEU:HD13	1.88	0.54
2:D:121:HIS:HB3	2:D:124:MET:HG2	1.89	0.54
2:H:349:ARG:O	2:H:352:GLU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:229:SER:O	2:L:233:MET:HG3	2.08	0.54
2:D:210:LEU:HB2	2:D:223:THR:HA	1.89	0.54
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.90	0.54
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.72	0.54
2:J:27:ARG:HH12	2:J:30:GLN:NE2	2.05	0.54
1:K:301:ASP:O	1:K:304:PRO:HD2	2.08	0.54
2:F:121:HIS:HB3	2:F:124:MET:HG2	1.90	0.53
1:E:296:LEU:CD2	1:E:322:MET:HE1	2.37	0.53
1:G:156:ILE:CG1	1:G:172:ARG:HH12	2.05	0.53
2:J:243:LYS:O	2:J:247:ARG:HG3	2.08	0.53
1:K:156:ILE:HD11	1:K:184:GLN:NE2	2.23	0.53
1:K:265:GLU:O	1:K:269:LEU:HD13	2.09	0.53
1:A:258:ARG:HH11	1:A:258:ARG:HB3	1.74	0.53
1:G:207:GLN:HG2	1:G:242:PHE:CE2	2.44	0.53
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.43	0.53
1:G:88:VAL:CG1	2:H:36:LEU:HD11	2.39	0.53
1:K:65:LEU:HD12	1:K:67:ARG:NH1	2.24	0.53
2:D:110:ASN:HB3	2:D:111:PRO:HD2	1.91	0.53
1:E:110:ASP:OD2	1:E:112:ARG:NE	2.36	0.53
2:F:210:LEU:HB2	2:F:223:THR:HA	1.89	0.53
2:H:267:PRO:HG2	8:H:413:HOH:O	2.08	0.53
1:I:191:ASP:O	1:I:194:ASN:HB2	2.08	0.53
1:E:326:GLN:HE21	1:E:326:GLN:H	1.56	0.53
1:A:78:VAL:O	1:A:104:ARG:HD2	2.09	0.53
1:A:261:GLN:O	1:A:265:GLU:HG2	2.08	0.53
2:J:22:ARG:O	2:J:26:VAL:HG23	2.08	0.53
1:A:214:ARG:HG3	1:A:214:ARG:O	2.08	0.53
1:C:91:ILE:CD1	2:D:38:GLU:H	2.22	0.53
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.44	0.53
1:K:348:LYS:HD2	8:K:464:HOH:O	2.07	0.53
1:E:100:TYR:O	1:E:104:ARG:HG3	2.08	0.52
1:G:265:GLU:O	1:G:269:LEU:HD13	2.09	0.52
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.73	0.52
2:D:269:ASP:HB3	2:D:272:TYR:HD2	1.74	0.52
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.44	0.52
2:H:334:GLU:HB3	2:H:337:ILE:HD12	1.91	0.52
1:K:91:ILE:HG13	2:L:36:LEU:O	2.09	0.52
2:H:115:HIS:ND1	2:H:116:PRO:HD2	2.24	0.52
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.44	0.52
2:F:352:GLU:HA	2:F:355:ARG:NH1	2.24	0.52
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:PRO:HG2	8:D:442:HOH:O	2.08	0.52
2:H:296:ASN:C	2:H:296:ASN:ND2	2.67	0.52
2:L:22:ARG:O	2:L:26:VAL:HG23	2.10	0.52
1:E:110:ASP:CG	1:E:112:ARG:HE	2.16	0.52
2:H:269:ASP:HB3	2:H:272:TYR:HD2	1.74	0.52
2:J:358:HIS:O	2:J:361:TRP:HB2	2.10	0.52
2:L:133:ILE:HG22	2:L:350:THR:HG23	1.91	0.52
2:L:103:ILE:HG23	2:L:104:PRO:HD2	1.91	0.52
2:L:121:HIS:HB3	2:L:124:MET:HG2	1.92	0.52
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.25	0.52
2:F:77:TYR:CE1	2:F:141:ARG:HB2	2.45	0.52
2:H:37:PRO:C	2:H:39:ARG:N	2.66	0.52
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.83	0.52
1:C:100:TYR:O	1:C:104:ARG:HG3	2.09	0.52
1:E:265:GLU:O	1:E:269:LEU:HD13	2.10	0.52
2:J:359:GLN:C	2:J:361:TRP:N	2.67	0.52
1:A:294:ASN:O	1:A:298:GLN:HG3	2.10	0.52
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.91	0.52
1:C:219:GLU:HA	1:C:219:GLU:OE1	2.10	0.52
1:E:91:ILE:HD11	2:F:38:GLU:H	1.75	0.52
2:F:96:ARG:HD3	8:F:431:HOH:O	2.09	0.52
1:C:334:LEU:HD22	1:C:367:HIS:O	2.10	0.51
2:F:26:VAL:O	2:F:30:GLN:HG3	2.10	0.51
1:I:323:LEU:HB3	1:I:367:HIS:CD2	2.45	0.51
1:A:255:VAL:HA	1:A:258:ARG:NH1	2.25	0.51
1:C:283:ILE:O	1:C:287:ARG:HD3	2.10	0.51
2:D:138:ASP:OD1	2:D:140:SER:HB3	2.10	0.51
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.75	0.51
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.45	0.51
2:L:312:TRP:O	2:L:315:SER:HB3	2.10	0.51
1:E:326:GLN:HE21	1:E:326:GLN:CA	2.23	0.51
1:G:287:ARG:O	1:G:291:ARG:HD3	2.10	0.51
1:I:149:GLN:NE2	1:I:179:LEU:HD13	2.25	0.51
2:J:69:LYS:O	2:J:73:ILE:HG13	2.11	0.51
2:J:351:SER:O	2:J:354:LEU:HB3	2.11	0.51
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.91	0.51
1:A:105:ALA:O	1:A:109:ARG:HG3	2.11	0.51
1:C:284:LEU:O	1:C:287:ARG:HG2	2.10	0.51
2:D:103:ILE:HG23	2:D:104:PRO:HD2	1.93	0.51
2:D:334:GLU:HB3	2:D:337:ILE:HD12	1.92	0.51
1:A:191:ASP:O	1:A:194:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:ARG:HD2	8:F:436:HOH:O	2.10	0.51
1:G:319:TYR:HA	1:G:322:MET:HE3	1.93	0.51
1:K:79:PRO:HA	1:K:101:ASP:OD1	2.10	0.51
2:L:22:ARG:HG2	2:L:22:ARG:NH1	2.26	0.51
2:D:79:LEU:O	2:D:96:ARG:HG3	2.10	0.51
2:H:121:HIS:HB3	2:H:124:MET:HG2	1.92	0.51
2:H:245:LEU:O	2:H:249:LYS:HG3	2.11	0.51
1:I:325:ASN:O	1:I:326:GLN:C	2.54	0.51
1:A:334:LEU:HD22	1:A:367:HIS:O	2.11	0.51
2:B:19:ASP:OD2	2:B:19:ASP:N	2.44	0.51
1:I:106:VAL:HG13	1:I:111:GLU:HB3	1.92	0.51
2:B:37:PRO:C	2:B:39:ARG:N	2.68	0.51
2:B:121:HIS:HB3	2:B:124:MET:HG2	1.93	0.51
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.41	0.51
2:B:29:PHE:O	2:B:33:LEU:HD22	2.10	0.50
2:F:360:SER:O	2:F:363:THR:HG23	2.11	0.50
2:L:144:LYS:HG2	2:L:185:LEU:HD22	1.93	0.50
2:H:180:CYS:O	2:H:184:MET:HG3	2.11	0.50
1:I:91:ILE:HG13	2:J:36:LEU:O	2.11	0.50
2:D:186:ASN:HB2	2:D:358:HIS:CE1	2.47	0.50
1:I:284:LEU:O	1:I:287:ARG:HG2	2.10	0.50
1:K:334:LEU:HD22	1:K:367:HIS:O	2.11	0.50
1:C:312:ILE:O	1:C:316:VAL:HG23	2.11	0.50
2:D:258:ASN:CG	2:D:259:GLY:H	2.19	0.50
1:E:173:ARG:HD2	8:E:393:HOH:O	2.10	0.50
2:J:77:TYR:HE2	2:J:137:ASP:OD2	1.95	0.50
1:K:214:ARG:O	1:K:214:ARG:HG2	2.11	0.50
1:A:328:ASP:O	1:A:329:ASN:HB2	2.12	0.50
1:A:334:LEU:O	1:A:338:LEU:HG	2.11	0.50
1:E:318:ILE:HG22	1:E:322:MET:CE	2.37	0.50
2:L:333:GLU:HA	8:L:464:HOH:O	2.11	0.50
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.93	0.50
2:H:40:TYR:CD1	2:H:40:TYR:N	2.78	0.50
2:J:359:GLN:HE21	2:J:359:GLN:CA	2.25	0.50
1:K:191:ASP:O	1:K:194:ASN:HB2	2.12	0.50
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.76	0.49
1:A:303:GLN:HB3	1:A:304:PRO:HD3	1.93	0.49
1:G:106:VAL:HG13	1:G:111:GLU:HB3	1.92	0.49
1:I:301:ASP:O	1:I:304:PRO:HD2	2.11	0.49
2:J:229:SER:O	2:J:233:MET:HG3	2.12	0.49
2:L:258:ASN:OD1	2:L:259:GLY:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.12	0.49
2:B:339:LYS:O	2:B:348:THR:HG23	2.11	0.49
1:A:150:GLU:HB3	8:A:423:HOH:O	2.12	0.49
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.47	0.49
2:J:121:HIS:HB3	2:J:124:MET:HG2	1.94	0.49
2:L:348:THR:HA	2:L:351:SER:CB	2.42	0.49
2:B:312:TRP:O	2:B:315:SER:HB3	2.13	0.49
1:E:334:LEU:HD22	1:E:367:HIS:O	2.12	0.49
2:J:258:ASN:OD1	2:J:259:GLY:N	2.39	0.49
1:A:173:ARG:HD2	8:A:400:HOH:O	2.13	0.49
2:D:29:PHE:O	2:D:33:LEU:HD22	2.12	0.49
1:G:138:ARG:O	1:G:142:ARG:HG3	2.12	0.49
1:G:219:GLU:HA	1:G:219:GLU:OE1	2.13	0.49
2:L:348:THR:O	2:L:351:SER:HB3	2.13	0.49
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.27	0.49
2:B:256:GLN:HE22	2:B:290:ASN:HB3	1.77	0.49
1:K:219:GLU:OE1	1:K:219:GLU:HA	2.13	0.49
2:F:155:GLN:HB2	2:F:161:PHE:CE2	2.48	0.49
1:I:285:GLN:NE2	2:J:247:ARG:HH11	2.11	0.49
1:C:177:GLU:HB3	8:C:434:HOH:O	2.13	0.49
2:H:202:ARG:HG3	2:H:202:ARG:NH1	2.24	0.49
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.48	0.49
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.94	0.49
2:F:339:LYS:NZ	2:F:339:LYS:HB3	2.28	0.49
2:H:138:ASP:OD1	2:H:140:SER:HB3	2.12	0.49
2:J:312:TRP:O	2:J:315:SER:HB3	2.13	0.49
1:K:107:LEU:CD1	2:L:117:TYR:HB2	2.43	0.49
2:L:353:ARG:HD2	2:L:353:ARG:O	2.12	0.49
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.95	0.48
2:F:37:PRO:C	2:F:39:ARG:H	2.21	0.48
2:F:250:ARG:O	2:F:254:MET:HG2	2.12	0.48
1:G:311:LEU:HD23	1:G:311:LEU:C	2.38	0.48
2:H:312:TRP:O	2:H:315:SER:HB3	2.14	0.48
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.95	0.48
1:A:296:LEU:HD22	1:A:322:MET:HE1	1.95	0.48
2:F:37:PRO:C	2:F:39:ARG:N	2.70	0.48
2:H:155:GLN:HB2	2:H:161:PHE:CE2	2.48	0.48
1:C:311:LEU:C	1:C:311:LEU:HD23	2.38	0.48
2:D:37:PRO:O	2:D:39:ARG:N	2.46	0.48
2:D:82:LEU:HD11	2:D:108:SER:HA	1.96	0.48
1:I:271:PRO:HG3	1:I:306:HIS:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:PHE:O	2:J:33:LEU:HD22	2.13	0.48
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.48	0.48
2:F:87:ARG:NH1	2:F:90:LEU:HD11	2.29	0.48
2:L:77:TYR:CZ	2:L:141:ARG:HB2	2.49	0.48
1:C:301:ASP:O	1:C:304:PRO:HD2	2.13	0.48
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.48	0.48
2:J:201:ARG:NH1	2:J:239:VAL:O	2.47	0.48
2:D:255:ARG:CZ	2:D:264:PRO:HG3	2.44	0.48
1:I:101:ASP:HA	1:I:104:ARG:HH11	1.78	0.48
1:A:258:ARG:HB3	1:A:258:ARG:NH1	2.29	0.48
2:D:155:GLN:HB2	2:D:161:PHE:CE2	2.48	0.48
1:G:325:ASN:O	1:G:326:GLN:C	2.56	0.48
2:J:63:SER:O	2:J:66:VAL:HG22	2.13	0.48
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.44	0.48
1:C:106:VAL:HG13	1:C:111:GLU:HB3	1.95	0.48
1:C:329:ASN:O	1:C:330:LYS:C	2.56	0.48
2:D:39:ARG:HG3	2:D:40:TYR:CD1	2.49	0.48
2:D:258:ASN:OD1	2:D:259:GLY:N	2.45	0.48
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.28	0.48
1:G:67:ARG:NH2	1:G:94:GLU:OE1	2.47	0.48
2:J:21:LEU:HD11	2:J:304:ARG:NH2	2.27	0.48
2:B:82:LEU:HD11	2:B:108:SER:HA	1.94	0.47
2:B:258:ASN:CG	2:B:259:GLY:H	2.21	0.47
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.14	0.47
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.29	0.47
2:F:130:SER:O	2:F:134:ILE:HG13	2.13	0.47
1:G:82:ASP:HB2	1:G:86:PRO:HB3	1.96	0.47
2:B:37:PRO:O	2:B:39:ARG:N	2.47	0.47
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.49	0.47
2:H:256:GLN:HG3	2:H:260:TYR:CZ	2.49	0.47
1:C:265:GLU:O	1:C:269:LEU:HD13	2.13	0.47
1:E:214:ARG:O	1:E:214:ARG:HG3	2.13	0.47
2:H:188:TRP:CE3	2:H:193:MET:HE2	2.50	0.47
1:C:88:VAL:HG13	2:D:36:LEU:HD11	1.96	0.47
2:L:82:LEU:HD11	2:L:108:SER:HA	1.96	0.47
2:B:79:LEU:O	2:B:96:ARG:HG3	2.15	0.47
2:J:353:ARG:HD3	2:J:353:ARG:C	2.39	0.47
2:D:312:TRP:O	2:D:315:SER:HB3	2.15	0.47
1:E:219:GLU:HA	1:E:219:GLU:OE1	2.14	0.47
2:B:37:PRO:C	2:B:39:ARG:H	2.22	0.47
1:C:214:ARG:O	1:C:214:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:VAL:O	2:D:30:GLN:HG3	2.15	0.47
2:D:37:PRO:CG	2:D:40:TYR:CE1	2.92	0.47
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.50	0.47
2:F:312:TRP:O	2:F:315:SER:HB3	2.13	0.47
1:G:88:VAL:HG13	2:H:36:LEU:HD11	1.96	0.47
1:G:224:ASP:O	1:G:228:LYS:HG3	2.15	0.47
1:G:334:LEU:O	1:G:338:LEU:HG	2.15	0.47
1:I:255:VAL:HG13	1:I:258:ARG:NH2	2.29	0.47
2:J:64:LEU:O	2:J:67:VAL:HG22	2.15	0.47
1:A:106:VAL:HG13	1:A:111:GLU:HB3	1.97	0.47
2:B:155:GLN:HB2	2:B:161:PHE:CE2	2.49	0.47
1:E:200:TYR:HB3	5:F:381:MGM:HC12	1.97	0.47
1:E:325:ASN:O	1:E:326:GLN:C	2.58	0.47
2:F:29:PHE:O	2:F:33:LEU:HD22	2.15	0.47
2:H:290:ASN:ND2	2:H:293:LYS:HG3	2.28	0.47
2:J:253:ILE:HD12	2:J:289:THR:HG22	1.97	0.47
2:B:22:ARG:O	2:B:26:VAL:HG23	2.14	0.47
1:E:329:ASN:O	1:E:330:LYS:C	2.58	0.47
1:I:311:LEU:HD23	1:I:311:LEU:C	2.40	0.47
2:L:348:THR:CA	2:L:351:SER:HB3	2.44	0.47
1:A:71:GLU:CD	1:A:71:GLU:H	2.18	0.46
1:E:106:VAL:HG13	1:E:111:GLU:HB3	1.96	0.46
2:F:70:ASP:O	2:F:74:GLU:HG2	2.15	0.46
1:G:318:ILE:HG22	1:G:322:MET:CE	2.45	0.46
2:J:232:LEU:HD13	2:J:343:ALA:HB1	1.97	0.46
2:B:92:ARG:HD2	2:B:119:SER:OG	2.15	0.46
1:C:101:ASP:HA	1:C:104:ARG:HH11	1.79	0.46
2:D:354:LEU:HD11	2:D:358:HIS:NE2	2.29	0.46
1:A:66:TYR:CE1	1:A:119:LEU:HD13	2.51	0.46
1:C:207:GLN:OE1	2:D:216:LEU:HD13	2.16	0.46
1:C:291:ARG:HH11	1:C:291:ARG:HB2	1.81	0.46
2:D:245:LEU:O	2:D:249:LYS:HG3	2.15	0.46
2:F:24:ARG:HB2	2:F:24:ARG:NH1	2.29	0.46
1:G:184:GLN:HG3	8:G:402:HOH:O	2.15	0.46
1:C:340:LEU:HD23	1:C:343:ILE:HD12	1.98	0.46
2:D:250:ARG:O	2:D:254:MET:HG2	2.16	0.46
1:E:239:GLN:OE1	1:E:239:GLN:HA	2.15	0.46
2:H:130:SER:O	2:H:134:ILE:HG13	2.16	0.46
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.98	0.46
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.55	0.46
1:C:308:SER:O	1:C:312:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:LEU:CD2	2:J:54:ALA:HB1	2.46	0.46
1:A:91:ILE:CD1	2:B:38:GLU:H	2.28	0.46
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.78	0.46
2:L:186:ASN:HB2	2:L:358:HIS:CE1	2.51	0.46
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.50	0.46
1:A:214:ARG:O	1:A:214:ARG:CG	2.64	0.46
1:C:286:ASP:HB2	8:C:424:HOH:O	2.16	0.46
2:F:172:MET:HE1	2:F:200:ILE:HA	1.98	0.46
1:G:328:ASP:O	1:G:329:ASN:HB2	2.15	0.46
1:I:60:SER:OG	1:I:61:PRO:HD2	2.16	0.46
1:I:265:GLU:O	1:I:269:LEU:HD13	2.15	0.46
2:J:353:ARG:NH1	2:J:357:LEU:HD12	2.31	0.46
2:B:39:ARG:NH1	2:B:40:TYR:OH	2.49	0.46
1:C:69:ARG:HB3	1:C:71:GLU:OE1	2.15	0.46
1:C:78:VAL:O	1:C:104:ARG:HD2	2.16	0.46
2:H:87:ARG:HB3	2:H:87:ARG:NH1	2.30	0.46
2:J:353:ARG:HD3	2:J:353:ARG:O	2.15	0.46
1:A:97:ARG:HG2	1:A:101:ASP:OD2	2.15	0.46
2:B:130:SER:O	2:B:134:ILE:HG13	2.16	0.46
2:B:256:GLN:HG3	2:B:260:TYR:CZ	2.51	0.46
1:E:191:ASP:O	1:E:194:ASN:HB2	2.16	0.46
2:F:40:TYR:CD1	2:F:40:TYR:N	2.83	0.46
2:H:235:LYS:O	2:H:239:VAL:HG23	2.16	0.46
2:J:82:LEU:HD11	2:J:108:SER:HA	1.97	0.46
1:G:267:ILE:HD13	1:G:277:TRP:CE2	2.51	0.45
1:K:149:GLN:HG3	8:K:478:HOH:O	2.14	0.45
2:H:230:LEU:HD22	2:H:239:VAL:HG21	1.99	0.45
2:D:208:ASN:ND2	2:D:247:ARG:HB3	2.31	0.45
1:E:58:LEU:HD22	1:E:95:LYS:CD	2.47	0.45
1:E:65:LEU:O	1:E:69:ARG:HG3	2.15	0.45
2:F:82:LEU:HD11	2:F:108:SER:HA	1.97	0.45
2:J:27:ARG:NH1	2:J:27:ARG:HG3	2.32	0.45
1:E:357:ARG:HH11	1:E:357:ARG:HG3	1.81	0.45
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.31	0.45
2:H:22:ARG:HH11	2:H:22:ARG:HG2	1.82	0.45
2:H:82:LEU:HD11	2:H:108:SER:HA	1.97	0.45
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.51	0.45
2:B:207:ASP:O	2:B:208:ASN:HB2	2.17	0.45
1:K:81:ASN:HD21	2:L:105:PHE:H	1.63	0.45
2:L:361:TRP:C	2:L:363:THR:H	2.24	0.45
1:A:267:ILE:HD13	1:A:277:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ILE:HD11	2:H:38:GLU:H	1.81	0.45
1:G:329:ASN:O	1:G:330:LYS:C	2.59	0.45
2:J:155:GLN:HB2	2:J:161:PHE:CE2	2.52	0.45
1:A:355:TYR:O	1:A:358:TYR:HB3	2.17	0.45
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.81	0.45
2:B:250:ARG:O	2:B:254:MET:HG2	2.16	0.45
2:F:258:ASN:CG	2:F:259:GLY:H	2.25	0.45
1:G:312:ILE:O	1:G:316:VAL:HG23	2.17	0.45
2:H:18:LEU:N	2:H:18:LEU:CD2	2.79	0.45
2:J:19:ASP:OD2	2:J:19:ASP:N	2.50	0.45
2:L:77:TYR:CE1	2:L:141:ARG:HB2	2.51	0.45
1:E:148:LEU:CB	1:E:179:LEU:HD21	2.44	0.45
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.52	0.45
2:L:29:PHE:O	2:L:33:LEU:HD22	2.16	0.45
1:A:200:TYR:HB3	5:B:379:MGM:HC12	1.98	0.44
1:A:329:ASN:O	1:A:330:LYS:C	2.59	0.44
1:C:148:LEU:CB	1:C:179:LEU:HD21	2.44	0.44
1:E:329:ASN:HB3	1:E:332:ASP:CB	2.47	0.44
2:H:26:VAL:O	2:H:30:GLN:HG3	2.16	0.44
2:D:255:ARG:NH1	2:D:264:PRO:HG3	2.33	0.44
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.51	0.44
1:A:252:ASP:OD2	1:A:255:VAL:HG23	2.17	0.44
2:F:64:LEU:HD23	2:F:64:LEU:HA	1.82	0.44
2:H:77:TYR:CE1	2:H:141:ARG:HB2	2.51	0.44
2:J:22:ARG:HG2	2:J:22:ARG:HH11	1.82	0.44
1:C:325:ASN:O	1:C:326:GLN:C	2.60	0.44
2:H:249:LYS:HB3	2:H:285:ILE:HD13	2.00	0.44
1:I:334:LEU:O	1:I:338:LEU:HG	2.17	0.44
1:K:251:SER:HB2	8:K:459:HOH:O	2.18	0.44
1:A:325:ASN:O	1:A:326:GLN:C	2.61	0.44
1:E:71:GLU:OE1	1:E:71:GLU:N	2.44	0.44
1:E:340:LEU:HA	1:E:343:ILE:HD12	2.00	0.44
1:A:274:GLU:O	1:A:278:ASN:ND2	2.51	0.44
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.99	0.44
2:H:339:LYS:HE3	2:H:348:THR:HG21	2.00	0.44
1:I:148:LEU:CB	1:I:179:LEU:HD21	2.45	0.44
1:I:200:TYR:HB3	5:J:379:MGM:HC12	2.00	0.44
1:C:55:PHE:HE2	1:C:118:LYS:HZ3	1.64	0.44
2:D:303:ASP:OD1	2:D:306:VAL:HG13	2.18	0.44
2:D:353:ARG:HH12	2:D:357:LEU:HG	1.80	0.44
2:H:33:LEU:HD22	2:H:54:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HE1	2:B:200:ILE:HA	1.99	0.44
1:K:214:ARG:HB2	8:K:453:HOH:O	2.17	0.44
2:D:255:ARG:HD3	2:D:261:HIS:CD2	2.53	0.43
2:H:86:ASP:OD2	2:H:86:ASP:N	2.42	0.43
1:I:107:LEU:HD11	2:J:117:TYR:HB2	1.99	0.43
1:A:91:ILE:HD12	2:B:38:GLU:HB2	2.00	0.43
2:H:29:PHE:O	2:H:33:LEU:HD22	2.19	0.43
2:J:188:TRP:CE3	2:J:193:MET:HE2	2.53	0.43
1:K:91:ILE:HD11	2:L:37:PRO:HA	2.00	0.43
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.52	0.43
2:D:22:ARG:O	2:D:26:VAL:HG23	2.18	0.43
2:B:40:TYR:CD1	2:B:40:TYR:N	2.86	0.43
2:F:138:ASP:HA	2:F:357:LEU:HD11	2.01	0.43
1:G:91:ILE:HD12	2:H:38:GLU:HB2	1.99	0.43
2:H:22:ARG:O	2:H:26:VAL:HG23	2.18	0.43
2:B:18:LEU:HB3	2:B:19:ASP:H	1.59	0.43
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.33	0.43
2:H:250:ARG:O	2:H:254:MET:HG2	2.19	0.43
2:H:255:ARG:CZ	2:H:264:PRO:HG3	2.48	0.43
2:B:86:ASP:OD2	2:B:86:ASP:N	2.50	0.43
2:B:249:LYS:HB3	2:B:285:ILE:HD13	2.00	0.43
2:J:27:ARG:HG3	2:J:27:ARG:HH11	1.82	0.43
1:A:151:GLU:HG3	1:A:175:LEU:HD11	2.00	0.43
2:D:282:LEU:HD21	2:D:342:PRO:HB2	2.00	0.43
1:E:334:LEU:O	1:E:338:LEU:HG	2.18	0.43
2:L:92:ARG:HD2	2:L:119:SER:OG	2.19	0.43
2:L:155:GLN:HB2	2:L:161:PHE:CE2	2.53	0.43
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.82	0.43
2:H:24:ARG:HG2	2:H:24:ARG:HH11	1.83	0.43
1:C:65:LEU:O	1:C:69:ARG:HG3	2.19	0.43
1:C:353:LYS:HG3	1:C:354:GLU:N	2.34	0.43
2:F:122:ILE:HG22	2:F:163:ALA:HA	2.01	0.43
2:F:163:ALA:HB2	2:F:174:PHE:CZ	2.54	0.43
2:H:37:PRO:O	2:H:39:ARG:N	2.52	0.43
2:H:163:ALA:HB2	2:H:174:PHE:CZ	2.54	0.43
1:K:329:ASN:O	1:K:330:LYS:C	2.62	0.43
1:A:225:GLN:HE21	1:A:225:GLN:HB3	1.52	0.43
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.19	0.43
2:D:197:ILE:HD11	2:D:235:LYS:HD2	2.00	0.43
2:D:256:GLN:HB2	2:D:260:TYR:CE2	2.53	0.43
1:E:58:LEU:HD22	1:E:95:LYS:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LEU:CB	1:G:179:LEU:HD21	2.47	0.43
2:H:258:ASN:CG	2:H:259:GLY:H	2.24	0.43
2:H:332:MET:O	2:H:333:GLU:HB2	2.19	0.43
1:I:283:ILE:O	1:I:287:ARG:HD3	2.18	0.43
2:J:235:LYS:O	2:J:239:VAL:HG23	2.18	0.43
2:J:357:LEU:HD22	2:J:361:TRP:CZ2	2.54	0.43
1:A:88:VAL:HG13	2:B:36:LEU:HD11	2.00	0.42
2:D:163:ALA:HB2	2:D:174:PHE:CZ	2.54	0.42
2:F:103:ILE:HG23	2:F:104:PRO:HD2	2.01	0.42
2:H:21:LEU:HD23	2:H:24:ARG:HD2	2.01	0.42
2:H:133:ILE:HG22	2:H:350:THR:HG23	1.99	0.42
2:J:236:LEU:HD22	2:J:245:LEU:HD21	2.00	0.42
1:K:60:SER:OG	1:K:61:PRO:HD2	2.19	0.42
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.54	0.42
2:H:21:LEU:N	2:H:21:LEU:CD1	2.82	0.42
2:J:172:MET:HE1	2:J:200:ILE:HA	2.00	0.42
2:J:186:ASN:HB2	2:J:358:HIS:NE2	2.34	0.42
1:K:223:VAL:HG11	1:K:240:ARG:HB2	2.00	0.42
1:E:326:GLN:CA	1:E:326:GLN:NE2	2.83	0.42
1:I:106:VAL:HG11	1:I:116:ALA:CB	2.48	0.42
1:I:207:GLN:OE1	2:J:216:LEU:HD13	2.19	0.42
1:I:355:TYR:O	1:I:358:TYR:HB3	2.19	0.42
1:K:106:VAL:HG13	1:K:111:GLU:HB3	1.99	0.42
2:L:249:LYS:HB3	2:L:285:ILE:HD13	2.01	0.42
1:C:328:ASP:O	1:C:329:ASN:CB	2.68	0.42
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.55	0.42
2:F:37:PRO:O	2:F:39:ARG:N	2.52	0.42
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.83	0.42
1:K:344:LEU:HD13	1:K:356:TRP:CE2	2.54	0.42
2:L:253:ILE:HD12	2:L:289:THR:HG22	2.01	0.42
1:C:124:ILE:HD13	1:C:134:TRP:CH2	2.55	0.42
1:E:106:VAL:HG11	1:E:116:ALA:CB	2.49	0.42
1:E:180:LYS:HD3	1:E:180:LYS:HA	1.88	0.42
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.93	0.42
2:H:64:LEU:O	2:H:67:VAL:HG22	2.20	0.42
1:K:225:GLN:NE2	1:K:229:GLU:OE2	2.53	0.42
2:L:90:LEU:HD23	2:L:90:LEU:HA	1.85	0.42
2:L:363:THR:C	8:L:481:HOH:O	2.62	0.42
2:B:122:ILE:HG22	2:B:163:ALA:HA	2.01	0.42
2:D:236:LEU:HD22	2:D:245:LEU:HD21	2.01	0.42
2:H:208:ASN:CG	2:H:247:ARG:HB3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:LEU:O	1:I:69:ARG:HG3	2.19	0.42
2:L:172:MET:HE1	2:L:200:ILE:HA	2.02	0.42
1:A:88:VAL:CG1	2:B:36:LEU:HD11	2.50	0.42
1:A:255:VAL:CG1	1:A:258:ARG:HH12	2.23	0.42
2:D:253:ILE:HD12	2:D:289:THR:HG22	2.01	0.42
1:G:91:ILE:H	1:G:91:ILE:HG13	1.74	0.42
1:K:311:LEU:C	1:K:311:LEU:HD23	2.45	0.42
2:D:74:GLU:CD	2:D:141:ARG:HH22	2.28	0.42
2:H:207:ASP:O	2:H:208:ASN:HB2	2.20	0.42
1:A:255:VAL:HA	1:A:258:ARG:HH12	1.84	0.42
1:C:232:ARG:NH2	1:C:272:HIS:O	2.53	0.42
1:G:65:LEU:O	1:G:69:ARG:HG3	2.20	0.42
2:J:103:ILE:HG23	2:J:104:PRO:HD2	2.02	0.42
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.86	0.41
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.55	0.41
1:C:88:VAL:HG12	2:D:36:LEU:HD11	2.01	0.41
2:D:77:TYR:CE1	2:D:141:ARG:HB2	2.55	0.41
1:E:214:ARG:O	1:E:214:ARG:CG	2.67	0.41
2:J:36:LEU:HA	2:J:37:PRO:HD3	1.92	0.41
2:J:37:PRO:HD2	2:J:40:TYR:CE1	2.55	0.41
1:K:114:GLU:OE2	1:K:146:LYS:NZ	2.39	0.41
1:C:114:GLU:OE2	1:C:146:LYS:NZ	2.38	0.41
2:D:332:MET:O	2:D:333:GLU:HB2	2.20	0.41
1:I:267:ILE:HD13	1:I:277:TRP:CE2	2.55	0.41
1:K:101:ASP:HA	1:K:104:ARG:HH11	1.85	0.41
1:A:103:PHE:CZ	1:A:133:VAL:HG22	2.56	0.41
2:B:173:ARG:HG2	5:B:379:MGM:H112	2.02	0.41
2:D:172:MET:HE1	2:D:200:ILE:HA	2.01	0.41
1:E:328:ASP:O	1:E:329:ASN:HB2	2.20	0.41
2:J:21:LEU:CD1	2:J:21:LEU:N	2.83	0.41
2:J:290:ASN:OD1	2:J:290:ASN:C	2.63	0.41
1:E:200:TYR:CB	5:F:381:MGM:HC12	2.50	0.41
1:E:296:LEU:O	1:E:300:LEU:HG	2.21	0.41
2:F:36:LEU:HA	2:F:37:PRO:HD3	1.87	0.41
1:I:100:TYR:C	1:I:104:ARG:NH1	2.79	0.41
2:J:90:LEU:HD23	2:J:90:LEU:HA	1.90	0.41
1:K:180:LYS:HD3	1:K:180:LYS:HA	1.93	0.41
1:E:344:LEU:HD13	1:E:356:TRP:CE2	2.55	0.41
2:F:202:ARG:HH11	2:F:202:ARG:HG2	1.85	0.41
1:G:255:VAL:HG13	1:G:258:ARG:NH2	2.35	0.41
1:I:219:GLU:OE1	1:I:219:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:130:SER:O	2:J:134:ILE:HG13	2.21	0.41
1:K:91:ILE:HG13	1:K:91:ILE:H	1.75	0.41
2:D:208:ASN:CG	2:D:247:ARG:HB3	2.46	0.41
1:A:338:LEU:HD11	1:A:364:GLN:HG2	2.02	0.41
2:D:40:TYR:CD1	2:D:40:TYR:N	2.87	0.41
2:D:130:SER:O	2:D:134:ILE:HG13	2.21	0.41
1:E:227:LEU:HD23	1:E:227:LEU:HA	1.91	0.41
1:G:308:SER:HB2	1:G:309:PRO:HD2	2.02	0.41
2:H:253:ILE:HD12	2:H:289:THR:HG22	2.03	0.41
2:J:173:ARG:HG2	5:J:379:MGM:H112	2.03	0.41
2:J:295:ARG:HG2	2:J:295:ARG:HH11	1.86	0.41
2:L:38:GLU:O	2:L:38:GLU:HG2	2.20	0.41
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.29	0.41
2:L:258:ASN:CG	2:L:259:GLY:H	2.26	0.41
1:C:112:ARG:O	1:C:144:LEU:HD21	2.20	0.41
2:H:137:ASP:OD1	2:H:139:LEU:N	2.45	0.41
2:H:158:ASP:OD2	2:H:158:ASP:C	2.63	0.41
2:J:30:GLN:O	2:J:34:GLN:HG3	2.20	0.41
1:A:311:LEU:C	1:A:311:LEU:HD23	2.45	0.41
2:D:37:PRO:C	2:D:39:ARG:N	2.77	0.41
2:H:172:MET:HE1	2:H:200:ILE:HA	2.03	0.41
2:H:187:ASN:OD1	2:H:187:ASN:C	2.64	0.41
2:H:255:ARG:HD3	2:H:261:HIS:CD2	2.56	0.41
2:J:122:ILE:HG22	2:J:163:ALA:HA	2.01	0.41
2:J:207:ASP:O	2:J:208:ASN:HB2	2.20	0.41
2:J:250:ARG:O	2:J:254:MET:HG2	2.21	0.41
2:J:253:ILE:CD1	2:J:289:THR:HG22	2.50	0.41
1:K:124:ILE:HD13	1:K:134:TRP:CH2	2.56	0.41
2:L:236:LEU:HD22	2:L:245:LEU:HD21	2.02	0.41
2:L:266:LYS:HE3	2:L:266:LYS:HB3	1.98	0.41
2:B:349:ARG:HH11	2:B:349:ARG:HG2	1.86	0.41
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.85	0.41
2:D:22:ARG:HG2	2:D:22:ARG:NH1	2.35	0.41
1:E:103:PHE:CZ	1:E:133:VAL:HG22	2.56	0.41
2:F:188:TRP:CE3	2:F:193:MET:HE2	2.56	0.41
2:F:339:LYS:NZ	2:F:339:LYS:CB	2.84	0.41
2:H:344:LEU:HD12	2:H:344:LEU:HA	1.93	0.41
1:I:112:ARG:O	1:I:144:LEU:HD21	2.21	0.41
2:J:163:ALA:HB2	2:J:174:PHE:CZ	2.56	0.41
1:K:189:ILE:HD11	1:K:205:HIS:CD2	2.52	0.41
1:K:232:ARG:HD3	8:L:477:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ASP:O	2:B:74:GLU:HG2	2.21	0.40
2:B:193:MET:O	2:B:197:ILE:HG13	2.21	0.40
1:E:66:TYR:CE1	1:E:119:LEU:HD13	2.56	0.40
1:E:107:LEU:HD11	2:F:117:TYR:HB2	2.02	0.40
1:G:200:TYR:HB3	5:H:380:MGM:HC12	2.03	0.40
2:J:138:ASP:HA	2:J:357:LEU:HD11	2.03	0.40
1:C:287:ARG:HG2	1:C:287:ARG:H	1.67	0.40
1:C:308:SER:HB2	1:C:309:PRO:HD2	2.03	0.40
2:D:110:ASN:CB	2:D:111:PRO:HD2	2.51	0.40
1:E:75:ILE:CG1	1:E:115:ARG:NH2	2.84	0.40
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.88	0.40
8:I:430:HOH:O	2:J:99:SER:HB2	2.20	0.40
1:A:106:VAL:HG11	1:A:116:ALA:CB	2.51	0.40
2:B:205:SER:OG	2:B:206:TYR:N	2.55	0.40
2:H:338:CYS:HB3	8:H:415:HOH:O	2.21	0.40
1:K:340:LEU:HD23	1:K:343:ILE:HD12	2.03	0.40
2:L:110:ASN:CB	2:L:111:PRO:HD2	2.51	0.40
2:L:180:CYS:O	2:L:184:MET:HG3	2.21	0.40
2:L:255:ARG:HD3	2:L:261:HIS:CD2	2.57	0.40
2:B:236:LEU:HD22	2:B:245:LEU:HD21	2.03	0.40
1:C:92:TYR:O	1:C:97:ARG:NH2	2.54	0.40
2:H:232:LEU:HD12	2:H:232:LEU:HA	1.93	0.40
1:K:83:GLY:HA3	2:L:105:PHE:CE1	2.56	0.40
1:K:308:SER:HB2	1:K:309:PRO:HD2	2.04	0.40
1:A:112:ARG:HA	1:A:140:LEU:CD2	2.52	0.40
1:A:127:ASN:ND2	1:A:130:ASN:HB2	2.36	0.40
2:D:344:LEU:HD12	2:D:344:LEU:HA	1.85	0.40
1:E:207:GLN:HG2	1:E:242:PHE:CE2	2.57	0.40
1:E:267:ILE:HD13	1:E:277:TRP:CE2	2.56	0.40
2:H:20:PHE:CE2	2:H:337:ILE:HD11	2.57	0.40
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.51	0.40
2:J:193:MET:HG3	2:J:233:MET:HE2	2.03	0.40
1:K:81:ASN:ND2	2:L:105:PHE:H	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/377 (83%)	288 (92%)	24 (8%)	0	100	100
1	C	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	E	312/377 (83%)	289 (93%)	23 (7%)	0	100	100
1	G	312/377 (83%)	289 (93%)	23 (7%)	0	100	100
1	I	312/377 (83%)	290 (93%)	22 (7%)	0	100	100
1	K	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
2	B	344/377 (91%)	326 (95%)	16 (5%)	2 (1%)	21	38
2	D	344/377 (91%)	329 (96%)	12 (4%)	3 (1%)	14	28
2	F	344/377 (91%)	327 (95%)	16 (5%)	1 (0%)	36	54
2	H	344/377 (91%)	326 (95%)	17 (5%)	1 (0%)	36	54
2	J	344/377 (91%)	322 (94%)	20 (6%)	2 (1%)	21	38
2	L	344/377 (91%)	328 (95%)	14 (4%)	2 (1%)	21	38
3	M	3/10 (30%)	3 (100%)	0	0	100	100
3	N	3/10 (30%)	3 (100%)	0	0	100	100
3	O	3/10 (30%)	3 (100%)	0	0	100	100
3	P	3/10 (30%)	3 (100%)	0	0	100	100
3	Q	3/10 (30%)	3 (100%)	0	0	100	100
3	R	3/10 (30%)	3 (100%)	0	0	100	100
All	All	3954/4584 (86%)	3715 (94%)	228 (6%)	11 (0%)	36	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	38	GLU
2	B	258	ASN
2	D	258	ASN
2	F	258	ASN

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Mol	Chain	Res	Type
2	H	258	ASN
2	J	258	ASN
2	L	258	ASN
2	B	362	LYS
2	D	333	GLU
2	J	34	GLN
2	L	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	282/338 (83%)	271 (96%)	11 (4%)	28	54
1	C	286/338 (85%)	277 (97%)	9 (3%)	35	60
1	E	289/338 (86%)	280 (97%)	9 (3%)	35	60
1	G	285/338 (84%)	279 (98%)	6 (2%)	47	70
1	I	285/338 (84%)	280 (98%)	5 (2%)	51	73
1	K	292/338 (86%)	287 (98%)	5 (2%)	53	75
2	B	291/326 (89%)	280 (96%)	11 (4%)	29	54
2	D	291/326 (89%)	276 (95%)	15 (5%)	21	43
2	F	295/326 (90%)	281 (95%)	14 (5%)	23	47
2	H	288/326 (88%)	277 (96%)	11 (4%)	29	54
2	J	291/326 (89%)	277 (95%)	14 (5%)	23	46
2	L	295/326 (90%)	281 (95%)	14 (5%)	23	47
3	M	5/10 (50%)	5 (100%)	0	100	100
3	N	5/10 (50%)	5 (100%)	0	100	100
3	O	5/10 (50%)	5 (100%)	0	100	100
3	P	5/10 (50%)	5 (100%)	0	100	100
3	Q	5/10 (50%)	5 (100%)	0	100	100
3	R	5/10 (50%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3500/4044 (86%)	3376 (96%)	124 (4%)	32 57

All (124) 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	225	GLN
1	A	281	LYS
1	A	287	ARG
1	A	348	LYS
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	114	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

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Mol	Chain	Res	Type
2	D	232	LEU
2	D	236	LEU
2	D	237	GLU
2	D	243	LYS
2	D	305	LEU
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
2	D	357	LEU
1	E	71	GLU
1	E	80	GLN
1	E	107	LEU
1	E	114	GLU
1	E	184	GLN
1	E	214	ARG
1	E	324	GLU
1	E	326	GLN
1	E	364	GLN
2	F	21	LEU
2	F	24	ARG
2	F	33	LEU
2	F	151	LEU
2	F	216	LEU
2	F	232	LEU
2	F	236	LEU
2	F	258	ASN
2	F	305	LEU
2	F	306	VAL
2	F	329	LEU
2	F	331	LEU
2	F	339	LYS
2	F	357	LEU
1	G	107	LEU
1	G	184	GLN
1	G	194	ASN
1	G	224	ASP
1	G	225	GLN
1	G	287	ARG
2	H	21	LEU
2	H	33	LEU
2	H	151	LEU
2	H	216	LEU

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Mol	Chain	Res	Type
2	H	232	LEU
2	H	236	LEU
2	H	296	ASN
2	H	305	LEU
2	H	306	VAL
2	H	329	LEU
2	H	331	LEU
1	I	107	LEU
1	I	114	GLU
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	305	LEU
2	J	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	357	LEU
1	K	71	GLU
1	K	80	GLN
1	K	107	LEU
1	K	114	GLU
1	K	357	ARG
2	L	21	LEU
2	L	33	LEU
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	284	LYS
2	L	305	LEU
2	L	306	VAL

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Mol	Chain	Res	Type
2	L	329	LEU
2	L	331	LEU
2	L	335	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	149	GLN
1	A	184	GLN
1	A	194	ASN
1	A	225	GLN
1	A	261	GLN
1	A	278	ASN
1	A	285	GLN
1	A	303	GLN
1	A	367	HIS
2	B	110	ASN
2	B	208	ASN
2	B	257	GLN
1	C	108	GLN
1	C	149	GLN
1	C	153	ASN
1	C	184	GLN
1	C	195	GLN
1	C	218	ASN
1	C	285	GLN
1	C	298	GLN
1	C	335	ASN
1	C	364	GLN
1	C	367	HIS
2	D	208	ASN
2	D	246	ASN
1	E	145	GLN
1	E	149	GLN
1	E	184	GLN
1	E	204	GLN
1	E	261	GLN
1	E	285	GLN
1	E	297	ASN
1	E	298	GLN
1	E	335	ASN

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Mol	Chain	Res	Type
1	E	364	GLN
2	F	208	ASN
2	F	246	ASN
1	G	81	ASN
1	G	89	GLN
1	G	135	HIS
1	G	149	GLN
1	G	184	GLN
1	G	225	GLN
1	G	278	ASN
1	G	297	ASN
1	G	303	GLN
1	G	367	HIS
2	H	34	GLN
2	H	296	ASN
1	I	89	GLN
1	I	130	ASN
1	I	149	GLN
1	I	184	GLN
1	I	218	ASN
1	I	285	GLN
1	I	335	ASN
1	I	367	HIS
2	J	30	GLN
2	J	34	GLN
2	J	208	ASN
2	J	246	ASN
2	J	294	ASN
2	J	296	ASN
2	J	359	GLN
1	K	81	ASN
1	K	108	GLN
1	K	184	GLN
1	K	195	GLN
1	K	234	ASN
1	K	294	ASN
1	K	326	GLN
1	K	367	HIS
2	L	212	GLN
2	L	257	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	MES	F	380	-	12,12,12	9.23	8 (66%)	15,16,16	2.15	5 (33%)
5	MGM	D	380	-	27,28,28	0.95	2 (7%)	34,37,37	2.03	6 (17%)
5	MGM	L	379	-	27,28,28	1.02	2 (7%)	34,37,37	2.04	6 (17%)
5	MGM	J	379	-	27,28,28	0.98	2 (7%)	34,37,37	2.02	6 (17%)
5	MGM	F	381	-	27,28,28	1.03	1 (3%)	34,37,37	2.09	6 (17%)
5	MGM	B	379	-	27,28,28	1.01	2 (7%)	34,37,37	2.02	7 (20%)
5	MGM	H	380	-	27,28,28	0.97	2 (7%)	34,37,37	2.00	6 (17%)

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
7	MES	F	380	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGM	D	380	-	-	10/31/31/31	-
5	MGM	L	379	-	-	10/31/31/31	-
5	MGM	J	379	-	-	10/31/31/31	-
5	MGM	F	381	-	-	10/31/31/31	-
5	MGM	B	379	-	-	10/31/31/31	-
5	MGM	H	380	-	-	10/31/31/31	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	380	MES	C8-S	-24.24	1.43	1.77
7	F	380	MES	O2S-S	12.77	1.81	1.45
7	F	380	MES	O1S-S	12.13	1.79	1.45
7	F	380	MES	O3S-S	8.56	1.79	1.47
7	F	380	MES	C7-C8	-4.81	1.39	1.52
7	F	380	MES	C3-C2	-2.86	1.39	1.50
7	F	380	MES	C5-C6	-2.67	1.40	1.50
5	L	379	MGM	C7-C8	2.57	1.39	1.33
7	F	380	MES	C7-N4	-2.54	1.41	1.47
5	F	381	MGM	C7-C8	2.45	1.38	1.33
5	H	380	MGM	C7-C8	2.40	1.38	1.33
5	B	379	MGM	C7-C8	2.37	1.38	1.33
5	J	379	MGM	C7-C8	2.35	1.38	1.33
5	B	379	MGM	C12-C13	2.34	1.38	1.33
5	J	379	MGM	C12-C13	2.26	1.38	1.33
5	L	379	MGM	C12-C13	2.21	1.38	1.33
5	D	380	MGM	C7-C8	2.14	1.38	1.33
5	D	380	MGM	C12-C13	2.13	1.38	1.33
5	H	380	MGM	C12-C13	2.11	1.37	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	381	MGM	C1-C2-N3	7.49	131.28	113.30
5	B	379	MGM	C1-C2-N3	7.21	130.61	113.30
5	J	379	MGM	C1-C2-N3	7.20	130.58	113.30
5	L	379	MGM	C1-C2-N3	7.15	130.47	113.30
5	H	380	MGM	C1-C2-N3	7.09	130.33	113.30
5	D	380	MGM	C1-C2-N3	7.09	130.33	113.30
5	D	380	MGM	C4-N3-C2	5.13	125.27	110.55
5	J	379	MGM	C4-N3-C2	5.12	125.24	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	381	MGM	C4-N3-C2	5.10	125.17	110.55
5	L	379	MGM	C4-N3-C2	5.06	125.06	110.55
5	H	380	MGM	C4-N3-C2	5.02	124.95	110.55
5	B	379	MGM	C4-N3-C2	5.01	124.94	110.55
7	F	380	MES	O1S-S-C8	4.40	113.38	106.73
5	F	381	MGM	O1-C1-C2	4.22	115.82	107.38
5	D	380	MGM	O1-C1-C2	4.17	115.71	107.38
5	L	379	MGM	O1-C1-C2	4.16	115.69	107.38
5	B	379	MGM	O1-C1-C2	4.12	115.62	107.38
7	F	380	MES	O3S-S-C8	4.02	113.87	106.00
5	H	380	MGM	O1-C1-C2	3.98	115.33	107.38
5	J	379	MGM	O1-C1-C2	3.65	114.68	107.38
5	L	379	MGM	O1B-PB-O3A	3.01	114.73	104.64
5	L	379	MGM	O1A-PA-O3A	2.99	115.35	107.27
5	J	379	MGM	O1B-PB-O3A	2.94	114.50	104.64
7	F	380	MES	O2S-S-C8	2.91	111.12	106.73
5	F	381	MGM	O1A-PA-O3A	2.87	115.03	107.27
5	F	381	MGM	O1B-PB-O3A	2.84	114.17	104.64
5	H	380	MGM	O1B-PB-O3A	2.82	114.08	104.64
5	D	380	MGM	O1A-PA-O3A	2.79	114.80	107.27
5	H	380	MGM	O1A-PA-O3A	2.78	114.79	107.27
5	B	379	MGM	O1A-PA-O3A	2.72	114.62	107.27
5	J	379	MGM	O1A-PA-O3A	2.72	114.61	107.27
5	B	379	MGM	O1B-PB-O3A	2.65	113.51	104.64
7	F	380	MES	O3S-S-O2S	-2.60	104.89	111.40
5	D	380	MGM	O1B-PB-O3A	2.57	113.24	104.64
7	F	380	MES	O2S-S-O1S	-2.52	105.63	113.82
5	F	381	MGM	C2-N3-C5	2.31	122.80	112.03
5	L	379	MGM	C2-N3-C5	2.30	122.75	112.03
5	B	379	MGM	C2-N3-C5	2.30	122.73	112.03
5	D	380	MGM	C2-N3-C5	2.26	122.58	112.03
5	H	380	MGM	C2-N3-C5	2.26	122.55	112.03
5	J	379	MGM	C2-N3-C5	2.21	122.35	112.03
5	B	379	MGM	C10-C8-C9	-2.02	111.72	115.23

There are no chirality outliers.

All (64) 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
5	B	379	MGM	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	D	380	MGM	C1-C2-N3-C4
5	D	380	MGM	O1-C1-C2-N3
5	D	380	MGM	PA-O3A-PB-O1B
5	F	381	MGM	C1-C2-N3-C4
5	F	381	MGM	O1-C1-C2-N3
5	F	381	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	380	MES	C7-C8-S-O3S
5	B	379	MGM	C6-C5-N3-C4
5	D	380	MGM	C6-C5-N3-C4
5	F	381	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	380	MES	N4-C7-C8-S
7	F	380	MES	C7-C8-S-O1S
7	F	380	MES	C7-C8-S-O2S
5	B	379	MGM	C10-C8-C9-C11
5	H	380	MGM	C10-C8-C9-C11
5	D	380	MGM	C10-C8-C9-C11
5	F	381	MGM	C10-C8-C9-C11
5	J	379	MGM	C10-C8-C9-C11
5	L	379	MGM	C10-C8-C9-C11
5	F	381	MGM	C7-C8-C9-C11
5	D	380	MGM	C7-C8-C9-C11
5	J	379	MGM	C7-C8-C9-C11
5	B	379	MGM	C7-C8-C9-C11
5	H	380	MGM	C7-C8-C9-C11
5	L	379	MGM	C7-C8-C9-C11
5	F	381	MGM	C6-C5-N3-C2
5	J	379	MGM	C6-C5-N3-C2
5	L	379	MGM	C6-C5-N3-C2
5	B	379	MGM	C14-C13-C15-C16
5	H	380	MGM	C14-C13-C15-C16

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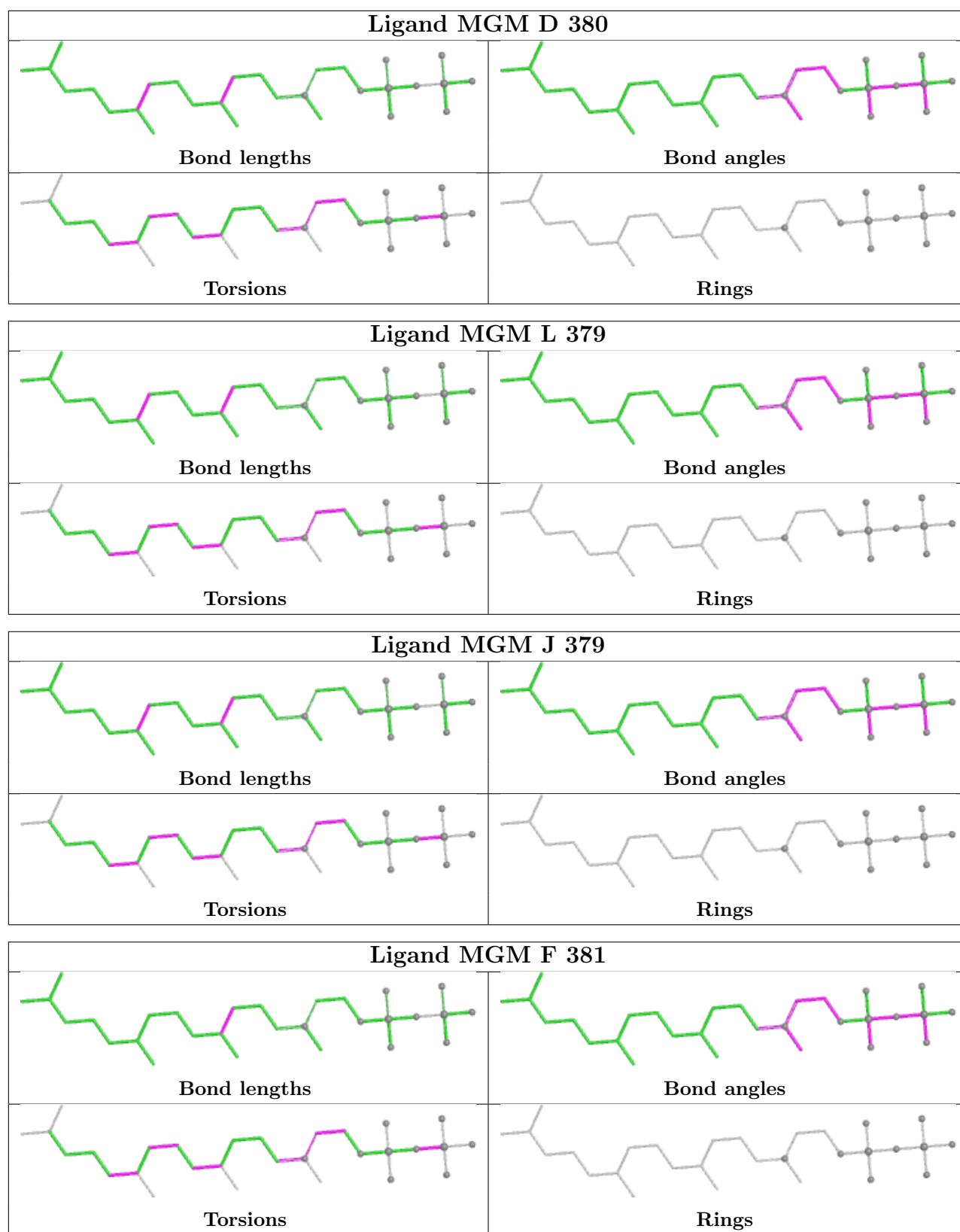
Mol	Chain	Res	Type	Atoms
5	D	380	MGM	C14-C13-C15-C16
5	B	379	MGM	C6-C5-N3-C2
5	F	381	MGM	C14-C13-C15-C16
5	J	379	MGM	C14-C13-C15-C16
5	B	379	MGM	PA-O3A-PB-O2B
5	D	380	MGM	PA-O3A-PB-O2B
5	F	381	MGM	PA-O3A-PB-O2B
5	H	380	MGM	PA-O3A-PB-O2B
5	J	379	MGM	PA-O3A-PB-O2B
5	L	379	MGM	PA-O3A-PB-O2B
5	L	379	MGM	C14-C13-C15-C16
5	D	380	MGM	C6-C5-N3-C2
5	H	380	MGM	C9-C11-C12-C13
5	D	380	MGM	C9-C11-C12-C13
5	J	379	MGM	C9-C11-C12-C13
5	L	379	MGM	C9-C11-C12-C13
5	B	379	MGM	C9-C11-C12-C13
5	F	381	MGM	C9-C11-C12-C13
5	H	380	MGM	C6-C5-N3-C2

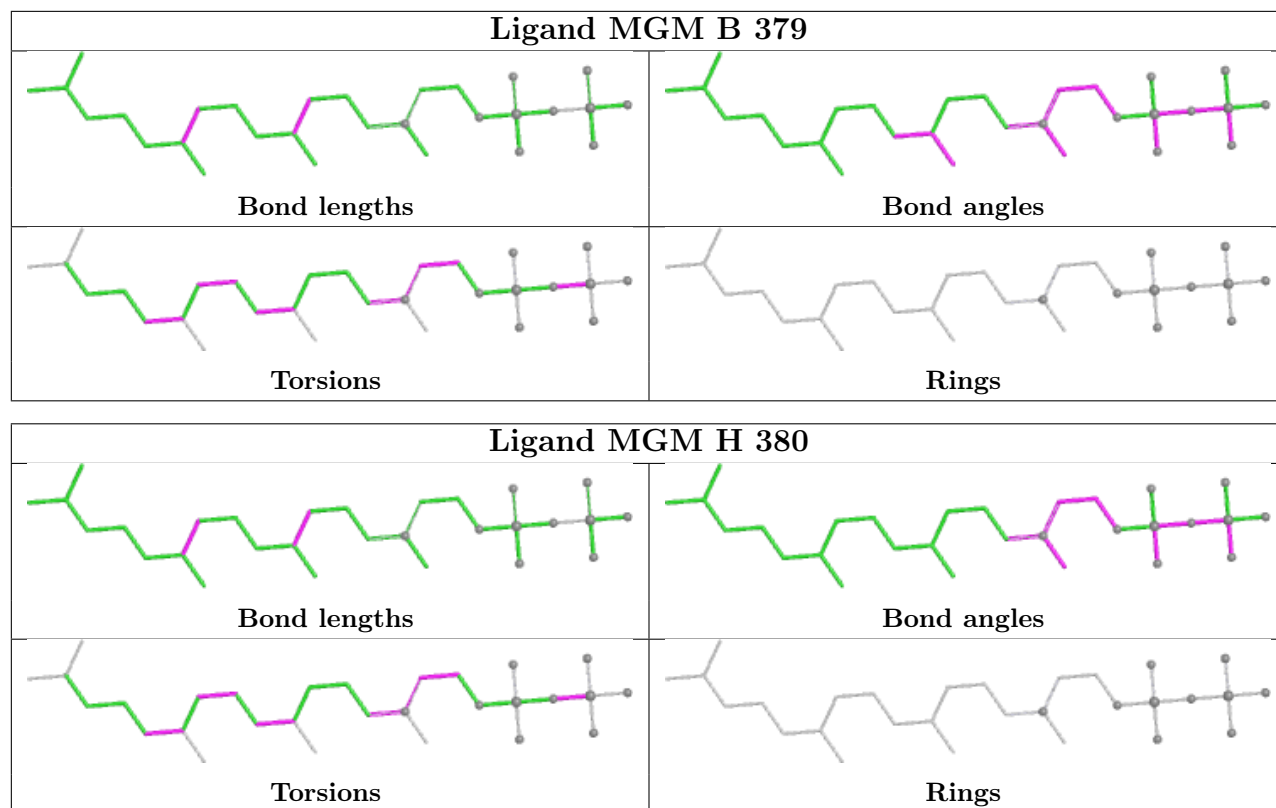
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	379	MGM	2	0
5	F	381	MGM	2	0
5	B	379	MGM	2	0
5	H	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%)	0.18	7 (2%) 62 53	31, 53, 86, 100	0
1	C	314/377 (83%)	0.09	10 (3%) 50 41	28, 49, 77, 98	0
1	E	314/377 (83%)	0.14	6 (1%) 66 59	28, 51, 77, 95	0
1	G	314/377 (83%)	0.14	12 (3%) 44 35	29, 49, 76, 98	0
1	I	314/377 (83%)	0.27	14 (4%) 38 29	27, 52, 82, 96	0
1	K	314/377 (83%)	-0.33	4 (1%) 75 68	21, 37, 63, 75	0
2	B	346/377 (91%)	-0.09	11 (3%) 50 41	30, 45, 67, 91	0
2	D	346/377 (91%)	-0.36	7 (2%) 65 57	26, 39, 62, 76	0
2	F	346/377 (91%)	-0.32	10 (2%) 53 45	24, 38, 64, 85	0
2	H	346/377 (91%)	0.02	15 (4%) 40 31	30, 50, 74, 96	0
2	J	346/377 (91%)	-0.03	10 (2%) 53 45	28, 48, 74, 94	0
2	L	346/377 (91%)	-0.48	6 (1%) 69 63	21, 34, 54, 77	0
3	M	5/10 (50%)	-0.25	0 100 100	35, 35, 43, 53	0
3	N	5/10 (50%)	-0.33	1 (20%) 3 3	35, 39, 41, 53	0
3	O	5/10 (50%)	-0.11	1 (20%) 3 3	34, 35, 41, 52	0
3	P	5/10 (50%)	0.18	1 (20%) 3 3	40, 41, 47, 59	0
3	Q	5/10 (50%)	0.11	1 (20%) 3 3	38, 39, 42, 54	0
3	R	5/10 (50%)	-0.28	0 100 100	33, 34, 39, 51	0
All	All	3990/4584 (87%)	-0.07	116 (2%) 53 45	21, 45, 73, 100	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	55	PHE	7.7
1	C	55	PHE	6.3
1	E	55	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
2	H	18	LEU	5.7
1	I	55	PHE	5.4
2	H	363	THR	4.8
2	J	110	ASN	4.5
2	J	363	THR	4.5
2	J	111	PRO	4.4
2	F	18	LEU	4.4
2	B	363	THR	4.4
1	K	55	PHE	4.3
2	J	108	SER	4.2
1	A	55	PHE	4.0
2	J	18	LEU	3.9
2	B	18	LEU	3.8
1	G	328	ASP	3.8
2	B	111	PRO	3.8
1	C	57	SER	3.7
1	A	368	SER	3.6
1	G	59	ASP	3.6
2	D	18	LEU	3.6
1	G	57	SER	3.5
1	I	368	SER	3.5
1	I	364	GLN	3.4
1	G	56	LEU	3.4
2	H	85	GLU	3.3
2	B	113	THR	3.3
2	D	363	THR	3.3
1	C	328	ASP	3.3
2	H	40	TYR	3.2
2	F	111	PRO	3.2
1	A	331	GLU	3.2
2	H	111	PRO	3.1
2	L	111	PRO	3.1
2	B	362	LYS	3.0
2	F	363	THR	3.0
1	K	59	ASP	2.9
3	P	6	LYS	2.9
1	E	56	LEU	2.9
1	E	331	GLU	2.9
2	B	40	TYR	2.9
1	G	60	SER	2.9
1	C	60	SER	2.8
1	G	62	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	328	ASP	2.8
1	I	326	GLN	2.8
2	J	113	THR	2.7
1	C	331	GLU	2.7
2	H	316	HIS	2.7
1	I	328	ASP	2.7
1	C	368	SER	2.7
2	F	113	THR	2.6
2	L	113	THR	2.6
1	G	326	GLN	2.6
1	E	330	LYS	2.6
1	A	364	GLN	2.6
2	F	316	HIS	2.5
2	H	305	LEU	2.5
1	C	62	THR	2.5
2	F	110	ASN	2.5
2	F	40	TYR	2.5
2	B	292	GLU	2.5
1	K	326	GLN	2.5
1	A	330	LYS	2.5
3	Q	6	LYS	2.5
1	I	59	ASP	2.4
2	L	18	LEU	2.4
2	D	111	PRO	2.4
2	B	112	GLY	2.4
1	I	367	HIS	2.4
2	D	40	TYR	2.4
2	J	314	ASP	2.4
2	B	109	LYS	2.3
2	J	89	ASN	2.3
1	E	57	SER	2.3
2	H	108	SER	2.3
1	A	326	GLN	2.3
1	G	58	LEU	2.3
1	K	56	LEU	2.3
2	F	85	GLU	2.3
2	H	38	GLU	2.3
2	D	37	PRO	2.3
2	H	35	VAL	2.3
2	H	362	LYS	2.2
2	J	85	GLU	2.2
2	B	37	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	368	SER	2.2
2	F	112	GLY	2.2
1	I	327	CYS	2.2
1	G	305	SER	2.2
2	H	360	SER	2.2
2	H	110	ASN	2.1
1	C	304	PRO	2.1
1	C	59	ASP	2.1
2	L	112	GLY	2.1
2	H	359	GLN	2.1
1	I	366	LYS	2.1
3	O	6	LYS	2.1
1	I	91	ILE	2.1
1	I	225	GLN	2.1
2	F	359	GLN	2.1
2	D	305	LEU	2.1
2	L	314	ASP	2.1
2	L	363	THR	2.1
1	I	329	ASN	2.1
1	I	288	GLY	2.1
1	G	142	ARG	2.1
2	H	65	ASP	2.1
1	C	195	GLN	2.0
2	J	109	LYS	2.0
2	D	316	HIS	2.0
3	N	6	LYS	2.0
1	E	303	GLN	2.0
1	I	305	SER	2.0
2	B	314	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

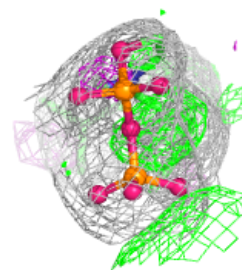
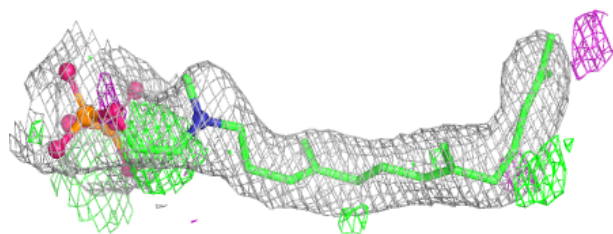
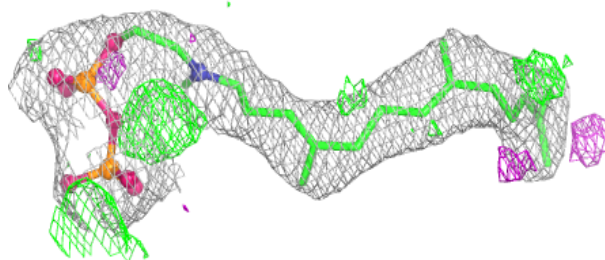
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MES	F	380	12/12	0.92	0.17	72,77,79,79	0
5	MGM	H	380	29/29	0.95	0.12	30,38,53,54	0
5	MGM	B	379	29/29	0.95	0.12	33,40,53,54	0
5	MGM	D	380	29/29	0.96	0.10	29,35,47,47	0
5	MGM	L	379	29/29	0.96	0.10	18,29,42,44	0
5	MGM	F	381	29/29	0.96	0.10	27,39,47,47	0
5	MGM	J	379	29/29	0.97	0.10	24,34,43,44	0
6	CL	F	379	1/1	0.99	0.04	35,35,35,35	0
6	CL	H	379	1/1	0.99	0.04	47,47,47,47	0
6	CL	D	379	1/1	0.99	0.05	37,37,37,37	0
4	ZN	J	378	1/1	1.00	0.01	33,33,33,33	0
4	ZN	L	378	1/1	1.00	0.01	29,29,29,29	0
4	ZN	B	378	1/1	1.00	0.02	33,33,33,33	0
4	ZN	D	378	1/1	1.00	0.02	31,31,31,31	0
4	ZN	F	378	1/1	1.00	0.02	32,32,32,32	0
4	ZN	H	378	1/1	1.00	0.01	43,43,43,43	0

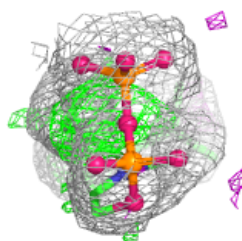
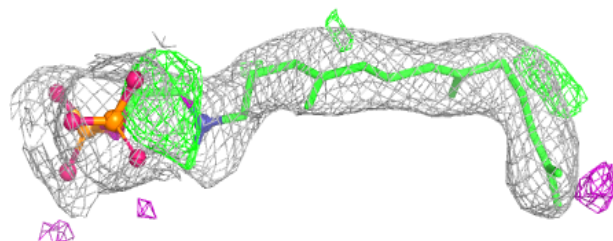
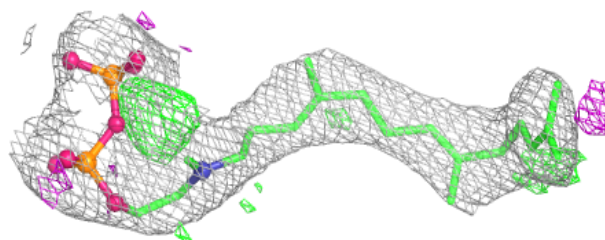
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

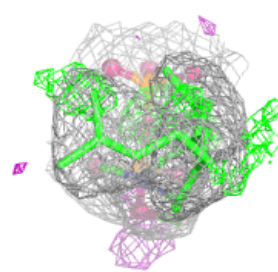
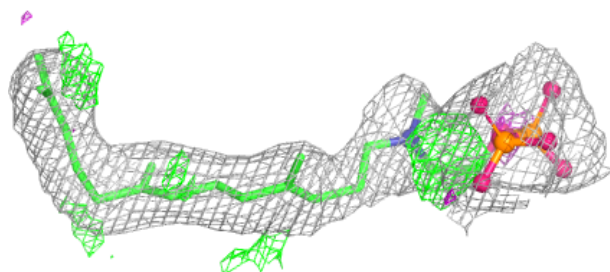
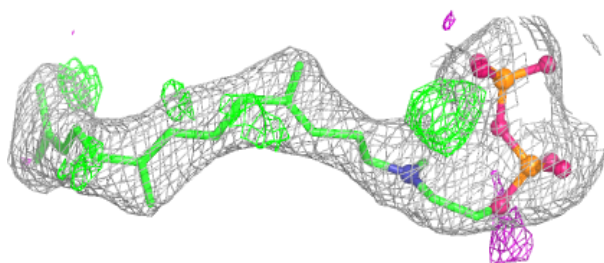
**Electron density around MGM B 379:**

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

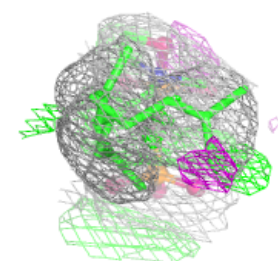
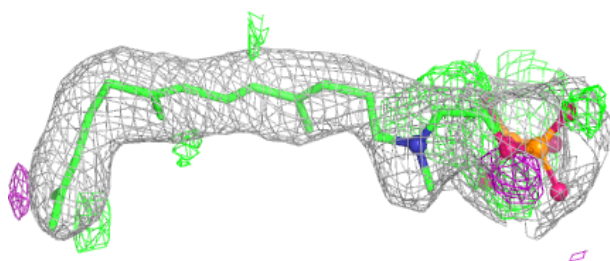
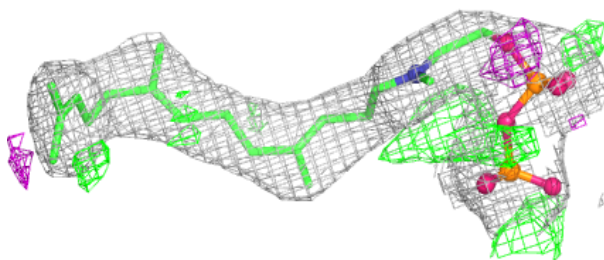


Electron density around MGM D 380:

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

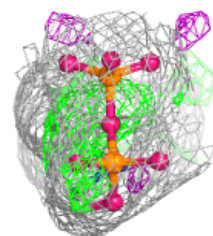
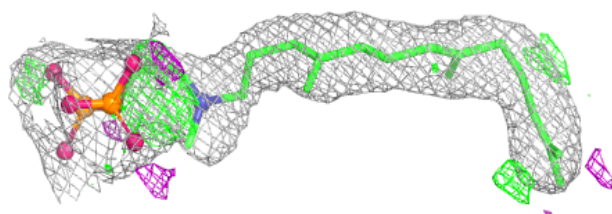
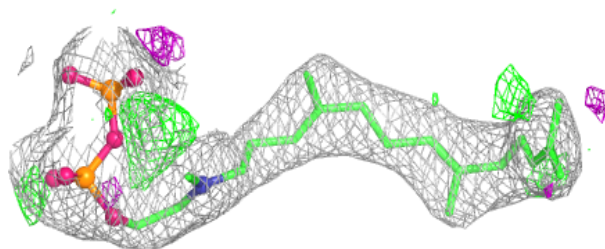
**Electron density around MGM L 379:**

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

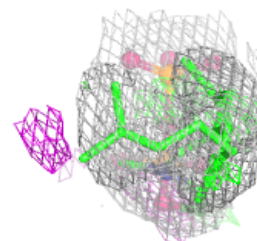
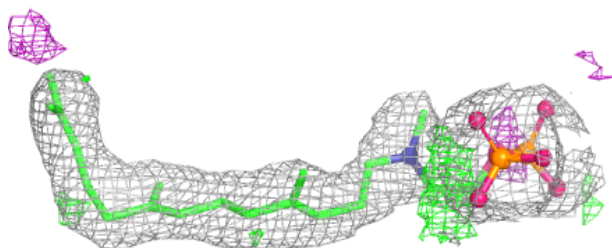
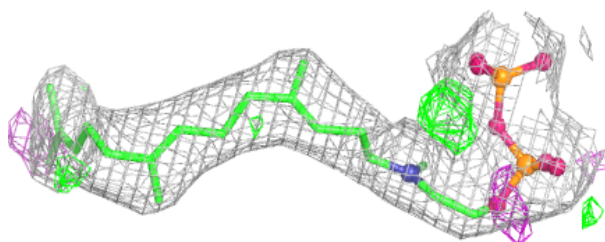


Electron density around MGM F 381:

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

**Electron density around MGM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.