



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 AM UTC

PDB ID : 1TNO / pdb_00001tno
Title : Rat Protein Geranylgeranyltransferase Type-I Complexed with a GGPP analog and a KKKSCTKCVIM Peptide Derived from K-Ras4B
Authors : Reid, T.S.; Terry, K.L.; Casey, P.J.; Beese, L.S.
Deposited on : 2004-06-11
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

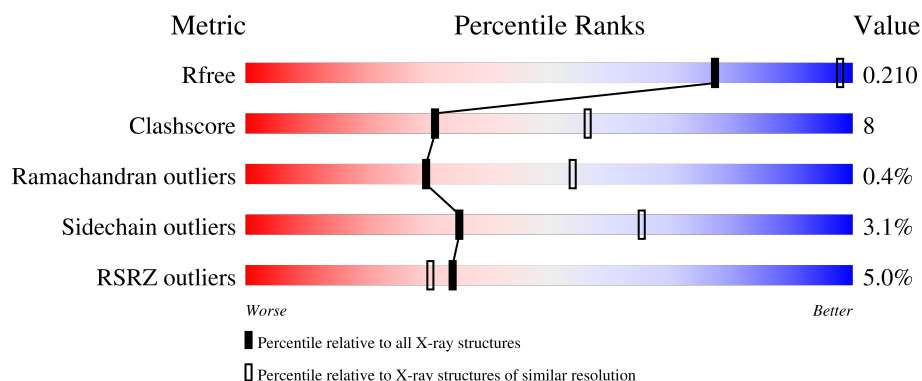
1 Overall quality at a glance

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	5% 65% 17% • 17%
1	C	377	4% 67% 16% • 17%
1	E	377	4% 64% 18% • 17%
1	G	377	6% 67% 16% • 17%
1	I	377	4% 66% 17% • 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	11	
3	N	11	
3	O	11	
3	P	11	
3	Q	11	
3	R	11	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2629	1679	463	482	5			
1	C	314	Total	C	N	O	S	0	0	0
			2643	1689	461	488	5			
1	E	314	Total	C	N	O	S	0	0	0
			2642	1686	461	490	5			
1	G	314	Total	C	N	O	S	0	0	0
			2633	1683	459	486	5			
1	I	314	Total	C	N	O	S	0	0	0
			2656	1694	465	492	5			
1	K	314	Total	C	N	O	S	0	0	0
			2671	1703	467	496	5			

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

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

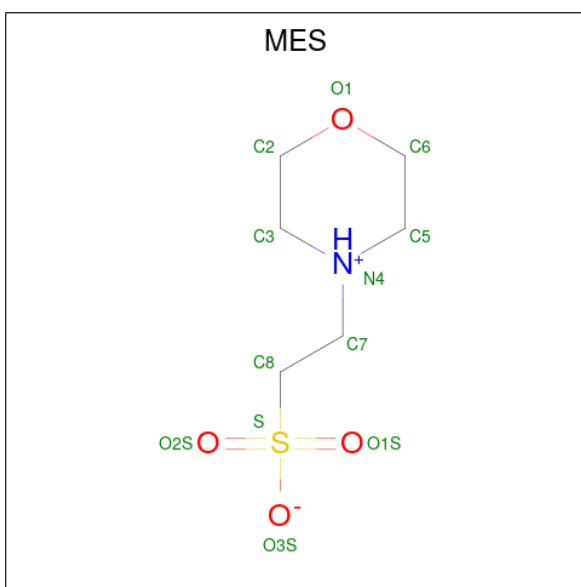
- Molecule 3 is a protein called c-K-ras2 protein isoform b.

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

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

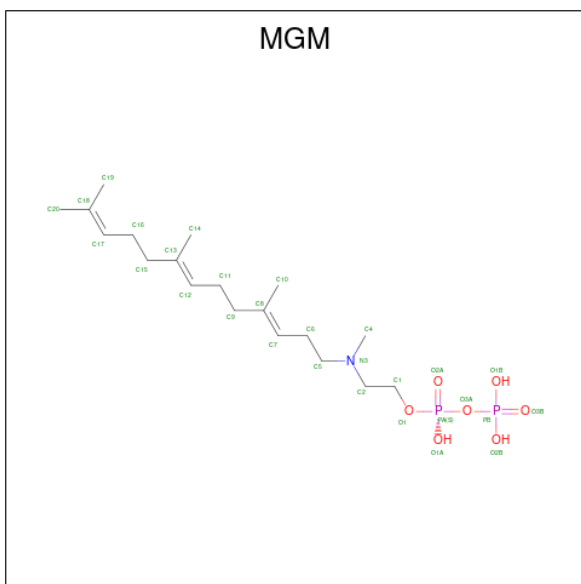
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 6 is 2-[METHYL-(5-GERANYL-4-METHYL-PENT-3-ENYL)-AMINO]-ETHYL-DIPHOSPHATE (CCD ID: MGM) (formula: $C_{19}H_{37}NO_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			29	19	1	7	2		

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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

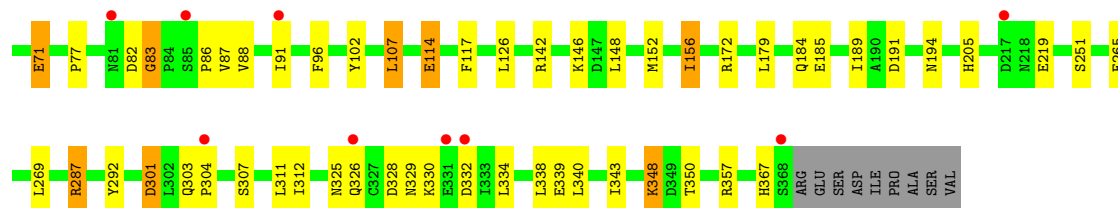
- Molecule 8 is water.

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

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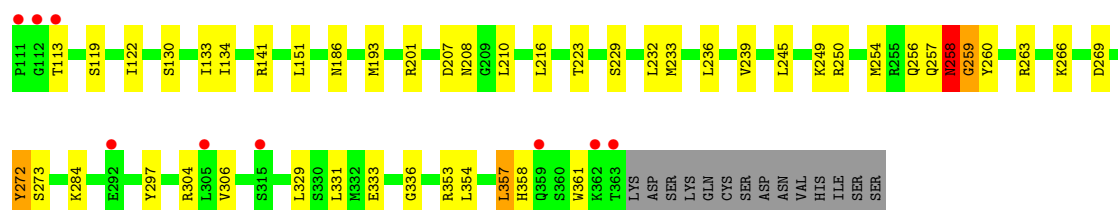
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	52	Total 52	O 52	0	0
8	J	47	Total 47	O 47	0	0
8	K	123	Total 123	O 123	0	0
8	L	93	Total 93	O 93	0	0
8	N	2	Total 2	O 2	0	0
8	O	2	Total 2	O 2	0	0
8	P	4	Total 4	O 4	0	0
8	Q	2	Total 2	O 2	0	0
8	R	4	Total 4	O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



Chain B:

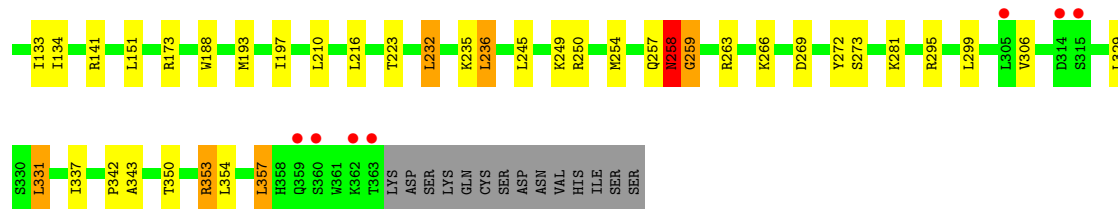
Amino Acid	Count
MET	1
ALA	1
ALA	1
THR	1
GLU	1
ASP	1
ASP	1
ARG	1
LEU	1
ALA	1
GLY	1
SER	1
GLY	1
GLU	1
GLY	1
GLU	1
ARG	1
L18	1
L21	1
R22	1
V26	1
F29	1
Q30	1
L33	1
L36	1
P37	1
E38	1
R39	1
Y40	1
T49	1
I50	1
A54	1
L64	1
S65	1
K69	1
D70	1
I73	1
E74	1
Y77	1
E85	1
R92	1
P104	1
F105	1
H106	1
V108	1



Chain D:

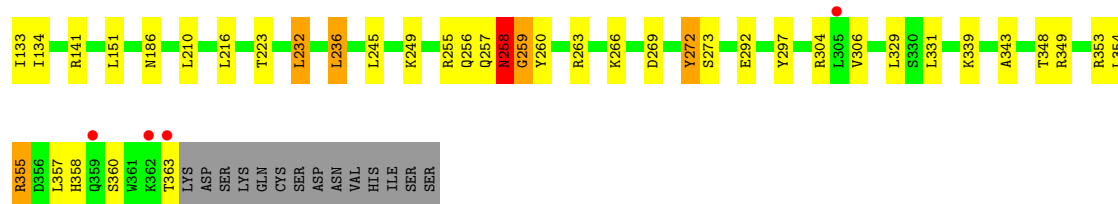
Amino Acid	Percentage
Red	4%
Green	75%
Yellow	14%
Grey	8%

MET ALA ALA THR GLU ASP ASP ARG ARG LEU LEU GLY SER GLY GLU GLU GLY ARG L18 D19 F20 L21 R22 V26 F29 Q30 L33 Q34 V35 L36 P37 E38 R39 Y40 T49 K69 I73 Y77 E85 L101 G102 I103 P104 F105 N106 K109 N110 I122 L120

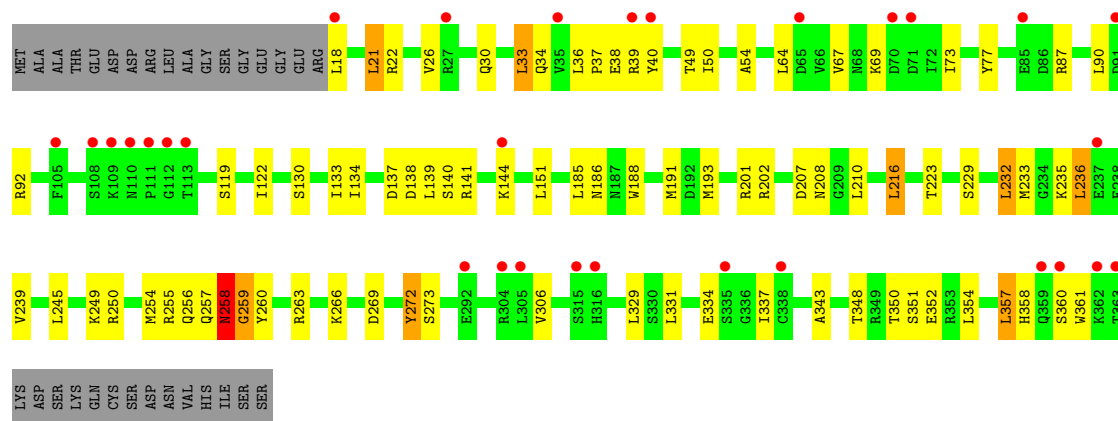


Chain F:

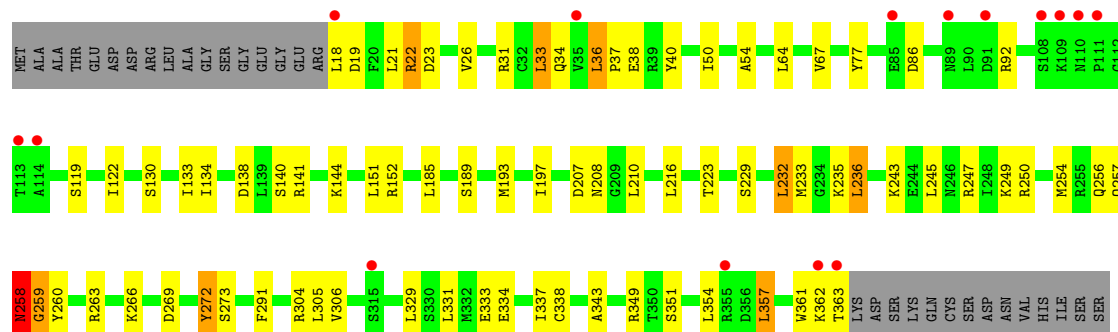
Residue	Category
MET	Grey
ALA	Grey
ALA	Grey
THR	Grey
GLU	Grey
ASP	Grey
ASP	Grey
ARG	Grey
LEU	Grey
ALA	Grey
GLY	Grey
SER	Grey
GLY	Grey
GLY	Grey
GLY	Grey
GLU	Grey
ARG	Grey
L18	Red
L21	Orange
F29	Yellow
Q30	Yellow
L33	Orange
Q34	Green
V35	Green
L36	Yellow
P37	Yellow
E38	Yellow
R39	Orange
Y40	Red
K69	Yellow
I73	Yellow
Y77	Yellow
E85	Red
R92	Yellow
M10	Red
P11	Red
G12	Yellow
T13	Red
A14	Yellow
H15	Yellow
P16	Yellow
S19	Yellow
G20	Yellow
H21	Yellow
I22	Yellow
A23	Yellow
M24	Yellow
S30	Yellow



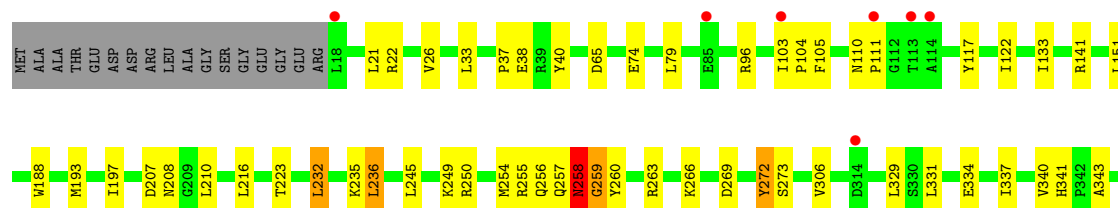
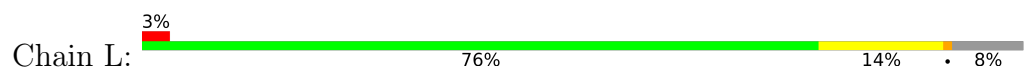
• Molecule 2: Geranylgeranyl transferase type I beta subunit

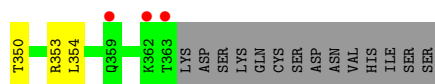


• Molecule 2: Geranylgeranyl transferase type I beta subunit

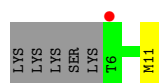


• Molecule 2: Geranylgeranyl transferase type I beta subunit

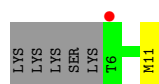




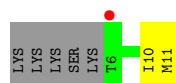
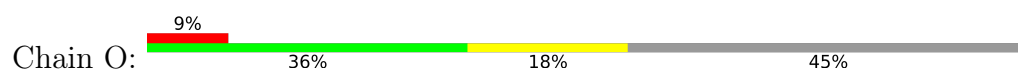
- Molecule 3: c-K-ras2 protein isoform b



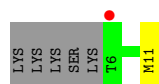
- Molecule 3: c-K-ras2 protein isoform b



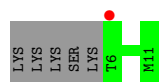
- Molecule 3: c-K-ras2 protein isoform b



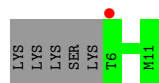
- Molecule 3: c-K-ras2 protein isoform b



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	272.53Å 268.48Å 185.94Å 90.00° 131.48° 90.00°	Depositor
Resolution (Å)	29.98 – 2.70 29.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.98-2.70) 92.2 (29.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.54Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.211 0.193 , 0.210	Depositor DCC
R_{free} test set	12637 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.089 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33292	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MGM, CL, MES, ZN

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	0/2695	0.84	5/3668 (0.1%)
1	C	0.42	0/2709	0.86	5/3684 (0.1%)
1	E	0.44	0/2708	0.85	5/3684 (0.1%)
1	G	0.43	0/2699	0.86	3/3672 (0.1%)
1	I	0.43	0/2722	0.84	6/3700 (0.2%)
1	K	0.46	0/2737	0.86	7/3717 (0.2%)
2	B	0.43	0/2759	0.91	10/3733 (0.3%)
2	D	0.44	0/2775	0.89	7/3752 (0.2%)
2	F	0.45	0/2780	0.91	7/3758 (0.2%)
2	H	0.41	0/2756	0.91	6/3729 (0.2%)
2	J	0.41	0/2773	0.91	10/3750 (0.3%)
2	L	0.47	0/2785	0.91	5/3764 (0.1%)
3	M	0.51	0/45	0.88	0/57
3	N	0.49	0/45	0.93	0/57
3	O	0.50	0/45	0.97	0/57
3	P	0.50	0/45	0.94	0/57
3	Q	0.55	0/45	0.98	0/57
3	R	0.55	0/45	0.89	0/57
All	All	0.44	0/33168	0.88	76/44953 (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	1
2	F	0	2
2	H	0	1
2	J	0	1

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

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	259	GLY	N-CA-C	-9.98	98.33	112.60
2	L	259	GLY	N-CA-C	-9.95	98.37	112.60
2	F	259	GLY	N-CA-C	-9.72	98.69	112.60
2	H	259	GLY	N-CA-C	-9.71	98.71	112.60
2	B	259	GLY	N-CA-C	-9.58	98.90	112.60
2	D	259	GLY	N-CA-C	-9.56	98.93	112.60
1	C	185	GLU	N-CA-C	9.01	122.02	111.02
1	E	185	GLU	N-CA-C	9.00	122.00	111.02
1	A	185	GLU	N-CA-C	8.91	121.89	111.02
1	I	185	GLU	N-CA-C	8.84	121.80	111.02
1	K	185	GLU	N-CA-C	8.79	121.75	111.02
1	G	185	GLU	N-CA-C	8.68	121.61	111.02
1	K	348	LYS	N-CA-C	7.61	121.82	112.23
2	D	258	ASN	N-CA-C	-6.98	95.93	110.80
2	J	22	ARG	N-CA-C	6.94	119.44	111.11
2	H	258	ASN	N-CA-C	-6.75	96.43	110.80
2	B	258	ASN	N-CA-C	-6.62	96.70	110.80
2	J	258	ASN	N-CA-C	-6.62	96.71	110.80
2	L	258	ASN	N-CA-C	-6.60	96.75	110.80
1	K	292	TYR	CA-C-N	6.51	126.75	119.32
1	K	292	TYR	C-N-CA	6.51	126.75	119.32
2	F	258	ASN	N-CA-C	-6.43	97.11	110.80
2	L	257	GLN	N-CA-C	-6.16	105.79	113.55
2	J	257	GLN	N-CA-C	-6.11	105.86	113.55
1	K	350	THR	N-CA-C	6.09	118.71	111.71
2	D	257	GLN	N-CA-C	-6.04	105.94	113.55
2	H	257	GLN	N-CA-C	-6.03	105.96	113.55
1	C	350	THR	N-CA-C	6.00	118.61	111.71
2	F	257	GLN	N-CA-C	-5.83	106.20	113.55
2	B	257	GLN	N-CA-C	-5.79	106.26	113.55
1	K	83	GLY	CA-C-N	5.71	125.39	119.05
1	K	83	GLY	C-N-CA	5.71	125.39	119.05
1	I	83	GLY	CA-C-N	5.69	125.37	119.05
1	I	83	GLY	C-N-CA	5.69	125.37	119.05
1	C	346	LYS	N-CA-C	5.67	118.39	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	292	TYR	CA-C-N	5.59	125.69	119.32
1	I	292	TYR	C-N-CA	5.59	125.69	119.32
2	H	122	ILE	N-CA-C	5.55	116.95	110.62
2	J	122	ILE	N-CA-C	5.51	116.90	110.62
2	L	273	SER	N-CA-C	-5.44	105.74	112.38
2	D	122	ILE	N-CA-C	5.44	116.82	110.62
1	A	347	GLU	N-CA-C	5.40	120.77	114.62
2	D	273	SER	N-CA-C	-5.40	105.80	112.38
2	F	353	ARG	N-CA-C	-5.37	104.83	111.33
2	L	122	ILE	N-CA-C	5.37	116.74	110.62
1	G	83	GLY	CA-C-N	5.36	125.00	119.05
1	G	83	GLY	C-N-CA	5.36	125.00	119.05
1	A	83	GLY	CA-C-N	5.35	124.99	119.05
1	A	83	GLY	C-N-CA	5.35	124.99	119.05
2	H	273	SER	N-CA-C	-5.34	106.03	112.54
1	E	350	THR	N-CA-C	5.33	118.58	111.75
2	B	273	SER	N-CA-C	-5.32	105.89	112.38
1	E	347	GLU	N-CA-C	5.31	120.68	114.62
2	B	36	LEU	CA-C-N	5.28	125.19	119.85
2	B	36	LEU	C-N-CA	5.28	125.19	119.85
2	F	273	SER	N-CA-C	-5.28	105.94	112.38
1	C	83	GLY	CA-C-N	5.27	124.90	119.05
1	C	83	GLY	C-N-CA	5.27	124.90	119.05
2	B	122	ILE	N-CA-C	5.25	116.60	110.62
2	J	273	SER	N-CA-C	-5.25	105.98	112.38
2	F	122	ILE	N-CA-C	5.22	116.57	110.62
1	I	217	ASP	N-CA-C	5.19	121.86	110.80
1	E	292	TYR	CA-C-N	5.18	125.22	119.32
1	E	292	TYR	C-N-CA	5.18	125.22	119.32
2	B	284	LYS	N-CA-C	5.13	118.66	111.74
2	D	342	PRO	N-CA-C	5.12	120.65	113.53
2	J	291	PHE	N-CA-C	5.10	116.53	111.07
1	A	350	THR	N-CA-C	5.07	117.46	111.33
2	B	22	ARG	N-CA-C	5.04	119.68	111.37
2	F	292	GLU	N-CA-C	5.03	116.45	111.07
2	J	36	LEU	CA-C-N	5.03	125.01	120.03
2	J	36	LEU	C-N-CA	5.03	125.01	120.03
2	H	50	ILE	N-CA-C	-5.03	105.64	110.72
2	J	50	ILE	N-CA-C	-5.03	105.64	110.72
2	D	353	ARG	N-CA-C	-5.01	105.82	111.28
2	B	50	ILE	N-CA-C	-5.00	105.67	110.72

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	272	TYR	Sidechain
2	B	297	TYR	Sidechain
2	D	272	TYR	Sidechain
2	F	272	TYR	Sidechain
2	F	297	TYR	Sidechain
2	H	272	TYR	Sidechain
2	J	272	TYR	Sidechain
2	L	272	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2520	53	0
1	C	2643	0	2540	40	0
1	E	2642	0	2534	48	0
1	G	2633	0	2524	48	0
1	I	2656	0	2560	45	0
1	K	2671	0	2588	39	0
2	B	2697	0	2600	48	0
2	D	2713	0	2628	47	0
2	F	2718	0	2635	37	0
2	H	2694	0	2590	55	0
2	J	2711	0	2616	50	0
2	L	2723	0	2643	30	0
3	M	46	0	52	1	0
3	N	46	0	52	1	0
3	O	46	0	52	1	0
3	P	46	0	52	1	0
3	Q	46	0	52	0	0
3	R	46	0	52	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	12	0	13	0	0
5	F	12	0	13	0	0
6	B	29	0	34	0	0
6	D	29	0	34	1	0
6	F	29	0	34	0	0
6	H	29	0	34	1	0
6	J	29	0	34	0	0
6	L	29	0	34	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
8	A	44	0	0	1	0
8	B	34	0	0	0	0
8	C	41	0	0	2	0
8	D	51	0	0	1	0
8	E	50	0	0	1	0
8	F	58	0	0	0	0
8	G	40	0	0	0	0
8	H	31	0	0	0	0
8	I	52	0	0	1	0
8	J	47	0	0	0	0
8	K	123	0	0	2	0
8	L	93	0	0	0	0
8	N	2	0	0	0	0
8	O	2	0	0	0	0
8	P	4	0	0	0	0
8	Q	2	0	0	0	0
8	R	4	0	0	0	0
All	All	33292	0	31520	523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:ILE:HG12	1:K:172:ARG:HH12	1.02	1.10
1:I:156:ILE:HG12	1:I:172:ARG:HH12	1.09	1.09
1:A:156:ILE:HG12	1:A:172:ARG:HH12	1.18	1.07
1:E:156:ILE:HG12	1:E:172:ARG:HH12	1.10	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ILE:HG12	1:C:172:ARG:HH12	1.15	1.04
1:G:156:ILE:HG12	1:G:172:ARG:HH12	1.17	1.03
2:B:39:ARG:HB3	2:B:39:ARG:HH11	1.17	1.02
1:K:156:ILE:HG12	1:K:172:ARG:NH1	1.87	0.90
1:A:156:ILE:HG12	1:A:172:ARG:NH1	1.89	0.88
1:A:348:LYS:HA	1:A:348:LYS:HE2	1.64	0.78
1:A:152:MET:O	1:A:156:ILE:HG13	1.83	0.78
1:G:152:MET:O	1:G:156:ILE:HG13	1.84	0.77
1:I:152:MET:O	1:I:156:ILE:HG13	1.84	0.77
1:K:152:MET:O	1:K:156:ILE:HG13	1.85	0.76
2:F:355:ARG:HH11	2:F:355:ARG:HB3	1.50	0.76
1:E:156:ILE:HG12	1:E:172:ARG:NH1	1.96	0.75
1:I:156:ILE:HG12	1:I:172:ARG:NH1	1.95	0.74
1:E:312:ILE:HG23	1:E:340:LEU:HD22	1.70	0.73
1:A:339:GLU:O	1:A:343:ILE:HG13	1.90	0.72
1:C:152:MET:O	1:C:156:ILE:HG13	1.87	0.72
1:C:87:VAL:HG12	1:C:88:VAL:HG23	1.70	0.72
2:L:133:ILE:HD13	2:L:354:LEU:HD13	1.70	0.72
1:K:77:PRO:HG3	1:K:102:TYR:CZ	2.25	0.72
2:B:37:PRO:HD2	2:B:40:TYR:CD1	2.26	0.71
1:E:152:MET:O	1:E:156:ILE:HG13	1.90	0.71
1:E:318:ILE:HG22	1:E:322:MET:HE3	1.72	0.70
1:E:255:VAL:HG13	1:E:258:ARG:NH2	2.05	0.70
2:B:39:ARG:HH11	2:B:39:ARG:CB	1.99	0.70
2:H:348:THR:O	2:H:352:GLU:HG2	1.92	0.69
1:I:231:VAL:HG23	1:I:266:MET:HE3	1.73	0.69
1:C:189:ILE:HD11	1:C:205:HIS:HD2	1.55	0.69
1:I:333:ILE:HD13	1:I:336:LYS:HD2	1.75	0.69
2:J:138:ASP:HA	2:J:357:LEU:HD11	1.74	0.69
1:A:91:ILE:HD12	1:A:91:ILE:O	1.93	0.68
1:I:91:ILE:HD12	1:I:91:ILE:O	1.93	0.68
2:F:339:LYS:O	2:F:348:THR:HG23	1.93	0.68
1:E:189:ILE:HD11	1:E:205:HIS:HD2	1.59	0.67
2:F:37:PRO:HD2	2:F:40:TYR:CD1	2.30	0.67
1:C:156:ILE:HG12	1:C:172:ARG:NH1	2.00	0.67
1:I:353:LYS:HG3	1:I:354:GLU:N	2.10	0.67
1:K:91:ILE:HD12	1:K:91:ILE:O	1.95	0.66
1:I:189:ILE:HD11	1:I:205:HIS:HD2	1.61	0.66
2:H:202:ARG:HG3	2:H:202:ARG:HH11	1.61	0.66
1:K:189:ILE:HD11	1:K:205:HIS:HD2	1.61	0.66
1:C:339:GLU:O	1:C:343:ILE:HG13	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:O	1:C:91:ILE:HD12	1.96	0.65
1:I:339:GLU:O	1:I:343:ILE:HG13	1.96	0.65
1:E:91:ILE:O	1:E:91:ILE:HD12	1.96	0.65
1:G:91:ILE:HD12	1:G:91:ILE:O	1.95	0.65
1:G:189:ILE:HD11	1:G:205:HIS:HD2	1.60	0.65
2:D:110:ASN:N	2:D:110:ASN:ND2	2.44	0.64
2:F:133:ILE:HD13	2:F:354:LEU:HD13	1.78	0.64
2:D:37:PRO:HD2	2:D:40:TYR:CD1	2.32	0.64
1:E:87:VAL:HG12	1:E:88:VAL:HG23	1.78	0.64
2:B:39:ARG:HB3	2:B:39:ARG:NH1	2.02	0.64
1:I:329:ASN:HB3	1:I:332:ASP:HB3	1.80	0.64
1:E:296:LEU:HD22	1:E:322:MET:HE1	1.79	0.64
2:J:258:ASN:OD1	2:J:259:GLY:N	2.31	0.64
2:H:87:ARG:HH12	2:H:90:LEU:HD11	1.62	0.63
2:B:133:ILE:HD13	2:B:354:LEU:HD13	1.78	0.63
2:J:133:ILE:HD13	2:J:354:LEU:HD13	1.80	0.63
2:H:348:THR:O	2:H:351:SER:HB3	1.99	0.63
1:I:328:ASP:O	1:I:329:ASN:HB2	1.98	0.63
1:A:189:ILE:HD11	1:A:205:HIS:HD2	1.63	0.63
2:B:37:PRO:HD2	2:B:40:TYR:CE1	2.34	0.63
2:D:37:PRO:HB2	2:D:39:ARG:HG2	1.80	0.63
2:D:295:ARG:CZ	2:D:299:LEU:HD11	2.29	0.62
1:A:78:VAL:O	1:A:104:ARG:HD2	1.99	0.62
2:F:37:PRO:HD2	2:F:40:TYR:CE1	2.35	0.62
1:G:251:SER:HA	1:G:287:ARG:HH22	1.64	0.62
1:C:100:TYR:HB3	1:C:104:ARG:NH2	2.15	0.62
1:G:339:GLU:O	1:G:343:ILE:HG13	2.00	0.62
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.82	0.61
2:H:92:ARG:HD2	2:H:119:SER:HB3	1.81	0.61
1:I:87:VAL:HG12	1:I:88:VAL:HG23	1.81	0.61
2:F:355:ARG:HB3	2:F:355:ARG:NH1	2.14	0.61
1:K:87:VAL:HG12	1:K:88:VAL:HG23	1.81	0.61
1:E:339:GLU:O	1:E:343:ILE:HG13	2.01	0.61
1:G:87:VAL:HG12	1:G:88:VAL:HG23	1.81	0.61
1:K:251:SER:HA	1:K:287:ARG:HH22	1.65	0.61
2:B:26:VAL:O	2:B:30:GLN:HG3	2.01	0.60
1:E:117:PHE:CE2	1:E:146:LYS:HE2	2.36	0.60
2:L:232:LEU:HD13	2:L:343:ALA:HB1	1.83	0.60
2:B:353:ARG:HG2	2:B:353:ARG:HH11	1.65	0.60
1:K:303:GLN:HB3	1:K:304:PRO:HD3	1.84	0.60
1:E:231:VAL:HG23	1:E:266:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:ASN:N	2:D:110:ASN:HD22	2.00	0.60
1:C:303:GLN:O	1:C:307:SER:HB2	2.02	0.60
1:A:332:ASP:O	1:A:336:LYS:HG3	2.01	0.59
2:H:245:LEU:O	2:H:249:LYS:HG3	2.02	0.59
1:G:334:LEU:O	1:G:338:LEU:HG	2.02	0.59
2:H:37:PRO:HD2	2:H:40:TYR:CD1	2.38	0.59
2:H:69:LYS:O	2:H:73:ILE:HG13	2.01	0.59
2:H:18:LEU:HD22	2:H:18:LEU:N	2.17	0.58
1:E:156:ILE:CG1	1:E:172:ARG:HH12	2.01	0.58
1:G:312:ILE:HG23	1:G:340:LEU:HD22	1.84	0.58
1:C:78:VAL:HG21	1:C:108:GLN:NE2	2.18	0.58
1:I:148:LEU:HB2	1:I:179:LEU:HD21	1.86	0.58
1:G:207:GLN:OE1	2:H:216:LEU:HD13	2.03	0.58
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.19	0.57
1:C:312:ILE:HG23	1:C:340:LEU:HD22	1.84	0.57
2:F:232:LEU:HD13	2:F:343:ALA:HB1	1.86	0.57
2:J:144:LYS:HG2	2:J:185:LEU:HD22	1.86	0.57
2:B:256:GLN:HG3	2:B:260:TYR:CZ	2.40	0.57
1:C:148:LEU:HB2	1:C:179:LEU:HD21	1.86	0.57
2:B:229:SER:O	2:B:233:MET:HG3	2.04	0.57
1:C:180:LYS:HB2	1:E:214:ARG:HG2	1.86	0.57
2:D:353:ARG:NH1	2:D:357:LEU:HG	2.19	0.57
1:A:303:GLN:O	1:A:307:SER:HB2	2.05	0.57
1:A:87:VAL:HG12	1:A:88:VAL:HG23	1.85	0.57
1:A:274:GLU:HG3	1:A:310:TYR:CE2	2.40	0.57
1:I:303:GLN:N	1:I:304:PRO:HD2	2.20	0.57
2:L:133:ILE:CD1	2:L:354:LEU:HD13	2.35	0.57
1:A:287:ARG:O	1:A:291:ARG:HD3	2.05	0.57
1:C:214:ARG:O	1:C:214:ARG:HG2	2.03	0.57
1:G:334:LEU:HD22	1:G:367:HIS:O	2.04	0.57
2:H:133:ILE:HD13	2:H:354:LEU:HD13	1.87	0.57
1:G:69:ARG:HB3	1:G:71:GLU:OE1	2.05	0.56
2:L:197:ILE:HD11	2:L:235:LYS:HD3	1.87	0.56
2:H:232:LEU:HD13	2:H:343:ALA:HB1	1.86	0.56
1:I:312:ILE:HG23	1:I:340:LEU:HD22	1.87	0.56
1:I:334:LEU:HD22	1:I:367:HIS:O	2.06	0.56
2:H:210:LEU:HB2	2:H:223:THR:HA	1.87	0.56
1:E:303:GLN:N	1:E:304:PRO:HD2	2.21	0.56
1:K:303:GLN:O	1:K:307:SER:HB2	2.06	0.56
2:F:39:ARG:NH1	2:F:40:TYR:OH	2.39	0.56
2:D:69:LYS:O	2:D:73:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:PRO:HD2	2:L:40:TYR:CD1	2.41	0.55
2:D:37:PRO:HB2	2:D:39:ARG:HH11	1.72	0.55
1:E:148:LEU:HB2	1:E:179:LEU:HD21	1.87	0.55
2:D:281:LYS:HE3	2:D:331:LEU:HD12	1.89	0.55
2:F:69:LYS:O	2:F:73:ILE:HG13	2.06	0.55
2:D:30:GLN:O	2:D:34:GLN:HG3	2.06	0.55
2:D:133:ILE:HD13	2:D:354:LEU:HD13	1.88	0.55
1:C:78:VAL:HB	1:C:104:ARG:HB3	1.89	0.55
1:A:214:ARG:HG2	1:G:180:LYS:HB2	1.89	0.55
2:L:334:GLU:HB3	2:L:337:ILE:HD12	1.89	0.55
2:B:245:LEU:O	2:B:249:LYS:HG3	2.07	0.55
2:L:210:LEU:HB2	2:L:223:THR:HA	1.88	0.55
2:H:229:SER:O	2:H:233:MET:HG3	2.07	0.54
1:K:311:LEU:C	1:K:311:LEU:HD23	2.32	0.54
1:C:261:GLN:O	1:C:265:GLU:HG2	2.07	0.54
1:A:71:GLU:CD	1:A:71:GLU:H	2.15	0.54
2:L:353:ARG:HD3	2:L:353:ARG:O	2.07	0.54
1:E:303:GLN:O	1:E:307:SER:HB2	2.06	0.54
2:F:210:LEU:HB2	2:F:223:THR:HA	1.89	0.54
2:F:245:LEU:O	2:F:249:LYS:HG3	2.07	0.54
1:G:156:ILE:HG12	1:G:172:ARG:NH1	2.03	0.54
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.90	0.54
1:A:284:LEU:O	1:A:287:ARG:HG2	2.08	0.54
2:D:295:ARG:NH2	2:D:299:LEU:HD11	2.22	0.54
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.23	0.54
1:I:311:LEU:HD23	1:I:311:LEU:C	2.33	0.53
1:K:334:LEU:HD22	1:K:367:HIS:O	2.08	0.53
2:B:333:GLU:OE1	2:J:23:ASP:HB2	2.08	0.53
2:J:77:TYR:CE1	2:J:141:ARG:HB2	2.43	0.53
2:D:197:ILE:HD11	2:D:235:LYS:HD3	1.89	0.53
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.90	0.53
2:D:37:PRO:HD2	2:D:40:TYR:CE1	2.42	0.53
1:I:231:VAL:CG2	1:I:266:MET:HE3	2.38	0.53
2:J:210:LEU:HB2	2:J:223:THR:HA	1.88	0.53
2:D:39:ARG:HG3	2:D:40:TYR:CE1	2.44	0.53
1:G:59:ASP:OD1	1:G:59:ASP:N	2.41	0.53
1:I:323:LEU:HB3	1:I:367:HIS:CD2	2.44	0.53
2:J:334:GLU:HB3	2:J:337:ILE:HD12	1.90	0.53
1:G:101:ASP:HA	1:G:104:ARG:HH11	1.73	0.53
2:B:210:LEU:HB2	2:B:223:THR:HA	1.90	0.53
1:G:303:GLN:O	1:G:307:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:64:LEU:O	2:J:67:VAL:HG22	2.09	0.53
2:J:193:MET:HG3	2:J:233:MET:HE2	1.90	0.53
1:K:339:GLU:O	1:K:343:ILE:HG13	2.08	0.53
2:L:110:ASN:HB3	2:L:111:PRO:HD2	1.91	0.53
2:D:210:LEU:HB2	2:D:223:THR:HA	1.90	0.52
2:H:188:TRP:CE3	2:H:193:MET:HE2	2.44	0.52
2:J:197:ILE:HD11	2:J:235:LYS:HD3	1.91	0.52
1:K:148:LEU:HB2	1:K:179:LEU:HD21	1.92	0.52
2:H:22:ARG:HH11	2:H:22:ARG:HG2	1.74	0.52
1:A:91:ILE:HD11	2:B:38:GLU:H	1.75	0.52
1:A:328:ASP:O	1:A:329:ASN:HB2	2.10	0.52
2:F:186:ASN:HB2	2:F:358:HIS:CE1	2.44	0.52
1:C:284:LEU:O	1:C:287:ARG:HG2	2.10	0.52
2:D:37:PRO:CB	2:D:39:ARG:HH11	2.23	0.52
1:G:100:TYR:O	1:G:104:ARG:HG3	2.10	0.52
1:K:77:PRO:HG3	1:K:102:TYR:CE1	2.44	0.52
1:A:214:ARG:HG3	1:A:214:ARG:O	2.10	0.52
2:J:22:ARG:O	2:J:26:VAL:HG23	2.10	0.52
2:J:361:TRP:C	2:J:363:THR:H	2.18	0.52
2:B:186:ASN:HB2	2:B:358:HIS:CE1	2.45	0.52
1:G:148:LEU:HB2	1:G:179:LEU:HD21	1.92	0.52
2:L:245:LEU:O	2:L:249:LYS:HG3	2.09	0.52
1:C:328:ASP:O	1:C:329:ASN:HB2	2.09	0.52
1:G:319:TYR:HD2	1:G:322:MET:HE3	1.75	0.52
2:H:186:ASN:HB2	2:H:358:HIS:CE1	2.45	0.52
2:B:69:LYS:O	2:B:73:ILE:HG13	2.09	0.51
1:A:261:GLN:O	1:A:265:GLU:HG2	2.10	0.51
2:B:336:GLY:HA2	2:J:305:LEU:HD13	1.93	0.51
1:C:156:ILE:HD11	1:C:172:ARG:HH22	1.74	0.51
1:K:82:ASP:HB2	1:K:86:PRO:HB3	1.92	0.51
2:H:258:ASN:OD1	2:H:259:GLY:N	2.38	0.51
1:I:340:LEU:HD23	1:I:343:ILE:HD12	1.91	0.51
1:A:265:GLU:O	1:A:269:LEU:HD13	2.11	0.51
1:G:311:LEU:HD23	1:G:311:LEU:C	2.36	0.51
1:E:340:LEU:HD23	1:E:343:ILE:HD12	1.93	0.51
2:H:64:LEU:HD11	2:H:134:ILE:HG22	1.92	0.51
1:I:325:ASN:O	1:I:326:GLN:C	2.53	0.51
2:D:106:ASN:HD21	2:D:109:LYS:H	1.58	0.51
2:D:245:LEU:O	2:D:249:LYS:HG3	2.11	0.51
1:I:100:TYR:O	1:I:104:ARG:HG3	2.11	0.51
1:G:78:VAL:O	1:G:104:ARG:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:117:PHE:CE2	1:K:146:LYS:HE2	2.46	0.50
1:A:334:LEU:O	1:A:338:LEU:HG	2.11	0.50
1:I:156:ILE:HD11	1:I:172:ARG:HH22	1.76	0.50
2:B:336:GLY:HA2	2:J:305:LEU:CD1	2.41	0.50
2:J:33:LEU:HD22	2:J:54:ALA:HB1	1.93	0.50
1:E:255:VAL:HG13	1:E:258:ARG:HH21	1.72	0.50
2:H:22:ARG:HG2	2:H:22:ARG:NH1	2.27	0.50
2:H:133:ILE:HG22	2:H:350:THR:HG23	1.92	0.50
1:A:334:LEU:HD22	1:A:367:HIS:O	2.11	0.50
1:G:117:PHE:CE2	1:G:146:LYS:HE2	2.47	0.50
2:B:258:ASN:OD1	2:B:259:GLY:N	2.43	0.50
1:I:303:GLN:O	1:I:307:SER:HB2	2.12	0.50
2:J:338:CYS:SG	2:J:349:ARG:NH2	2.84	0.50
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.47	0.49
1:C:334:LEU:HD22	1:C:367:HIS:O	2.12	0.49
1:G:82:ASP:HB2	1:G:86:PRO:HB3	1.94	0.49
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.47	0.49
1:C:104:ARG:HG2	2:D:101:LEU:O	2.12	0.49
1:E:325:ASN:O	1:E:326:GLN:C	2.54	0.49
1:E:284:LEU:O	1:E:287:ARG:HG2	2.12	0.49
1:E:353:LYS:HE3	1:E:357:ARG:HH12	1.77	0.49
1:G:319:TYR:CD2	1:G:322:MET:HE3	2.48	0.49
1:G:340:LEU:HD23	1:G:343:ILE:HD12	1.94	0.49
1:K:251:SER:HA	1:K:287:ARG:NH2	2.28	0.49
1:K:265:GLU:O	1:K:269:LEU:HD13	2.13	0.49
1:I:78:VAL:O	1:I:104:ARG:HD2	2.13	0.49
2:B:258:ASN:CG	2:B:259:GLY:H	2.20	0.49
1:C:97:ARG:HG2	1:C:101:ASP:OD2	2.12	0.49
2:D:133:ILE:HG22	2:D:350:THR:HG23	1.95	0.49
2:B:22:ARG:HG2	2:B:22:ARG:HH11	1.77	0.48
2:B:22:ARG:HG2	2:B:22:ARG:NH1	2.28	0.48
1:K:312:ILE:HG23	1:K:340:LEU:HD22	1.94	0.48
1:K:88:VAL:HG12	1:K:88:VAL:O	2.13	0.48
2:D:39:ARG:HG2	2:D:39:ARG:HH11	1.78	0.48
2:J:351:SER:O	2:J:354:LEU:HB3	2.13	0.48
1:K:156:ILE:HD11	1:K:172:ARG:HH22	1.77	0.48
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.94	0.48
1:A:344:LEU:HA	1:A:348:LYS:HB2	1.96	0.48
2:H:130:SER:O	2:H:134:ILE:HG13	2.13	0.48
2:H:30:GLN:O	2:H:34:GLN:HG3	2.13	0.48
1:E:296:LEU:CD2	1:E:322:MET:HE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:344:LEU:HD13	1:I:356:TRP:CE2	2.49	0.48
1:G:343:ILE:HG22	1:G:348:LYS:HG3	1.96	0.48
1:E:334:LEU:O	1:E:338:LEU:HG	2.13	0.48
1:G:328:ASP:O	1:G:329:ASN:HB2	2.14	0.48
1:I:144:LEU:HB2	1:I:146:LYS:HD3	1.96	0.48
1:I:324:GLU:HA	1:I:324:GLU:OE1	2.13	0.48
2:L:188:TRP:CE3	2:L:193:MET:HE2	2.48	0.48
2:B:250:ARG:O	2:B:254:MET:HG2	2.14	0.47
1:K:83:GLY:HA3	2:L:105:PHE:CD1	2.49	0.47
2:B:29:PHE:O	2:B:33:LEU:HD22	2.13	0.47
2:H:64:LEU:O	2:H:67:VAL:HG22	2.14	0.47
2:H:138:ASP:OD1	2:H:140:SER:HB3	2.15	0.47
2:J:229:SER:O	2:J:233:MET:HG3	2.14	0.47
1:A:311:LEU:C	1:A:311:LEU:HD23	2.39	0.47
2:F:130:SER:O	2:F:134:ILE:HG13	2.14	0.47
2:B:21:LEU:HD11	2:B:304:ARG:NH2	2.28	0.47
1:C:311:LEU:C	1:C:311:LEU:HD23	2.40	0.47
1:E:334:LEU:HD22	1:E:367:HIS:O	2.14	0.47
1:C:91:ILE:HD11	2:D:38:GLU:H	1.80	0.47
2:D:232:LEU:HD13	2:D:343:ALA:HB1	1.96	0.47
1:E:265:GLU:O	1:E:269:LEU:HD13	2.15	0.47
1:G:261:GLN:O	1:G:265:GLU:HG2	2.15	0.47
1:G:265:GLU:O	1:G:269:LEU:HD13	2.14	0.47
2:J:33:LEU:CD2	2:J:54:ALA:HB1	2.45	0.47
2:B:193:MET:HG3	2:B:233:MET:HE2	1.97	0.47
1:E:91:ILE:HD11	2:F:38:GLU:H	1.79	0.47
1:G:325:ASN:O	1:G:326:GLN:C	2.57	0.47
1:A:191:ASP:O	1:A:194:ASN:HB2	2.15	0.47
1:E:96:PHE:CE1	1:E:126:LEU:HB3	2.50	0.47
2:J:245:LEU:O	2:J:249:LYS:HG3	2.15	0.47
1:K:114:GLU:OE2	1:K:146:LYS:NZ	2.41	0.47
1:K:325:ASN:O	1:K:326:GLN:C	2.58	0.47
1:C:265:GLU:O	1:C:269:LEU:HD13	2.14	0.46
2:D:258:ASN:CG	2:D:259:GLY:H	2.22	0.46
2:D:353:ARG:HH11	2:D:357:LEU:HG	1.79	0.46
1:A:332:ASP:OD1	1:A:336:LYS:HD2	2.15	0.46
1:C:325:ASN:O	1:C:326:GLN:C	2.58	0.46
2:J:138:ASP:OD1	2:J:140:SER:HB3	2.14	0.46
1:E:329:ASN:HB3	1:E:332:ASP:HB3	1.97	0.46
1:E:331:GLU:O	1:E:335:ASN:ND2	2.48	0.46
1:A:325:ASN:O	1:A:326:GLN:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:TYR:CZ	2:B:141:ARG:HB2	2.50	0.46
1:C:82:ASP:HB2	1:C:86:PRO:HB3	1.97	0.46
1:G:318:ILE:HG22	1:G:322:MET:HE2	1.98	0.46
1:I:302:LEU:C	1:I:304:PRO:HD2	2.41	0.46
1:K:334:LEU:O	1:K:338:LEU:HG	2.16	0.46
1:C:117:PHE:CE2	1:C:146:LYS:HE2	2.51	0.46
1:I:156:ILE:CG1	1:I:172:ARG:HH12	2.01	0.46
1:I:191:ASP:O	1:I:194:ASN:HB2	2.15	0.46
1:K:191:ASP:O	1:K:194:ASN:HB2	2.16	0.46
2:J:256:GLN:HB2	2:J:260:TYR:CE2	2.51	0.46
2:H:26:VAL:O	2:H:30:GLN:HG3	2.16	0.45
1:I:334:LEU:O	1:I:338:LEU:HG	2.16	0.45
1:E:69:ARG:HB3	1:E:71:GLU:OE1	2.15	0.45
2:J:21:LEU:HD11	2:J:304:ARG:NH2	2.30	0.45
2:L:133:ILE:HG22	2:L:350:THR:HG23	1.98	0.45
1:A:92:TYR:O	1:A:97:ARG:NH2	2.49	0.45
2:B:39:ARG:HG2	2:B:40:TYR:CE1	2.52	0.45
1:C:283:ILE:O	1:C:287:ARG:HD3	2.16	0.45
1:G:252:ASP:OD2	1:G:252:ASP:C	2.57	0.45
2:H:137:ASP:OD1	2:H:139:LEU:N	2.40	0.45
2:J:207:ASP:O	2:J:208:ASN:HB2	2.15	0.45
2:H:77:TYR:CZ	2:H:141:ARG:HB2	2.52	0.45
1:A:156:ILE:HD11	1:A:172:ARG:HH22	1.81	0.45
1:A:214:ARG:O	1:A:214:ARG:CG	2.64	0.45
1:K:96:PHE:CE1	1:K:126:LEU:HB3	2.52	0.45
2:D:188:TRP:CE3	2:D:193:MET:HE2	2.51	0.45
1:E:302:LEU:C	1:E:304:PRO:HD2	2.42	0.45
2:H:202:ARG:HG3	2:H:202:ARG:NH1	2.30	0.45
2:L:256:GLN:HB2	2:L:260:TYR:CE2	2.52	0.45
1:A:283:ILE:O	1:A:287:ARG:HD3	2.17	0.44
2:H:33:LEU:HD22	2:H:54:ALA:HB1	1.99	0.44
1:I:332:ASP:O	1:I:336:LYS:HG3	2.17	0.44
2:J:77:TYR:CZ	2:J:141:ARG:HB2	2.52	0.44
1:A:251:SER:HA	1:A:287:ARG:HH22	1.82	0.44
2:F:258:ASN:OD1	2:F:259:GLY:N	2.46	0.44
2:H:250:ARG:O	2:H:254:MET:HG2	2.18	0.44
2:D:130:SER:O	2:D:134:ILE:HG13	2.17	0.44
1:E:106:VAL:HG13	1:E:111:GLU:HB3	1.98	0.44
2:H:357:LEU:HD22	2:H:361:TRP:CZ2	2.53	0.44
2:J:22:ARG:HG2	2:J:22:ARG:HH11	1.82	0.44
2:L:236:LEU:HD22	2:L:245:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:353:ARG:HD3	2:L:353:ARG:C	2.42	0.44
1:A:296:LEU:CD2	1:A:322:MET:HE1	2.48	0.44
2:D:20:PHE:CZ	2:D:337:ILE:HD11	2.52	0.44
2:H:256:GLN:HB2	2:H:260:TYR:CE2	2.52	0.44
1:K:348:LYS:HD2	8:K:462:HOH:O	2.17	0.44
2:F:30:GLN:O	2:F:34:GLN:HG3	2.18	0.44
2:F:269:ASP:HB3	2:F:272:TYR:HD2	1.83	0.44
1:I:173:ARG:HD2	8:I:403:HOH:O	2.17	0.44
2:J:138:ASP:OD1	2:J:140:SER:CB	2.66	0.44
2:F:92:ARG:HB3	2:F:119:SER:HB3	1.99	0.44
1:G:88:VAL:HG13	2:H:36:LEU:HD11	2.00	0.44
2:L:258:ASN:OD1	2:L:259:GLY:N	2.45	0.44
2:B:36:LEU:HA	2:B:37:PRO:HD3	1.85	0.44
2:B:49:THR:HG21	3:M:11:MET:HE1	2.00	0.44
2:F:77:TYR:CZ	2:F:141:ARG:HB2	2.53	0.44
1:G:251:SER:HA	1:G:287:ARG:NH2	2.31	0.44
2:H:21:LEU:CD1	2:H:21:LEU:N	2.81	0.44
2:H:144:LYS:HD2	2:H:185:LEU:HD22	2.00	0.44
1:I:255:VAL:HG13	1:I:258:ARG:NH2	2.33	0.44
2:D:236:LEU:HD22	2:D:245:LEU:HD21	2.00	0.43
2:F:92:ARG:HB3	2:F:119:SER:CB	2.47	0.43
2:H:263:ARG:HB2	2:H:266:LYS:HG3	2.00	0.43
1:K:329:ASN:HB3	1:K:332:ASP:HB3	1.99	0.43
1:A:81:ASN:ND2	2:B:105:PHE:H	2.16	0.43
2:B:130:SER:O	2:B:134:ILE:HG13	2.17	0.43
1:G:65:LEU:HD12	1:G:67:ARG:NH1	2.33	0.43
2:D:29:PHE:O	2:D:33:LEU:HD22	2.18	0.43
2:D:106:ASN:ND2	2:D:109:LYS:H	2.16	0.43
2:H:235:LYS:O	2:H:239:VAL:HG23	2.17	0.43
2:H:236:LEU:HD22	2:H:245:LEU:HD21	2.00	0.43
2:H:357:LEU:O	2:H:360:SER:HB3	2.18	0.43
1:K:328:ASP:O	1:K:329:ASN:HB2	2.19	0.43
2:L:74:GLU:CD	2:L:141:ARG:HH22	2.26	0.43
2:L:38:GLU:O	2:L:38:GLU:HG2	2.17	0.43
1:K:219:GLU:OE1	1:K:219:GLU:HA	2.19	0.43
2:L:263:ARG:HB2	2:L:266:LYS:HG3	2.00	0.43
1:C:78:VAL:HG21	1:C:108:GLN:HE22	1.82	0.43
1:K:184:GLN:HB2	8:K:379:HOH:O	2.18	0.43
1:K:311:LEU:HD23	1:K:311:LEU:O	2.19	0.43
2:B:357:LEU:HD22	2:B:361:TRP:NE1	2.34	0.43
1:E:65:LEU:HD12	1:E:67:ARG:NH1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:207:ASP:O	2:H:208:ASN:HB2	2.19	0.43
1:I:344:LEU:HA	1:I:348:LYS:HB2	2.00	0.43
2:J:86:ASP:OD2	2:J:86:ASP:N	2.49	0.43
2:L:22:ARG:O	2:L:26:VAL:HG23	2.18	0.43
1:A:81:ASN:HD21	2:B:105:PHE:H	1.67	0.43
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.56	0.43
2:D:77:TYR:CZ	2:D:141:ARG:HB2	2.54	0.43
2:H:202:ARG:HH11	2:H:202:ARG:CG	2.31	0.43
2:J:232:LEU:HD13	2:J:343:ALA:HB1	2.00	0.43
1:C:105:ALA:O	1:C:109:ARG:HG3	2.18	0.43
1:E:239:GLN:OE1	1:E:239:GLN:HA	2.19	0.43
2:H:33:LEU:CD2	2:H:54:ALA:HB1	2.49	0.43
2:H:37:PRO:C	2:H:39:ARG:H	2.27	0.43
2:J:130:SER:O	2:J:134:ILE:HG13	2.19	0.43
2:L:22:ARG:NH1	2:L:22:ARG:HG2	2.33	0.43
2:L:103:ILE:HG23	2:L:104:PRO:HD2	2.00	0.43
2:F:29:PHE:O	2:F:33:LEU:HD22	2.19	0.43
1:G:252:ASP:OD1	1:G:255:VAL:HG23	2.19	0.43
2:H:49:THR:HG21	3:P:11:MET:HE1	2.01	0.43
2:L:22:ARG:HG2	2:L:22:ARG:HH11	1.82	0.43
2:F:256:GLN:HB2	2:F:260:TYR:CE2	2.54	0.42
2:F:269:ASP:OD1	2:F:269:ASP:C	2.62	0.42
1:G:287:ARG:O	1:G:291:ARG:HD3	2.19	0.42
1:C:100:TYR:HB3	1:C:104:ARG:HH21	1.82	0.42
2:D:36:LEU:HA	2:D:37:PRO:HD3	1.89	0.42
2:B:70:ASP:O	2:B:74:GLU:HG2	2.19	0.42
2:B:269:ASP:HB3	2:B:272:TYR:HD2	1.84	0.42
1:E:198:LYS:NZ	8:E:403:HOH:O	2.52	0.42
2:J:19:ASP:OD2	2:J:19:ASP:N	2.50	0.42
2:B:133:ILE:CD1	2:B:354:LEU:HD13	2.49	0.42
1:G:353:LYS:HE2	1:G:353:LYS:HB3	1.82	0.42
2:H:334:GLU:HB3	2:H:337:ILE:HD12	2.01	0.42
2:J:38:GLU:HG2	2:J:38:GLU:O	2.19	0.42
2:J:92:ARG:HB3	2:J:119:SER:HB3	2.00	0.42
2:J:236:LEU:HD22	2:J:245:LEU:HD21	2.01	0.42
2:J:269:ASP:C	2:J:269:ASP:OD1	2.62	0.42
2:B:92:ARG:HB3	2:B:119:SER:CB	2.50	0.42
2:D:22:ARG:HG2	2:D:22:ARG:HH11	1.83	0.42
2:D:250:ARG:O	2:D:254:MET:HG2	2.20	0.42
2:F:39:ARG:HG2	2:F:40:TYR:CE1	2.55	0.42
2:F:349:ARG:HG3	2:F:349:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:189:ILE:HD11	1:I:205:HIS:CD2	2.48	0.42
1:I:255:VAL:HG13	1:I:258:ARG:HH21	1.85	0.42
1:G:329:ASN:HB3	1:G:332:ASP:HB3	2.02	0.42
1:A:296:LEU:O	1:A:296:LEU:HD12	2.20	0.42
2:B:263:ARG:HB2	2:B:266:LYS:HG3	2.01	0.42
2:B:269:ASP:OD1	2:B:269:ASP:C	2.62	0.42
1:E:328:ASP:O	1:E:329:ASN:HB2	2.20	0.42
2:F:21:LEU:HD11	2:F:304:ARG:NH2	2.34	0.42
2:H:188:TRP:CZ3	2:H:191:MET:HE3	2.54	0.42
6:H:380:MGM:O1	6:H:380:MGM:HC41	2.20	0.42
2:J:92:ARG:HB3	2:J:119:SER:CB	2.49	0.42
1:K:71:GLU:CD	1:K:71:GLU:H	2.27	0.42
1:A:184:GLN:HB2	8:A:379:HOH:O	2.20	0.42
2:D:22:ARG:O	2:D:26:VAL:HG23	2.19	0.42
2:D:49:THR:HG21	3:N:11:MET:HE1	2.00	0.42
1:E:329:ASN:O	1:E:330:LYS:C	2.63	0.42
2:F:36:LEU:HA	2:F:37:PRO:HD3	1.87	0.42
2:F:266:LYS:HE3	2:F:266:LYS:HB3	1.91	0.42
2:F:360:SER:O	2:F:363:THR:HG23	2.20	0.42
2:H:18:LEU:N	2:H:18:LEU:CD2	2.83	0.42
2:H:37:PRO:C	2:H:39:ARG:N	2.76	0.42
1:I:91:ILE:HG13	2:J:36:LEU:O	2.19	0.42
2:J:138:ASP:OD1	2:J:140:SER:N	2.53	0.42
2:J:269:ASP:HB3	2:J:272:TYR:HD2	1.85	0.42
2:B:207:ASP:O	2:B:208:ASN:HB2	2.19	0.42
1:C:296:LEU:CD2	1:C:322:MET:HE1	2.50	0.42
1:E:65:LEU:O	1:E:69:ARG:HG3	2.20	0.42
1:G:156:ILE:CG1	1:G:172:ARG:HH12	2.08	0.42
1:A:303:GLN:HB3	1:A:304:PRO:HD3	2.02	0.42
2:B:201:ARG:NH1	2:B:239:VAL:O	2.52	0.42
2:D:263:ARG:HB2	2:D:266:LYS:HG3	2.01	0.42
1:E:74:ASP:OD2	1:E:75:ILE:HG12	2.20	0.42
2:F:115:HIS:HA	2:F:116:PRO:HD3	1.95	0.42
1:K:301:ASP:O	1:K:304:PRO:HD2	2.20	0.42
2:D:266:LYS:HE3	2:D:266:LYS:HB3	1.93	0.41
1:G:227:LEU:HD23	1:G:227:LEU:HA	1.93	0.41
1:I:265:GLU:O	1:I:269:LEU:HD13	2.20	0.41
1:A:156:ILE:CD1	1:A:172:ARG:HH22	2.33	0.41
1:C:231:VAL:HG23	1:C:266:MET:HE3	2.02	0.41
2:D:103:ILE:HG23	2:D:104:PRO:HD2	2.02	0.41
2:J:18:LEU:HB3	2:J:19:ASP:H	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:37:PRO:HD2	2:J:40:TYR:CD1	2.56	0.41
1:A:82:ASP:HB2	1:A:86:PRO:HB3	2.02	0.41
2:D:26:VAL:O	2:D:30:GLN:HG3	2.20	0.41
1:G:101:ASP:HA	1:G:104:ARG:NH1	2.35	0.41
1:G:106:VAL:HG13	1:G:111:GLU:HB3	2.02	0.41
1:I:355:TYR:O	1:I:358:TYR:HB3	2.20	0.41
2:J:152:ARG:HD3	2:J:189:SER:O	2.21	0.41
1:K:330:LYS:HE2	1:K:367:HIS:HB3	2.01	0.41
2:L:269:ASP:HB3	2:L:272:TYR:HD2	1.85	0.41
2:D:39:ARG:H	2:D:39:ARG:NH1	2.18	0.41
2:F:357:LEU:HD23	2:F:357:LEU:HA	1.93	0.41
2:L:79:LEU:O	2:L:96:ARG:HG3	2.20	0.41
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.85	0.41
2:B:357:LEU:HD22	2:B:361:TRP:CE2	2.56	0.41
1:E:308:SER:HB2	1:E:309:PRO:HD2	2.02	0.41
2:F:263:ARG:HB2	2:F:266:LYS:HG3	2.02	0.41
1:G:138:ARG:NH2	1:G:171:HIS:ND1	2.68	0.41
1:I:106:VAL:HG13	1:I:111:GLU:HB3	2.03	0.41
2:H:357:LEU:HD22	2:H:361:TRP:CE2	2.56	0.41
1:A:357:ARG:O	1:A:361:ARG:HG3	2.20	0.41
2:H:269:ASP:HB3	2:H:272:TYR:HD2	1.85	0.41
1:I:117:PHE:CE2	1:I:146:LYS:HE2	2.56	0.41
2:F:355:ARG:HH11	2:F:355:ARG:CB	2.24	0.41
2:J:258:ASN:CG	2:J:259:GLY:H	2.24	0.41
1:K:107:LEU:HD11	2:L:117:TYR:HB2	2.03	0.41
1:C:173:ARG:HD2	8:C:400:HOH:O	2.20	0.41
1:C:286:ASP:HB2	8:C:405:HOH:O	2.19	0.41
1:C:329:ASN:HB3	1:C:332:ASP:HB3	2.03	0.41
2:D:269:ASP:OD1	2:D:269:ASP:C	2.64	0.41
2:F:236:LEU:HD22	2:F:245:LEU:HD21	2.03	0.41
1:G:91:ILE:HD12	2:H:38:GLU:HB2	2.03	0.41
1:G:156:ILE:HD11	1:G:172:ARG:HH22	1.86	0.41
2:H:269:ASP:OD1	2:H:269:ASP:C	2.63	0.41
1:I:86:PRO:HB2	1:I:89:GLN:NE2	2.35	0.41
2:J:22:ARG:HG2	2:J:22:ARG:NH1	2.36	0.41
2:J:64:LEU:HD23	2:J:64:LEU:HA	1.90	0.41
2:L:250:ARG:O	2:L:254:MET:HG2	2.21	0.41
3:O:10:ILE:O	3:O:11:MET:HG3	2.20	0.41
2:B:64:LEU:HD11	2:B:134:ILE:HG22	2.03	0.41
1:C:348:LYS:HA	1:C:348:LYS:HD3	1.93	0.41
2:F:121:HIS:HB3	2:F:124:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:PRO:HD2	2:H:40:TYR:CE1	2.56	0.41
2:J:263:ARG:HB2	2:J:266:LYS:HG3	2.02	0.41
2:B:256:GLN:HG3	2:B:260:TYR:CE1	2.55	0.40
2:F:186:ASN:HB2	2:F:358:HIS:NE2	2.37	0.40
2:F:258:ASN:CG	2:F:259:GLY:H	2.29	0.40
1:G:287:ARG:H	1:G:287:ARG:HG2	1.60	0.40
2:J:266:LYS:HE3	2:J:266:LYS:HB3	1.94	0.40
1:K:287:ARG:H	1:K:287:ARG:HG2	1.63	0.40
2:L:207:ASP:O	2:L:208:ASN:HB2	2.21	0.40
2:L:340:VAL:HG22	2:L:341:HIS:N	2.35	0.40
1:A:81:ASN:HD21	2:B:104:PRO:HA	1.85	0.40
1:A:333:ILE:HD13	1:A:336:LYS:HD3	2.03	0.40
1:E:105:ALA:O	1:E:109:ARG:HG3	2.22	0.40
2:J:243:LYS:O	2:J:247:ARG:HG3	2.22	0.40
2:J:250:ARG:O	2:J:254:MET:HG2	2.21	0.40
2:B:33:LEU:CD2	2:B:54:ALA:HB1	2.52	0.40
1:C:88:VAL:HG13	2:D:36:LEU:HD11	2.03	0.40
1:C:106:VAL:HG13	1:C:111:GLU:HB3	2.03	0.40
2:D:254:MET:HE3	8:D:399:HOH:O	2.22	0.40
1:E:78:VAL:O	1:E:104:ARG:HD2	2.21	0.40
1:E:311:LEU:HD23	1:E:311:LEU:C	2.47	0.40
1:E:58:LEU:HD23	1:E:63:TYR:CE2	2.57	0.40
1:E:283:ILE:O	1:E:287:ARG:HD3	2.22	0.40
2:D:173:ARG:HG2	6:D:380:MGM:H112	2.03	0.40
1:E:328:ASP:O	1:E:329:ASN:CB	2.70	0.40
2:H:201:ARG:NH1	2:H:239:VAL:O	2.54	0.40
1:I:252:ASP:OD2	1:I:252:ASP:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/377 (83%)	289 (93%)	22 (7%)	1 (0%)	36	60
1	C	312/377 (83%)	293 (94%)	18 (6%)	1 (0%)	36	60
1	E	312/377 (83%)	290 (93%)	21 (7%)	1 (0%)	36	60
1	G	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	36	60
1	I	312/377 (83%)	292 (94%)	19 (6%)	1 (0%)	36	60
1	K	312/377 (83%)	293 (94%)	19 (6%)	0	100	100
2	B	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	36	60
2	D	344/377 (91%)	333 (97%)	10 (3%)	1 (0%)	36	60
2	F	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	36	60
2	H	344/377 (91%)	329 (96%)	14 (4%)	1 (0%)	36	60
2	J	344/377 (91%)	329 (96%)	11 (3%)	4 (1%)	10	27
2	L	344/377 (91%)	332 (96%)	11 (3%)	1 (0%)	36	60
3	M	4/11 (36%)	4 (100%)	0	0	100	100
3	N	4/11 (36%)	4 (100%)	0	0	100	100
3	O	4/11 (36%)	4 (100%)	0	0	100	100
3	P	4/11 (36%)	4 (100%)	0	0	100	100
3	Q	4/11 (36%)	4 (100%)	0	0	100	100
3	R	4/11 (36%)	4 (100%)	0	0	100	100
All	All	3960/4590 (86%)	3761 (95%)	185 (5%)	14 (0%)	30	54

All (14) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/338 (83%)	273 (98%)	7 (2%)	42	71
1	C	283/338 (84%)	276 (98%)	7 (2%)	42	71
1	E	284/338 (84%)	277 (98%)	7 (2%)	42	71
1	G	281/338 (83%)	276 (98%)	5 (2%)	51	78
1	I	287/338 (85%)	281 (98%)	6 (2%)	47	75
1	K	291/338 (86%)	283 (97%)	8 (3%)	39	69
2	B	289/326 (89%)	277 (96%)	12 (4%)	26	55
2	D	293/326 (90%)	280 (96%)	13 (4%)	25	53
2	F	294/326 (90%)	282 (96%)	12 (4%)	27	56
2	H	288/326 (88%)	277 (96%)	11 (4%)	29	58
2	J	292/326 (90%)	282 (97%)	10 (3%)	32	62
2	L	296/326 (91%)	285 (96%)	11 (4%)	30	59
3	M	6/11 (54%)	6 (100%)	0	100	100
3	N	6/11 (54%)	6 (100%)	0	100	100
3	O	6/11 (54%)	6 (100%)	0	100	100
3	P	6/11 (54%)	6 (100%)	0	100	100
3	Q	6/11 (54%)	6 (100%)	0	100	100
3	R	6/11 (54%)	6 (100%)	0	100	100
All	All	3494/4050 (86%)	3385 (97%)	109 (3%)	35	65

All (109) 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	182	PRO
1	A	194	ASN
1	A	214	ARG

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Mol	Chain	Res	Type
1	A	287	ARG
2	B	21	LEU
2	B	33	LEU
2	B	39	ARG
2	B	113	THR
2	B	151	LEU
2	B	216	LEU
2	B	232	LEU
2	B	236	LEU
2	B	306	VAL
2	B	329	LEU
2	B	331	LEU
2	B	357	LEU
1	C	59	ASP
1	C	71	GLU
1	C	107	LEU
1	C	194	ASN
1	C	287	ARG
1	C	324	GLU
1	C	364	GLN
2	D	21	LEU
2	D	33	LEU
2	D	39	ARG
2	D	110	ASN
2	D	151	LEU
2	D	216	LEU
2	D	232	LEU
2	D	236	LEU
2	D	258	ASN
2	D	306	VAL
2	D	329	LEU
2	D	331	LEU
2	D	357	LEU
1	E	71	GLU
1	E	107	LEU
1	E	214	ARG
1	E	225	GLN
1	E	265	GLU
1	E	287	ARG
1	E	324	GLU
2	F	21	LEU
2	F	33	LEU

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Mol	Chain	Res	Type
2	F	39	ARG
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	355	ARG
1	G	59	ASP
1	G	107	LEU
1	G	114	GLU
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	306	VAL
2	H	329	LEU
2	H	331	LEU
2	H	357	LEU
1	I	107	LEU
1	I	114	GLU
1	I	287	ARG
1	I	324	GLU
1	I	332	ASP
1	I	364	GLN
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	306	VAL
2	J	329	LEU
2	J	331	LEU
2	J	357	LEU

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Mol	Chain	Res	Type
1	K	71	GLU
1	K	107	LEU
1	K	114	GLU
1	K	142	ARG
1	K	156	ILE
1	K	287	ARG
1	K	301	ASP
1	K	357	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	255	ARG
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 (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	89	GLN
1	A	135	HIS
1	A	149	GLN
1	A	194	ASN
1	A	234	ASN
1	A	272	HIS
1	A	278	ASN
1	A	285	GLN
1	A	329	ASN
1	A	335	ASN
1	A	364	GLN
1	A	367	HIS
2	B	208	ASN
2	B	257	GLN
1	C	81	ASN
1	C	108	GLN
1	C	135	HIS
1	C	218	ASN

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Mol	Chain	Res	Type
1	C	272	HIS
1	C	285	GLN
1	C	298	GLN
1	C	364	GLN
1	C	367	HIS
2	D	30	GLN
2	D	106	ASN
2	D	110	ASN
2	D	208	ASN
2	D	212	GLN
2	D	246	ASN
2	D	257	GLN
1	E	81	ASN
1	E	89	GLN
1	E	135	HIS
1	E	184	GLN
1	E	205	HIS
1	E	218	ASN
1	E	225	GLN
1	E	285	GLN
1	E	325	ASN
1	E	335	ASN
2	F	30	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	162	GLN
1	G	184	GLN
1	G	234	ASN
1	G	272	HIS
1	G	285	GLN
1	G	297	ASN
1	G	335	ASN
1	G	367	HIS
2	H	208	ASN
1	I	81	ASN
1	I	89	GLN
1	I	135	HIS
1	I	149	GLN

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Mol	Chain	Res	Type
1	I	184	GLN
1	I	195	GLN
1	I	285	GLN
1	I	367	HIS
2	J	208	ASN
2	J	212	GLN
2	J	246	ASN
2	J	257	GLN
1	K	89	GLN
1	K	108	GLN
1	K	135	HIS
1	K	149	GLN
1	K	162	GLN
1	K	205	HIS
1	K	285	GLN
1	K	367	HIS
2	L	208	ASN
2	L	212	GLN
2	L	257	GLN

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MGM	L	380	-	27,28,28	1.00	2 (7%)	34,37,37	2.05	6 (17%)
6	MGM	J	379	-	27,28,28	1.00	2 (7%)	34,37,37	2.02	7 (20%)
5	MES	B	379	-	12,12,12	9.12	8 (66%)	15,16,16	2.07	5 (33%)
6	MGM	H	380	-	27,28,28	0.91	2 (7%)	34,37,37	1.97	6 (17%)
5	MES	F	380	-	12,12,12	9.31	8 (66%)	15,16,16	2.10	5 (33%)
6	MGM	D	380	-	27,28,28	0.97	2 (7%)	34,37,37	2.04	6 (17%)
6	MGM	B	380	-	27,28,28	1.00	2 (7%)	34,37,37	2.02	6 (17%)
6	MGM	F	381	-	27,28,28	0.99	2 (7%)	34,37,37	2.03	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
6	MGM	L	380	-	-	9/31/31/31	-
6	MGM	J	379	-	-	10/31/31/31	-
5	MES	B	379	-	-	1/6/14/14	0/1/1/1
6	MGM	H	380	-	-	9/31/31/31	-
5	MES	F	380	-	-	3/6/14/14	0/1/1/1
6	MGM	D	380	-	-	10/31/31/31	-
6	MGM	B	380	-	-	9/31/31/31	-
6	MGM	F	381	-	-	10/31/31/31	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	380	MES	C8-S	-24.47	1.43	1.77
5	B	379	MES	C8-S	-22.70	1.45	1.77
5	B	379	MES	O2S-S	13.57	1.83	1.45
5	F	380	MES	O2S-S	13.01	1.81	1.45
5	B	379	MES	O1S-S	13.00	1.81	1.45
5	F	380	MES	O1S-S	11.99	1.78	1.45
5	B	379	MES	O3S-S	9.28	1.82	1.47
5	F	380	MES	O3S-S	8.78	1.80	1.47
5	F	380	MES	C7-C8	-4.88	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	379	MES	C7-C8	-4.49	1.40	1.52
5	F	380	MES	C3-C2	-2.80	1.40	1.50
6	L	380	MGM	C7-C8	2.54	1.38	1.33
5	F	380	MES	C7-N4	-2.54	1.41	1.47
5	B	379	MES	C3-C2	-2.52	1.41	1.50
5	F	380	MES	C5-C6	-2.47	1.41	1.50
6	F	381	MGM	C7-C8	2.42	1.38	1.33
5	B	379	MES	C5-C6	-2.27	1.42	1.50
6	D	380	MGM	C7-C8	2.27	1.38	1.33
6	B	380	MGM	C12-C13	2.25	1.38	1.33
6	J	379	MGM	C7-C8	2.24	1.38	1.33
6	B	380	MGM	C7-C8	2.23	1.38	1.33
6	L	380	MGM	C12-C13	2.18	1.38	1.33
5	B	379	MES	C7-N4	-2.17	1.42	1.47
6	J	379	MGM	C12-C13	2.16	1.38	1.33
6	D	380	MGM	C12-C13	2.13	1.38	1.33
6	F	381	MGM	C12-C13	2.11	1.37	1.33
6	H	380	MGM	C7-C8	2.08	1.37	1.33
6	H	380	MGM	C12-C13	2.05	1.37	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	380	MGM	C1-C2-N3	7.48	131.26	113.30
6	F	381	MGM	C1-C2-N3	7.39	131.04	113.30
6	D	380	MGM	C1-C2-N3	7.35	130.95	113.30
6	L	380	MGM	C1-C2-N3	7.26	130.73	113.30
6	J	379	MGM	C1-C2-N3	7.23	130.65	113.30
6	H	380	MGM	C1-C2-N3	6.95	130.00	113.30
6	J	379	MGM	C4-N3-C2	5.28	125.70	110.55
6	D	380	MGM	C4-N3-C2	5.22	125.53	110.55
6	F	381	MGM	C4-N3-C2	5.13	125.27	110.55
6	L	380	MGM	C4-N3-C2	5.10	125.17	110.55
6	B	380	MGM	C4-N3-C2	5.07	125.08	110.55
6	H	380	MGM	C4-N3-C2	4.99	124.85	110.55
5	B	379	MES	O1S-S-C8	4.80	113.98	106.73
5	F	380	MES	O1S-S-C8	4.34	113.28	106.73
6	L	380	MGM	O1-C1-C2	4.07	115.51	107.38
6	D	380	MGM	O1-C1-C2	3.94	115.26	107.38
6	B	380	MGM	O1-C1-C2	3.92	115.21	107.38
6	F	381	MGM	O1-C1-C2	3.88	115.14	107.38
5	F	380	MES	O3S-S-C8	3.70	113.24	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	380	MGM	O1-C1-C2	3.65	114.68	107.38
5	B	379	MES	O3S-S-C8	3.63	113.10	106.00
6	J	379	MGM	O1-C1-C2	3.58	114.53	107.38
5	F	380	MES	O2S-S-C8	3.05	111.33	106.73
6	L	380	MGM	O1A-PA-O3A	3.04	115.49	107.27
6	F	381	MGM	O1A-PA-O3A	2.94	115.22	107.27
6	H	380	MGM	O1A-PA-O3A	2.90	115.12	107.27
6	D	380	MGM	O1A-PA-O3A	2.79	114.81	107.27
6	L	380	MGM	O1B-PB-O3A	2.76	113.88	104.64
6	J	379	MGM	O1B-PB-O3A	2.70	113.70	104.64
5	F	380	MES	O3S-S-O2S	-2.70	104.64	111.40
6	J	379	MGM	O1A-PA-O3A	2.65	114.42	107.27
6	D	380	MGM	O1B-PB-O3A	2.59	113.33	104.64
6	B	380	MGM	O1A-PA-O3A	2.58	114.25	107.27
6	B	380	MGM	O1B-PB-O3A	2.56	113.21	104.64
6	F	381	MGM	O1B-PB-O3A	2.55	113.19	104.64
6	H	380	MGM	O1B-PB-O3A	2.43	112.78	104.64
5	B	379	MES	O3S-S-O2S	-2.41	105.37	111.40
6	H	380	MGM	C2-N3-C5	2.29	122.72	112.03
5	B	379	MES	O2S-S-C8	2.28	110.18	106.73
5	F	380	MES	O2S-S-O1S	-2.27	106.43	113.82
5	B	379	MES	O2S-S-O1S	-2.27	106.43	113.82
6	B	380	MGM	C2-N3-C5	2.26	122.55	112.03
6	F	381	MGM	C2-N3-C5	2.23	122.44	112.03
6	L	380	MGM	C2-N3-C5	2.23	122.43	112.03
6	D	380	MGM	C2-N3-C5	2.17	122.13	112.03
6	J	379	MGM	C2-N3-C5	2.12	121.91	112.03
6	J	379	MGM	C10-C8-C9	-2.01	111.74	115.23

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	380	MES	C7-C8-S-O2S
5	F	380	MES	C7-C8-S-O3S
6	B	380	MGM	C1-C2-N3-C4
6	B	380	MGM	O1-C1-C2-N3
6	B	380	MGM	PA-O3A-PB-O1B
6	D	380	MGM	C1-C2-N3-C4
6	D	380	MGM	O1-C1-C2-N3
6	D	380	MGM	PA-O3A-PB-O1B
6	F	381	MGM	C1-C2-N3-C4

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Mol	Chain	Res	Type	Atoms
6	F	381	MGM	O1-C1-C2-N3
6	F	381	MGM	PA-O3A-PB-O1B
6	H	380	MGM	C1-C2-N3-C4
6	H	380	MGM	O1-C1-C2-N3
6	H	380	MGM	PA-O3A-PB-O1B
6	J	379	MGM	C1-C2-N3-C4
6	J	379	MGM	O1-C1-C2-N3
6	J	379	MGM	PA-O3A-PB-O1B
6	L	380	MGM	C1-C2-N3-C4
6	L	380	MGM	O1-C1-C2-N3
6	L	380	MGM	PA-O3A-PB-O1B
6	B	380	MGM	C6-C5-N3-C4
6	D	380	MGM	C6-C5-N3-C4
6	F	381	MGM	C6-C5-N3-C4
6	H	380	MGM	C6-C5-N3-C4
6	J	379	MGM	C6-C5-N3-C4
6	L	380	MGM	C6-C5-N3-C4
5	F	380	MES	C7-C8-S-O1S
5	B	379	MES	N4-C7-C8-S
6	B	380	MGM	C10-C8-C9-C11
6	D	380	MGM	C10-C8-C9-C11
6	H	380	MGM	C10-C8-C9-C11
6	J	379	MGM	C10-C8-C9-C11
6	L	380	MGM	C10-C8-C9-C11
6	F	381	MGM	C10-C8-C9-C11
6	B	380	MGM	C7-C8-C9-C11
6	H	380	MGM	C7-C8-C9-C11
6	D	380	MGM	C7-C8-C9-C11
6	F	381	MGM	C7-C8-C9-C11
6	J	379	MGM	C7-C8-C9-C11
6	L	380	MGM	C7-C8-C9-C11
6	F	381	MGM	PA-O3A-PB-O3B
6	J	379	MGM	PA-O3A-PB-O3B
6	B	380	MGM	PA-O3A-PB-O2B
6	D	380	MGM	PA-O3A-PB-O2B
6	F	381	MGM	PA-O3A-PB-O2B
6	H	380	MGM	PA-O3A-PB-O2B
6	J	379	MGM	PA-O3A-PB-O2B
6	L	380	MGM	PA-O3A-PB-O2B
6	B	380	MGM	C14-C13-C15-C16
6	H	380	MGM	C14-C13-C15-C16
6	J	379	MGM	C9-C11-C12-C13

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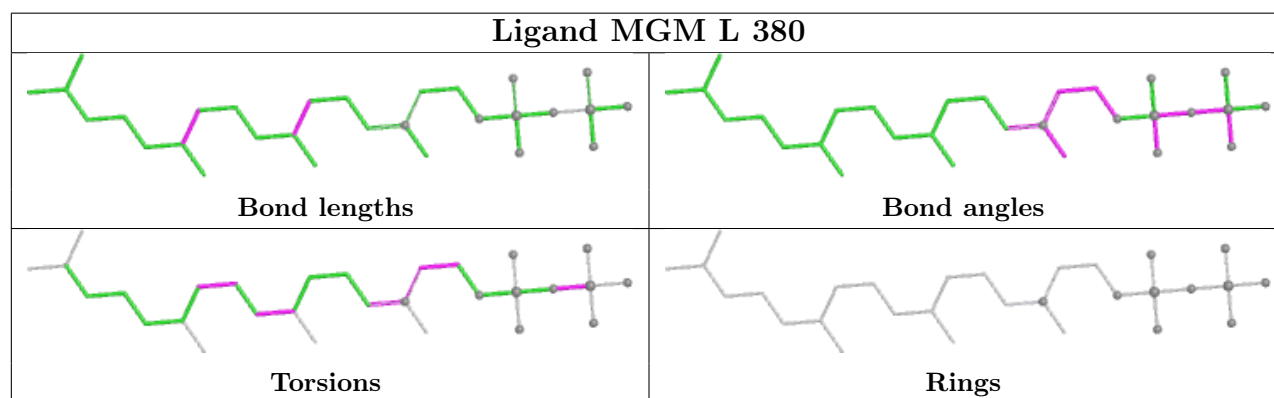
Mol	Chain	Res	Type	Atoms
6	B	380	MGM	C9-C11-C12-C13
6	F	381	MGM	C9-C11-C12-C13
6	H	380	MGM	C9-C11-C12-C13
6	L	380	MGM	C9-C11-C12-C13
6	D	380	MGM	C14-C13-C15-C16
6	D	380	MGM	C9-C11-C12-C13
6	D	380	MGM	C6-C5-N3-C2
6	F	381	MGM	C6-C5-N3-C2
6	J	379	MGM	C6-C5-N3-C2
6	L	380	MGM	C6-C5-N3-C2

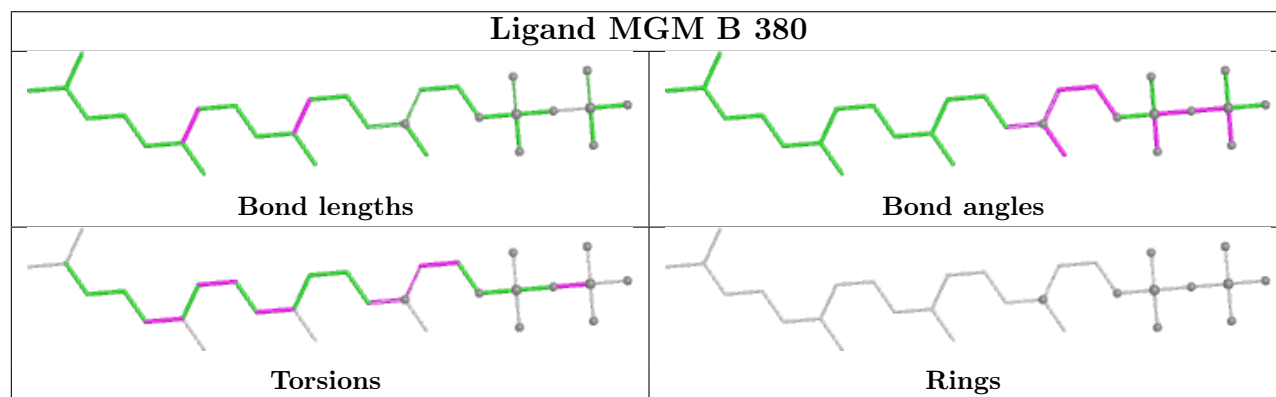
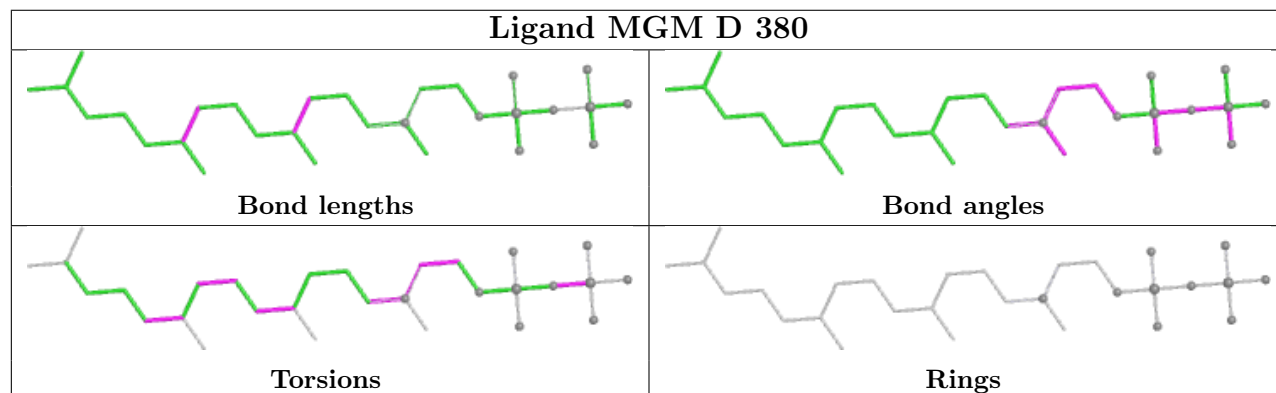
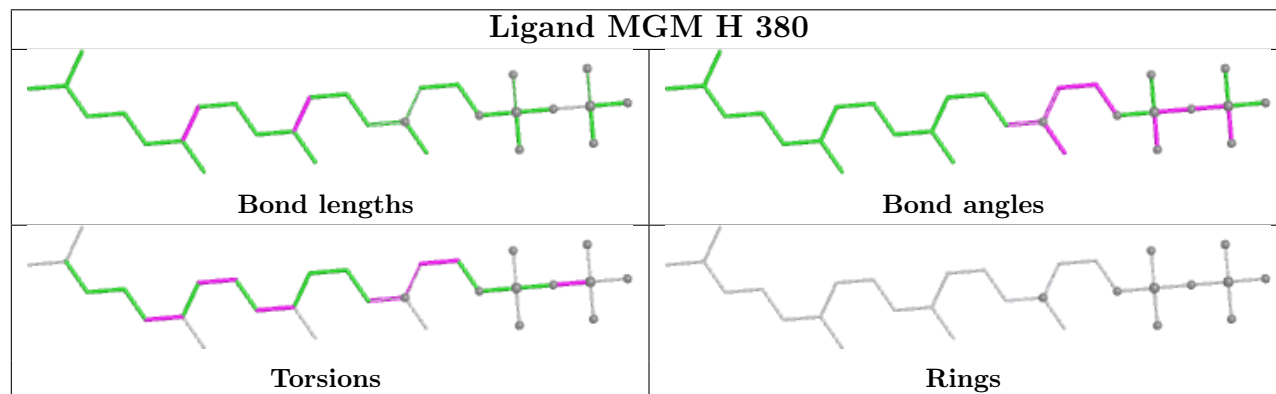
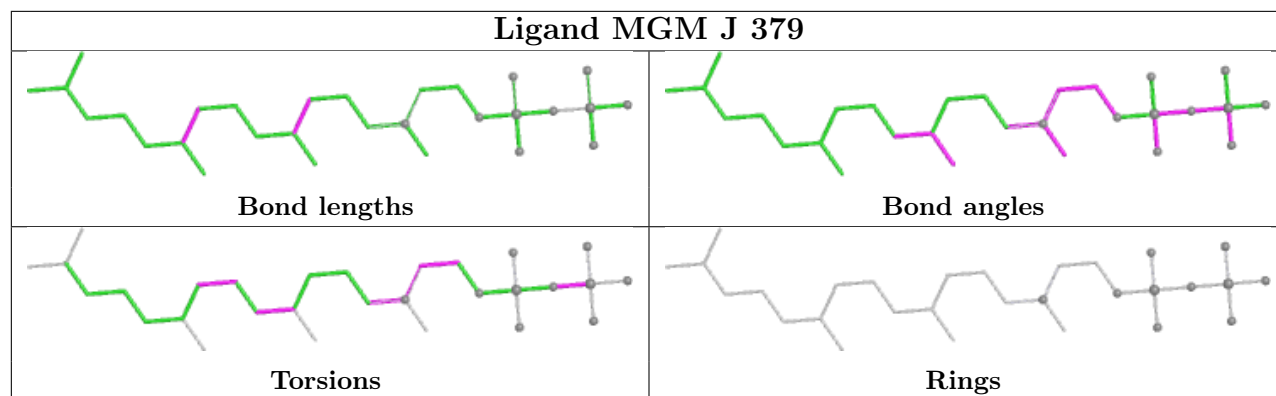
There are no ring outliers.

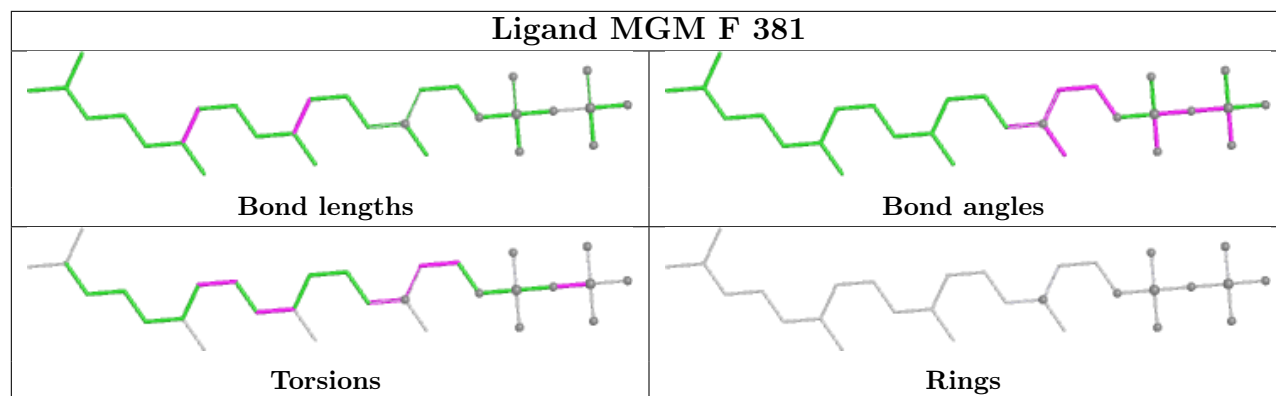
2 monomers are involved in 2 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	314/377 (83%)	0.37	20 (6%)	25	22	47, 69, 102, 119	0
1	C	314/377 (83%)	0.36	15 (4%)	35	32	44, 66, 94, 111	0
1	E	314/377 (83%)	0.39	16 (5%)	33	29	42, 67, 96, 113	0
1	G	314/377 (83%)	0.39	22 (7%)	22	19	43, 65, 96, 109	0
1	I	314/377 (83%)	0.45	14 (4%)	38	34	43, 68, 98, 109	0
1	K	314/377 (83%)	-0.06	13 (4%)	41	37	35, 55, 80, 94	0
2	B	346/377 (91%)	0.12	16 (4%)	37	34	48, 63, 89, 112	0
2	D	346/377 (91%)	0.01	14 (4%)	42	38	43, 59, 86, 103	0
2	F	346/377 (91%)	-0.06	10 (2%)	53	50	42, 56, 84, 108	0
2	H	346/377 (91%)	0.49	30 (8%)	16	13	44, 72, 102, 119	0
2	J	346/377 (91%)	0.21	15 (4%)	40	36	45, 65, 92, 117	0
2	L	346/377 (91%)	-0.14	10 (2%)	53	50	39, 53, 77, 106	0
3	M	6/11 (54%)	0.71	1 (16%)	4	3	53, 57, 78, 88	0
3	N	6/11 (54%)	0.45	1 (16%)	4	3	53, 59, 78, 83	0
3	O	6/11 (54%)	0.89	1 (16%)	4	3	50, 58, 77, 85	0
3	P	6/11 (54%)	1.07	1 (16%)	4	3	60, 69, 86, 92	0
3	Q	6/11 (54%)	0.97	1 (16%)	4	3	51, 63, 82, 91	0
3	R	6/11 (54%)	0.37	1 (16%)	4	3	47, 58, 76, 84	0
All	All	3996/4590 (87%)	0.21	201 (5%)	34	30	35, 63, 93, 119	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	LEU	7.0
1	E	55	PHE	6.7
2	F	18	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	55	PHE	6.2
1	G	55	PHE	6.1
2	J	363	THR	5.8
3	P	6	THR	5.6
2	L	363	THR	5.5
1	I	55	PHE	5.2
3	O	6	THR	5.1
2	J	110	ASN	5.0
2	H	18	LEU	5.0
2	B	363	THR	5.0
2	B	110	ASN	4.8
2	D	18	LEU	4.7
2	L	18	LEU	4.7
3	Q	6	THR	4.6
2	D	363	THR	4.5
2	F	110	ASN	4.5
3	M	6	THR	4.4
2	H	362	LYS	4.4
2	H	113	THR	4.4
1	A	331	GLU	4.4
1	K	55	PHE	4.3
2	H	363	THR	4.3
2	F	111	PRO	4.3
1	A	354	GLU	4.2
1	A	55	PHE	4.1
1	I	368	SER	4.1
3	N	6	THR	4.1
1	C	368	SER	4.1
2	D	359	GLN	4.0
1	E	332	ASP	4.0
2	J	18	LEU	4.0
3	R	6	THR	4.0
2	F	363	THR	3.9
1	I	364	GLN	3.9
1	I	327	CYS	3.8
2	H	359	GLN	3.8
1	G	57	SER	3.8
1	G	368	SER	3.8
1	E	56	LEU	3.7
2	H	85	GLU	3.7
1	C	328	ASP	3.7
2	J	111	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	326	GLN	3.6
2	B	113	THR	3.5
1	I	326	GLN	3.5
1	G	56	LEU	3.5
2	L	111	PRO	3.4
1	G	62	THR	3.4
2	J	362	LYS	3.3
1	C	62	THR	3.3
1	G	328	ASP	3.3
1	E	368	SER	3.2
1	C	57	SER	3.2
2	F	359	GLN	3.2
1	C	59	ASP	3.1
2	D	362	LYS	3.1
1	G	60	SER	3.1
2	B	111	PRO	3.0
2	B	362	LYS	3.0
2	D	109	LYS	3.0
2	H	39	ARG	3.0
1	A	327	CYS	3.0
1	A	326	GLN	3.0
2	J	91	ASP	3.0
1	C	251	SER	3.0
2	J	89	ASN	3.0
2	H	65	ASP	3.0
2	J	113	THR	3.0
2	H	110	ASN	3.0
1	G	61	PRO	2.9
2	H	335	SER	2.9
1	K	56	LEU	2.9
1	I	354	GLU	2.9
2	L	85	GLU	2.9
1	G	364	GLN	2.9
1	K	326	GLN	2.9
2	F	40	TYR	2.9
2	H	40	TYR	2.9
2	H	35	VAL	2.9
2	D	39	ARG	2.9
1	K	332	ASP	2.9
2	H	91	ASP	2.9
2	D	305	LEU	2.8
2	L	114	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	85	GLU	2.8
2	B	315	SER	2.8
1	E	294	ASN	2.8
1	K	368	SER	2.7
2	L	362	LYS	2.7
2	J	108	SER	2.7
1	G	304	PRO	2.7
2	H	305	LEU	2.7
1	K	59	ASP	2.7
2	H	112	GLY	2.6
2	J	114	ALA	2.6
1	A	332	ASP	2.6
2	D	314	ASP	2.6
2	H	70	ASP	2.6
1	A	142	ARG	2.6
1	C	60	SER	2.6
2	D	360	SER	2.6
2	B	359	GLN	2.6
1	I	328	ASP	2.6
1	A	217	ASP	2.6
2	J	315	SER	2.5
2	L	314	ASP	2.5
2	H	304	ARG	2.5
1	A	195	GLN	2.5
2	H	338	CYS	2.5
1	E	331	GLU	2.5
1	A	368	SER	2.5
2	B	305	LEU	2.5
2	D	315	SER	2.5
1	C	331	GLU	2.5
1	G	125	GLU	2.5
2	D	85	GLU	2.5
1	I	225	GLN	2.5
1	I	332	ASP	2.4
2	L	113	THR	2.4
1	A	305	SER	2.4
1	G	59	ASP	2.4
1	A	330	LYS	2.4
1	A	364	GLN	2.4
2	H	109	LYS	2.4
1	G	92	TYR	2.4
2	F	113	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	125	GLU	2.4
2	H	237	GLU	2.4
1	K	217	ASP	2.4
1	G	84	PRO	2.4
2	D	40	TYR	2.3
2	H	316	HIS	2.3
1	E	217	ASP	2.3
2	B	65	ASP	2.3
2	H	71	ASP	2.3
1	A	304	PRO	2.3
1	C	304	PRO	2.3
1	I	304	PRO	2.3
2	B	37	PRO	2.3
1	G	87	VAL	2.3
1	G	58	LEU	2.3
1	E	328	ASP	2.3
1	I	143	SER	2.3
2	B	85	GLU	2.3
2	B	292	GLU	2.3
2	F	85	GLU	2.3
2	D	37	PRO	2.3
1	E	195	GLN	2.3
1	E	326	GLN	2.3
2	F	362	LYS	2.2
2	H	292	GLU	2.2
1	C	81	ASN	2.2
1	K	81	ASN	2.2
2	L	359	GLN	2.2
1	A	177	GLU	2.2
1	E	265	GLU	2.2
2	B	40	TYR	2.2
2	J	35	VAL	2.2
2	H	111	PRO	2.2
1	C	217	ASP	2.2
1	C	332	ASP	2.2
1	E	288	GLY	2.2
2	H	144	LYS	2.2
2	F	305	LEU	2.2
1	G	335	ASN	2.1
1	I	288	GLY	2.1
2	B	112	GLY	2.1
1	E	71	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	304	PRO	2.1
2	J	109	LYS	2.1
1	A	300	LEU	2.1
1	I	59	ASP	2.1
1	G	85	SER	2.1
1	K	85	SER	2.1
2	H	315	SER	2.1
1	G	161	GLU	2.1
1	K	331	GLU	2.1
1	C	329	ASN	2.1
1	K	91	ILE	2.1
2	L	103	ILE	2.1
1	A	328	ASP	2.1
1	G	86	PRO	2.1
2	D	35	VAL	2.1
2	H	105	PHE	2.1
2	J	355	ARG	2.0
2	H	360	SER	2.0
1	K	62	THR	2.0
1	E	211	GLN	2.0
1	C	75	ILE	2.0
1	E	327	CYS	2.0
2	H	27	ARG	2.0
1	A	301	ASP	2.0
1	E	59	ASP	2.0
1	A	268	LYS	2.0
2	H	108	SER	2.0
1	A	288	GLY	2.0
2	B	106	ASN	2.0
1	G	64	VAL	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

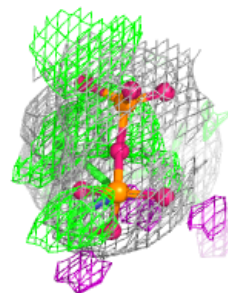
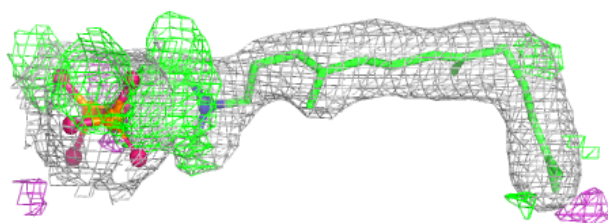
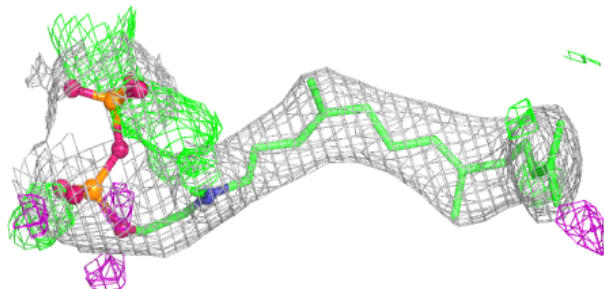
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MES	B	379	12/12	0.86	0.20	99,108,110,110	0
5	MES	F	380	12/12	0.93	0.15	86,94,97,97	0
6	MGM	J	379	29/29	0.94	0.13	50,58,70,71	0
6	MGM	L	380	29/29	0.94	0.13	41,54,65,67	0
6	MGM	H	380	29/29	0.95	0.13	56,65,74,75	0
6	MGM	D	380	29/29	0.95	0.12	50,59,67,69	0
6	MGM	F	381	29/29	0.95	0.11	49,56,66,69	0
6	MGM	B	380	29/29	0.96	0.11	52,59,69,72	0
7	CL	F	379	1/1	0.98	0.04	55,55,55,55	0
7	CL	H	379	1/1	0.98	0.06	69,69,69,69	0
7	CL	L	379	1/1	0.98	0.06	59,59,59,59	0
7	CL	D	379	1/1	0.99	0.06	62,62,62,62	0
4	ZN	B	378	1/1	1.00	0.01	51,51,51,51	0
4	ZN	D	378	1/1	1.00	0.01	53,53,53,53	0
4	ZN	F	378	1/1	1.00	0.01	48,48,48,48	0
4	ZN	H	378	1/1	1.00	0.01	60,60,60,60	0
4	ZN	J	378	1/1	1.00	0.01	53,53,53,53	0
4	ZN	L	378	1/1	1.00	0.01	46,46,46,46	0

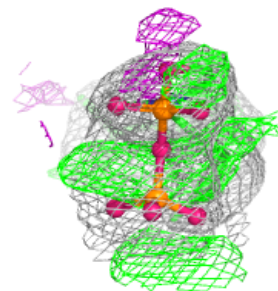
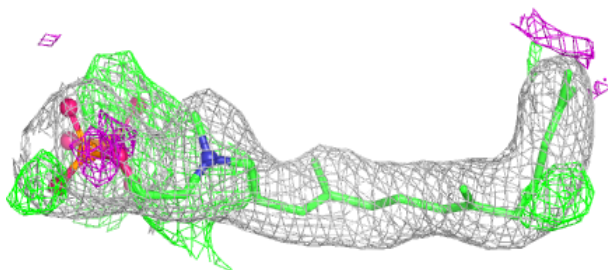
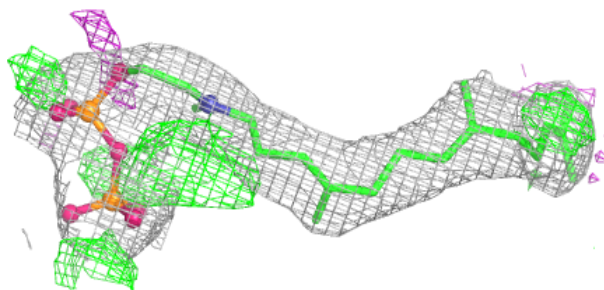
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

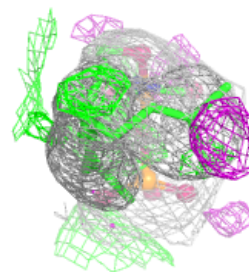
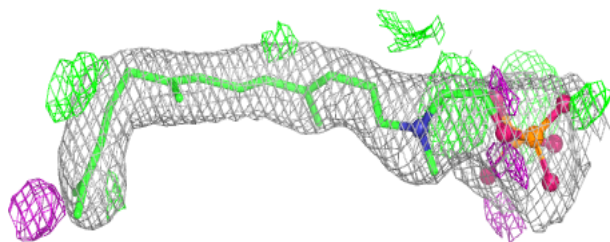
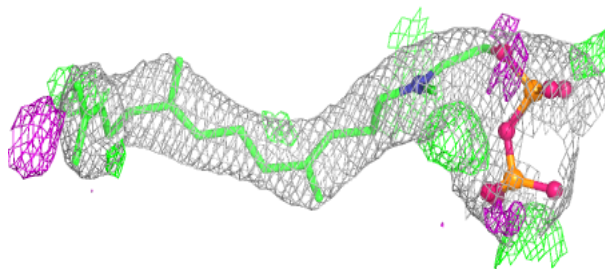
**Electron density around MGM L 380:**

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

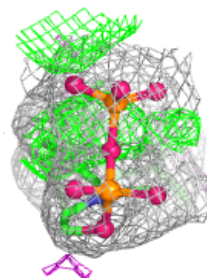
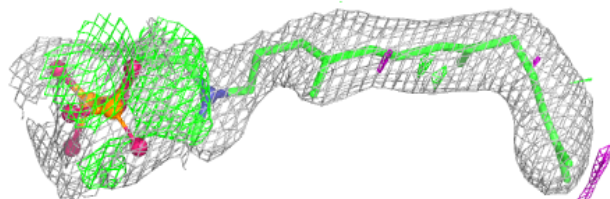
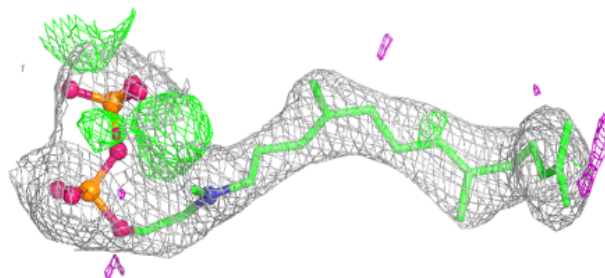


Electron density around MGM H 380:

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

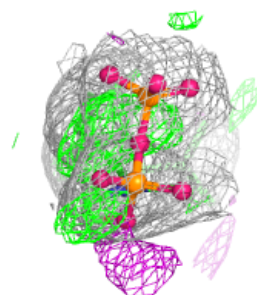
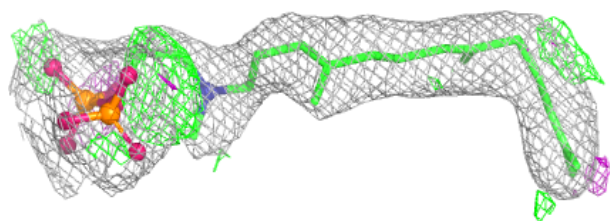
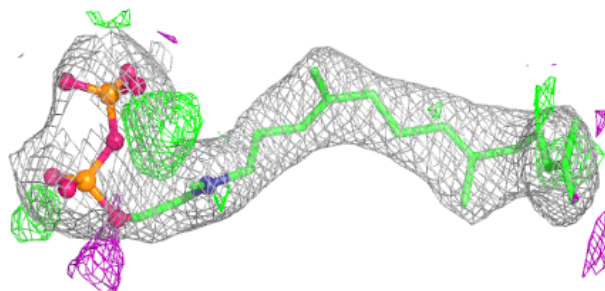
**Electron density around MGM D 380:**

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

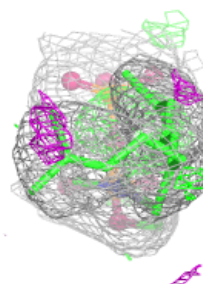
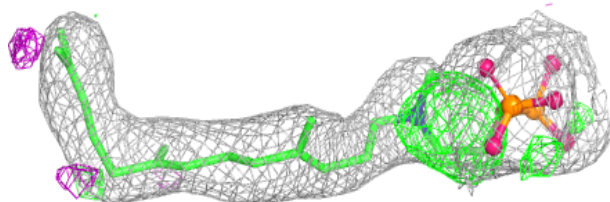
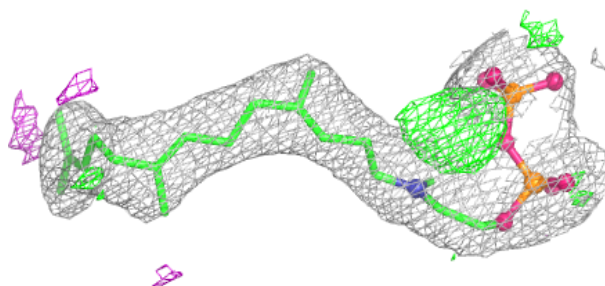


Electron density around MGM F 381:

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

**Electron density around MGM B 380:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.