



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:38 PM UTC

PDB ID : 4TNV / pdb_00004tnv
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab in a non-conducting conformation
Authors : Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.
Deposited on : 2014-06-05
Resolution : 3.60 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

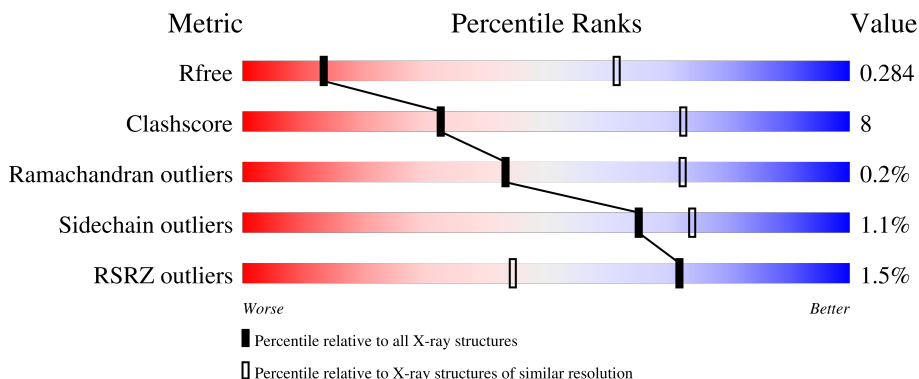
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	347	 2% 75% 22% •
1	B	347	 3% 74% 23% •
1	C	347	 % 75% 22% •
1	D	347	 2% 73% 24% •
1	E	347	 2% 75% 22% •

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Mol	Chain	Length	Quality of chain
1	P	347	
1	Q	347	
1	R	347	
1	S	347	
1	T	347	
2	F	224	
2	G	224	
2	H	224	
2	I	224	
2	J	224	
2	U	224	
2	V	224	
2	W	224	
2	X	224	
2	Y	224	
3	K	215	
3	L	215	
3	M	215	
3	N	215	
3	O	215	
3	Z	215	
3	f	215	
3	g	215	
3	h	215	
3	i	215	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 60408 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 Avermectin-sensitive glutamate-gated chloride channel GluCl alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	B	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	C	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	D	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	E	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	P	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	Q	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	R	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	S	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			
1	T	337	Total	C	N	O	S	0	0	0
			2695	1755	438	487	15			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	linker	UNP G5EBR3
A	304	GLY	-	linker	UNP G5EBR3
A	305	THR	-	linker	UNP G5EBR3
A	340	HIS	-	expression tag	UNP G5EBR3
A	341	HIS	-	expression tag	UNP G5EBR3
A	342	HIS	-	expression tag	UNP G5EBR3
A	343	HIS	-	expression tag	UNP G5EBR3
A	344	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	345	HIS	-	expression tag	UNP G5EBR3
A	346	HIS	-	expression tag	UNP G5EBR3
A	347	HIS	-	expression tag	UNP G5EBR3
B	303	ALA	-	linker	UNP G5EBR3
B	304	GLY	-	linker	UNP G5EBR3
B	305	THR	-	linker	UNP G5EBR3
B	340	HIS	-	expression tag	UNP G5EBR3
B	341	HIS	-	expression tag	UNP G5EBR3
B	342	HIS	-	expression tag	UNP G5EBR3
B	343	HIS	-	expression tag	UNP G5EBR3
B	344	HIS	-	expression tag	UNP G5EBR3
B	345	HIS	-	expression tag	UNP G5EBR3
B	346	HIS	-	expression tag	UNP G5EBR3
B	347	HIS	-	expression tag	UNP G5EBR3
C	303	ALA	-	linker	UNP G5EBR3
C	304	GLY	-	linker	UNP G5EBR3
C	305	THR	-	linker	UNP G5EBR3
C	340	HIS	-	expression tag	UNP G5EBR3
C	341	HIS	-	expression tag	UNP G5EBR3
C	342	HIS	-	expression tag	UNP G5EBR3
C	343	HIS	-	expression tag	UNP G5EBR3
C	344	HIS	-	expression tag	UNP G5EBR3
C	345	HIS	-	expression tag	UNP G5EBR3
C	346	HIS	-	expression tag	UNP G5EBR3
C	347	HIS	-	expression tag	UNP G5EBR3
D	303	ALA	-	linker	UNP G5EBR3
D	304	GLY	-	linker	UNP G5EBR3
D	305	THR	-	linker	UNP G5EBR3
D	340	HIS	-	expression tag	UNP G5EBR3
D	341	HIS	-	expression tag	UNP G5EBR3
D	342	HIS	-	expression tag	UNP G5EBR3
D	343	HIS	-	expression tag	UNP G5EBR3
D	344	HIS	-	expression tag	UNP G5EBR3
D	345	HIS	-	expression tag	UNP G5EBR3
D	346	HIS	-	expression tag	UNP G5EBR3
D	347	HIS	-	expression tag	UNP G5EBR3
E	303	ALA	-	linker	UNP G5EBR3
E	304	GLY	-	linker	UNP G5EBR3
E	305	THR	-	linker	UNP G5EBR3
E	340	HIS	-	expression tag	UNP G5EBR3
E	341	HIS	-	expression tag	UNP G5EBR3
E	342	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	expression tag	UNP G5EBR3
E	344	HIS	-	expression tag	UNP G5EBR3
E	345	HIS	-	expression tag	UNP G5EBR3
E	346	HIS	-	expression tag	UNP G5EBR3
E	347	HIS	-	expression tag	UNP G5EBR3
P	303	ALA	-	linker	UNP G5EBR3
P	304	GLY	-	linker	UNP G5EBR3
P	305	THR	-	linker	UNP G5EBR3
P	340	HIS	-	expression tag	UNP G5EBR3
P	341	HIS	-	expression tag	UNP G5EBR3
P	342	HIS	-	expression tag	UNP G5EBR3
P	343	HIS	-	expression tag	UNP G5EBR3
P	344	HIS	-	expression tag	UNP G5EBR3
P	345	HIS	-	expression tag	UNP G5EBR3
P	346	HIS	-	expression tag	UNP G5EBR3
P	347	HIS	-	expression tag	UNP G5EBR3
Q	303	ALA	-	linker	UNP G5EBR3
Q	304	GLY	-	linker	UNP G5EBR3
Q	305	THR	-	linker	UNP G5EBR3
Q	340	HIS	-	expression tag	UNP G5EBR3
Q	341	HIS	-	expression tag	UNP G5EBR3
Q	342	HIS	-	expression tag	UNP G5EBR3
Q	343	HIS	-	expression tag	UNP G5EBR3
Q	344	HIS	-	expression tag	UNP G5EBR3
Q	345	HIS	-	expression tag	UNP G5EBR3
Q	346	HIS	-	expression tag	UNP G5EBR3
Q	347	HIS	-	expression tag	UNP G5EBR3
R	303	ALA	-	linker	UNP G5EBR3
R	304	GLY	-	linker	UNP G5EBR3
R	305	THR	-	linker	UNP G5EBR3
R	340	HIS	-	expression tag	UNP G5EBR3
R	341	HIS	-	expression tag	UNP G5EBR3
R	342	HIS	-	expression tag	UNP G5EBR3
R	343	HIS	-	expression tag	UNP G5EBR3
R	344	HIS	-	expression tag	UNP G5EBR3
R	345	HIS	-	expression tag	UNP G5EBR3
R	346	HIS	-	expression tag	UNP G5EBR3
R	347	HIS	-	expression tag	UNP G5EBR3
S	303	ALA	-	linker	UNP G5EBR3
S	304	GLY	-	linker	UNP G5EBR3
S	305	THR	-	linker	UNP G5EBR3
S	340	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
S	341	HIS	-	expression tag	UNP G5EBR3
S	342	HIS	-	expression tag	UNP G5EBR3
S	343	HIS	-	expression tag	UNP G5EBR3
S	344	HIS	-	expression tag	UNP G5EBR3
S	345	HIS	-	expression tag	UNP G5EBR3
S	346	HIS	-	expression tag	UNP G5EBR3
S	347	HIS	-	expression tag	UNP G5EBR3
T	303	ALA	-	linker	UNP G5EBR3
T	304	GLY	-	linker	UNP G5EBR3
T	305	THR	-	linker	UNP G5EBR3
T	340	HIS	-	expression tag	UNP G5EBR3
T	341	HIS	-	expression tag	UNP G5EBR3
T	342	HIS	-	expression tag	UNP G5EBR3
T	343	HIS	-	expression tag	UNP G5EBR3
T	344	HIS	-	expression tag	UNP G5EBR3
T	345	HIS	-	expression tag	UNP G5EBR3
T	346	HIS	-	expression tag	UNP G5EBR3
T	347	HIS	-	expression tag	UNP G5EBR3

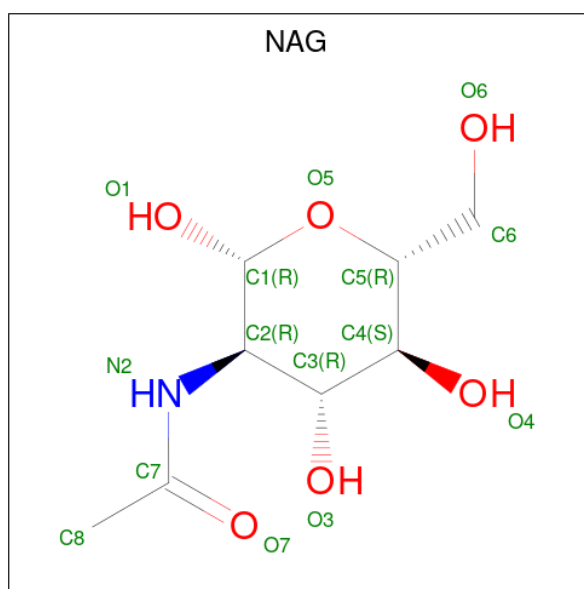
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			
2	G	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	H	223	Total	C	N	O	S	0	0	0
			1701	1077	278	338	8			
2	U	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	V	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	W	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	X	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	Y	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	J	223	Total	C	N	O	S	0	0	0
			1701	1077	278	338	8			
2	I	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			

- Molecule 3 is a protein called Mouse monoclonal Fab fragment, light chain.

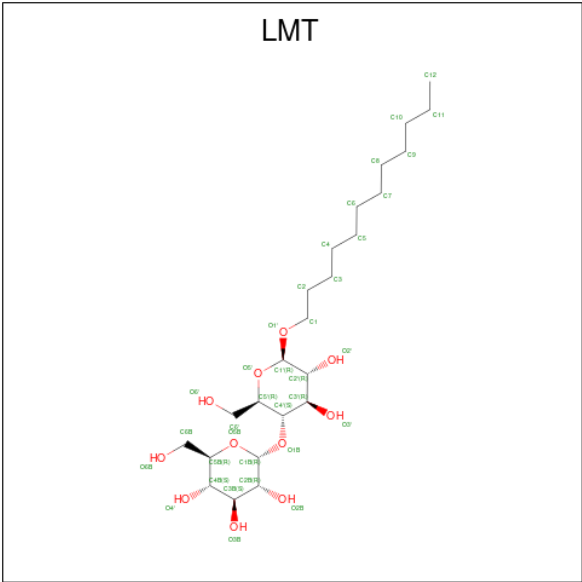
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	212	Total	C	N	O	S	0	0	0
			1606	1008	271	321	6			
3	L	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	N	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	O	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	Z	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	7			
3	f	214	Total	C	N	O	S	0	0	0
			1620	1015	273	325	7			
3	g	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	h	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	i	214	Total	C	N	O	S	0	0	0
			1620	1015	273	325	7			
3	M	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	R	1	Total	C	N	O	0	0
			14	8	1	5		
4	S	1	Total	C	N	O	0	0
			14	8	1	5		
4	T	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



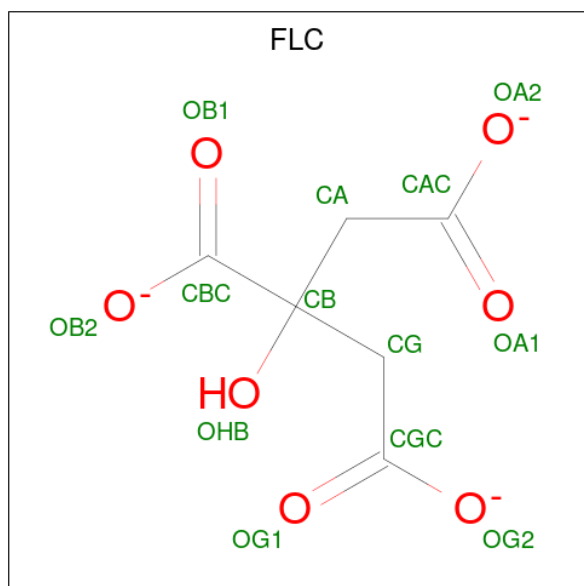
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	12	11		
5	B	1	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			23	12	11		
5	D	1	Total	C	O	0	0
			23	12	11		
5	E	1	Total	C	O	0	0
			23	12	11		
5	P	1	Total	C	O	0	0
			23	12	11		
5	Q	1	Total	C	O	0	0
			23	12	11		
5	R	1	Total	C	O	0	0
			23	12	11		
5	S	1	Total	C	O	0	0
			23	12	11		
5	T	1	Total	C	O	0	0
			25	14	11		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	6	7		
6	T	1	Total	C	O	0	0
			13	6	7		

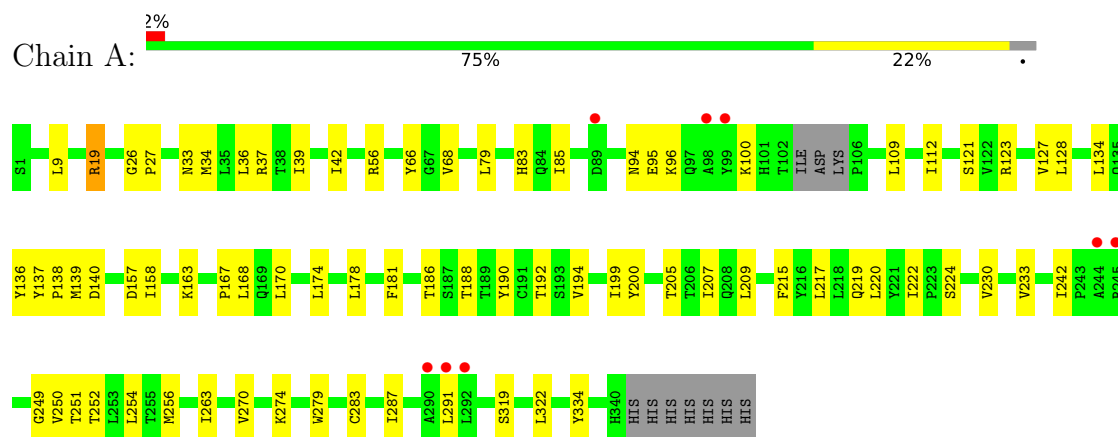
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	2	Total	Cl	0	0
			2	2		

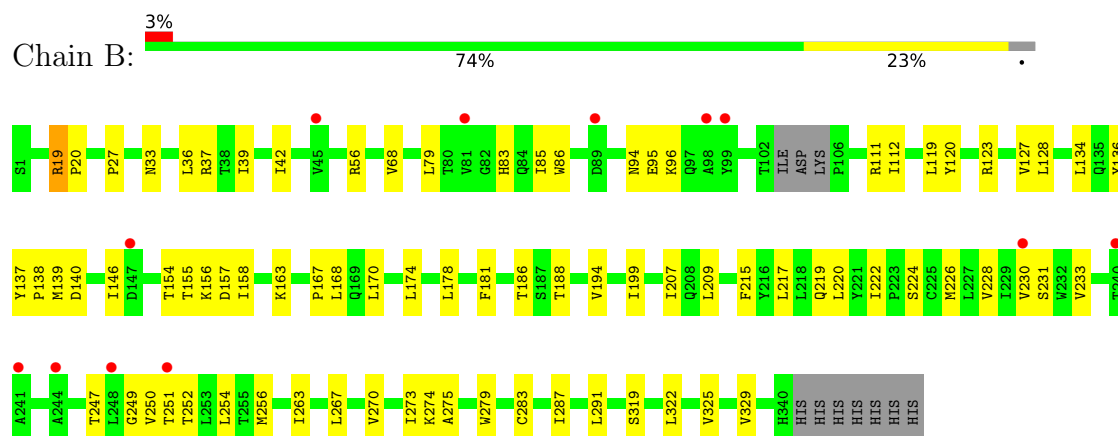
3 Residue-property plots

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.

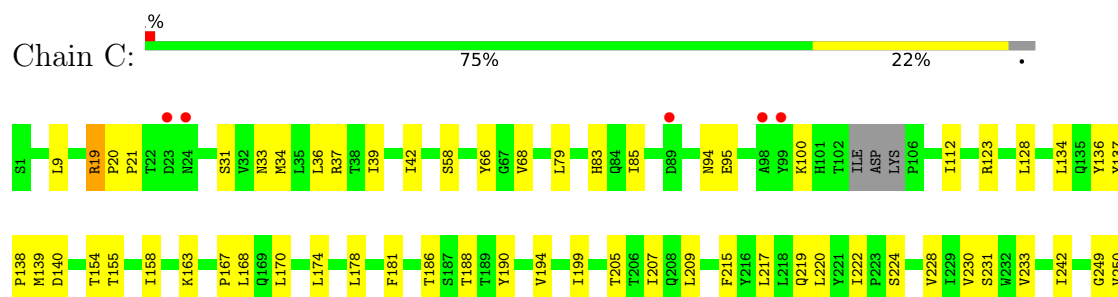
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

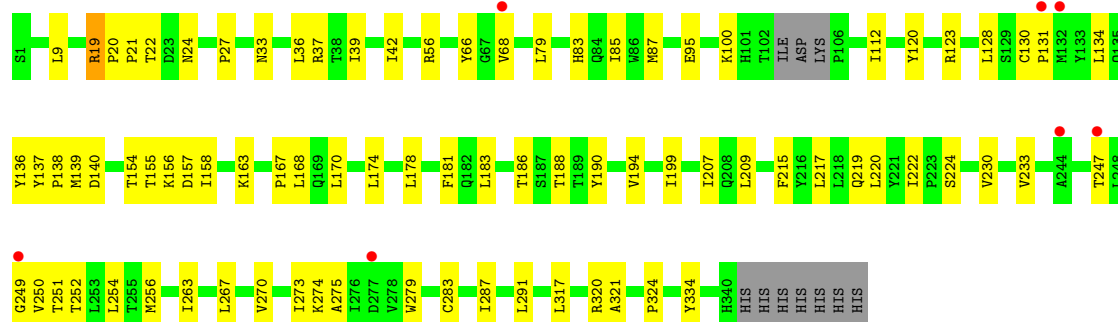
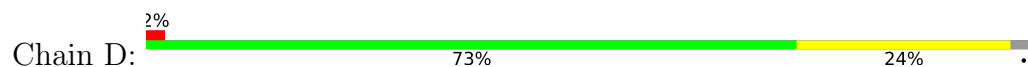


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

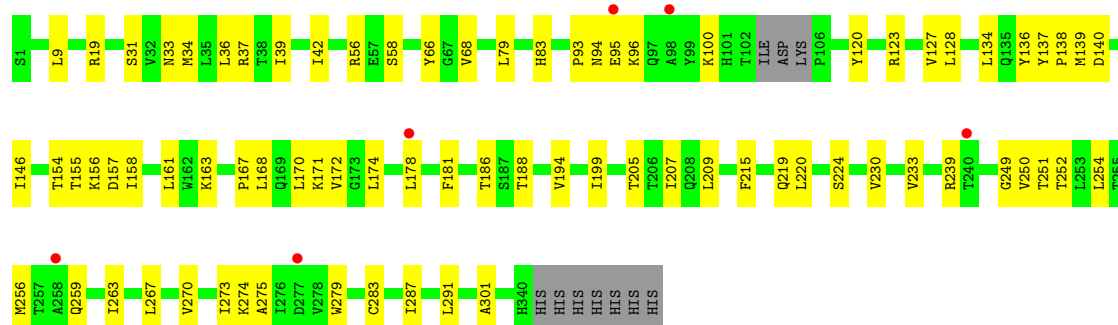




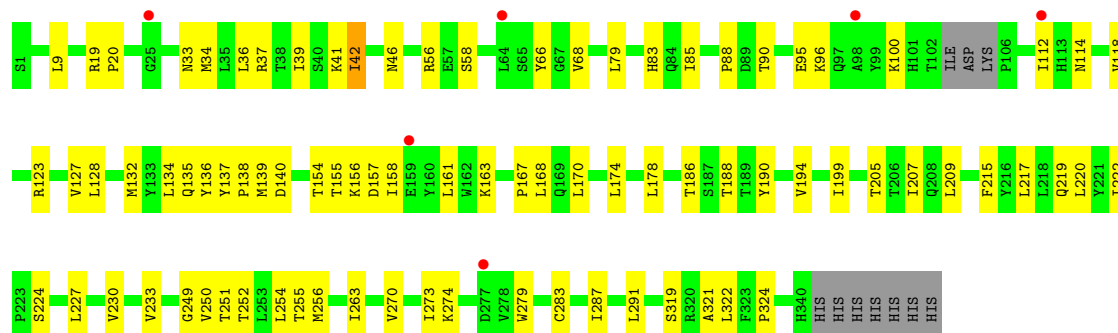
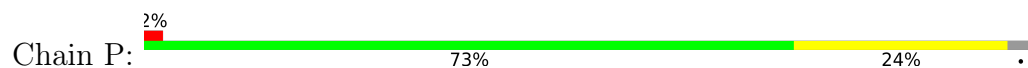
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



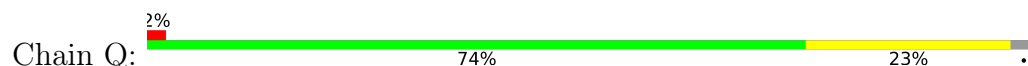
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

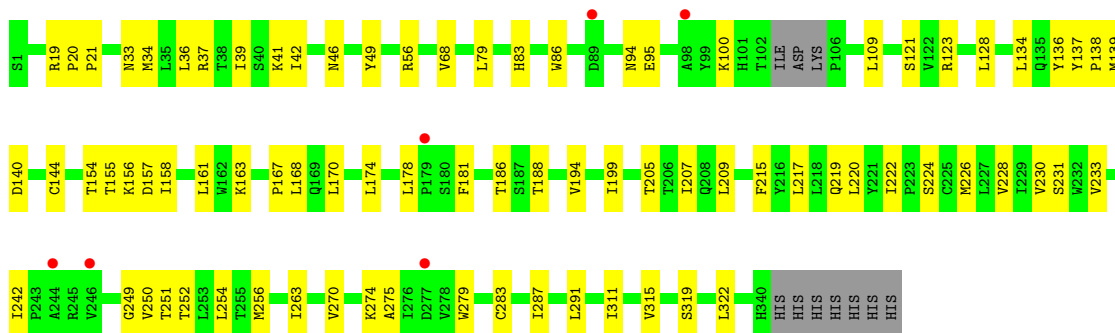


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

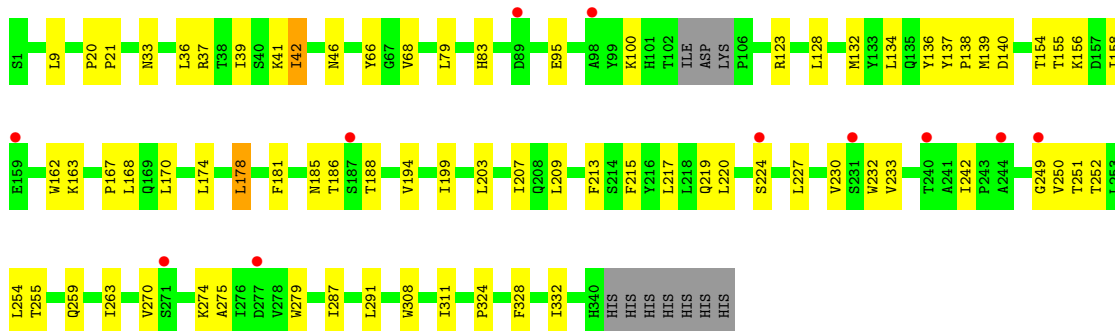
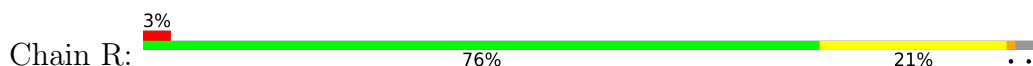


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

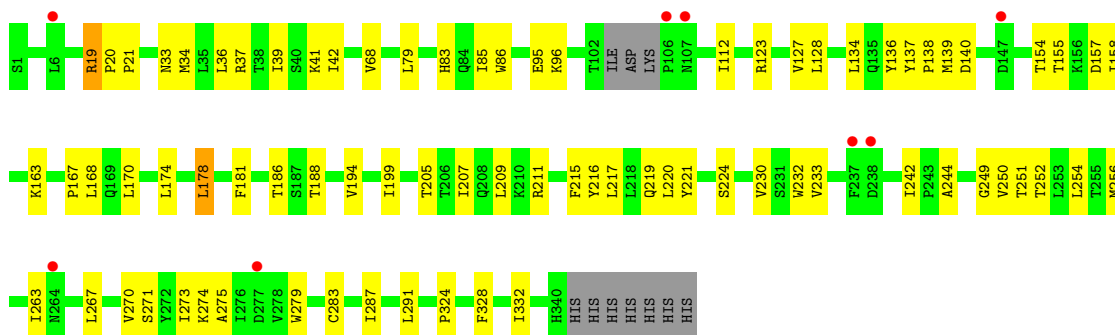
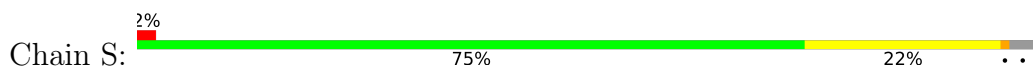




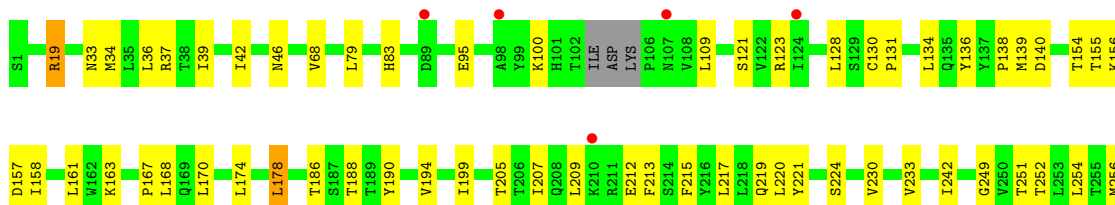
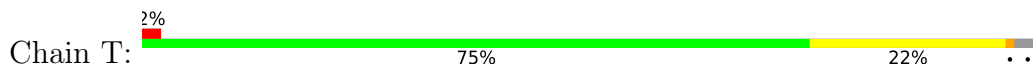
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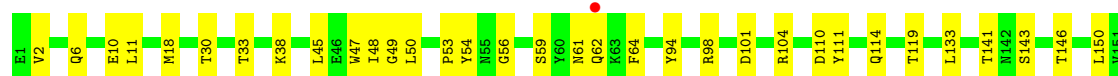
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha





- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F: 78% 21%



- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain G: 83% 17%



- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain H: 75% 24%



- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain U: 80% 19%

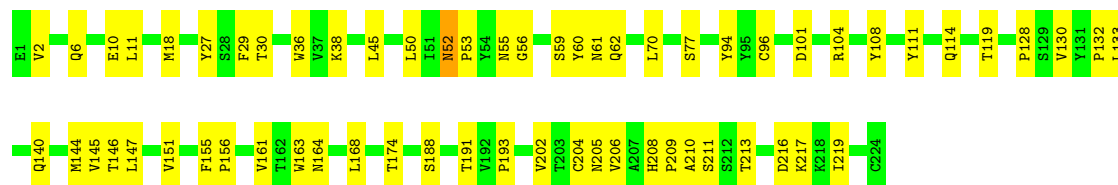


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

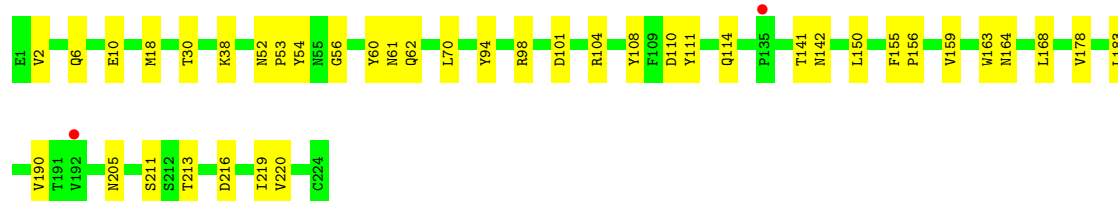
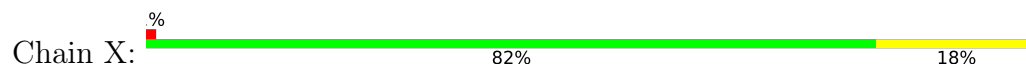
Chain V: 81% 19%



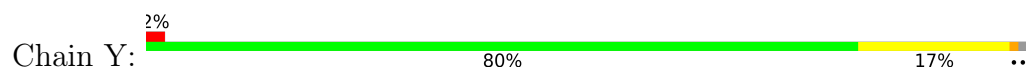
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



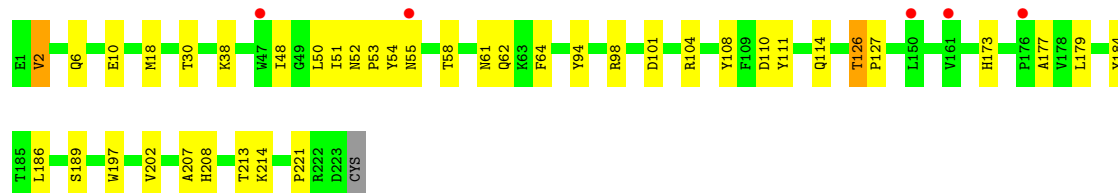
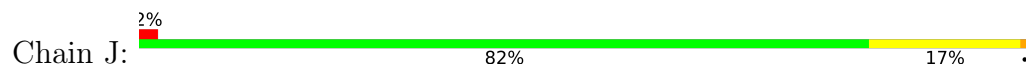
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



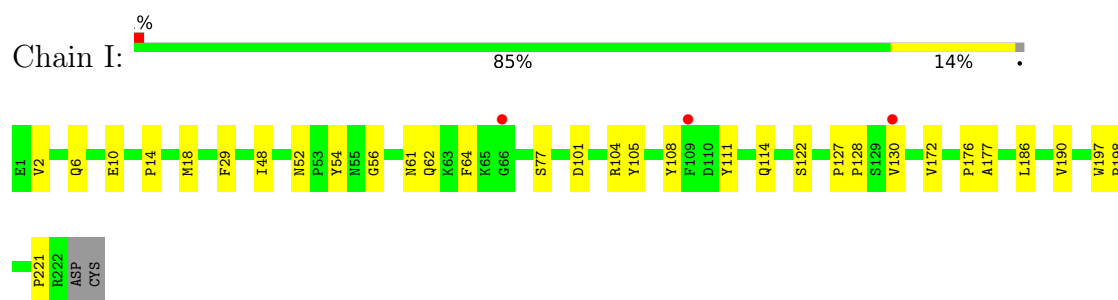
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



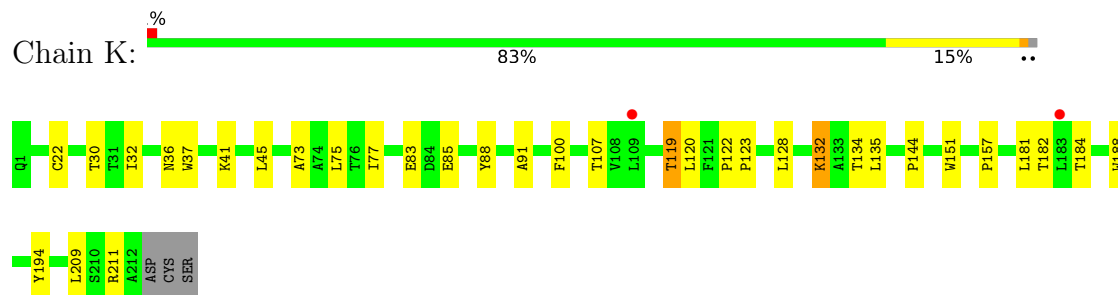
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



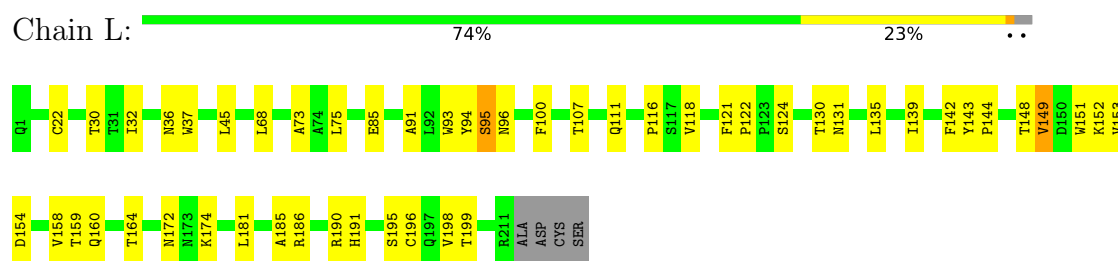
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



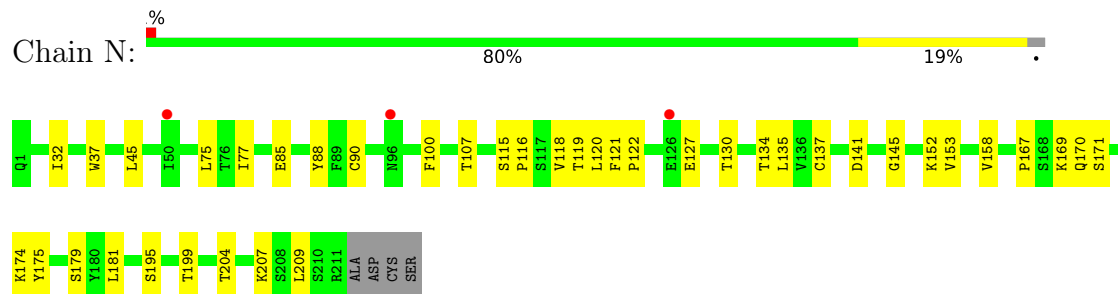
- Molecule 3: Mouse monoclonal Fab fragment, light chain



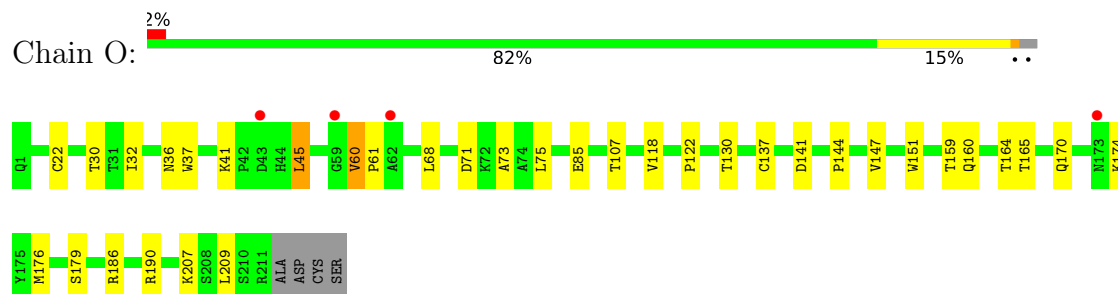
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



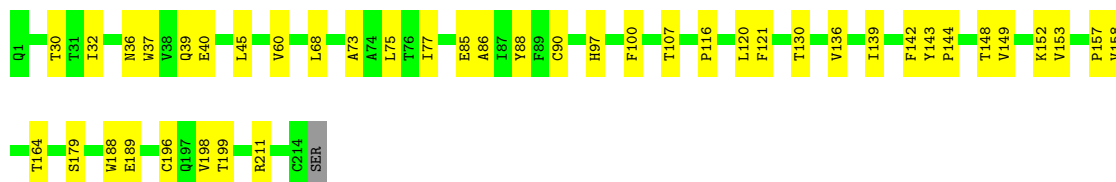
- Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain Z:  88% 11% .



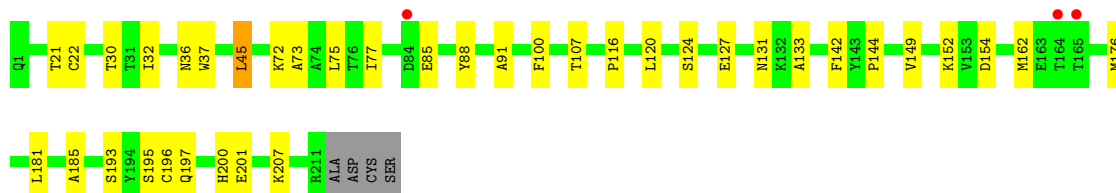
- Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain f:  80% 20%



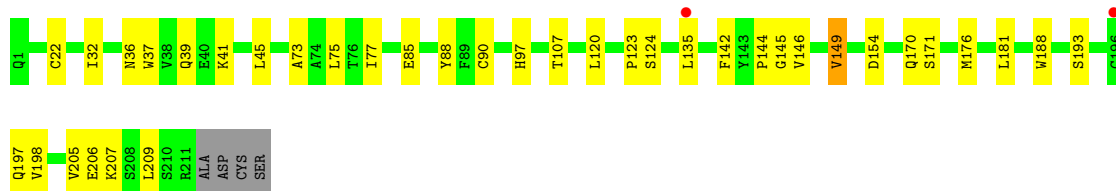
- Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain g:  80% 17% .



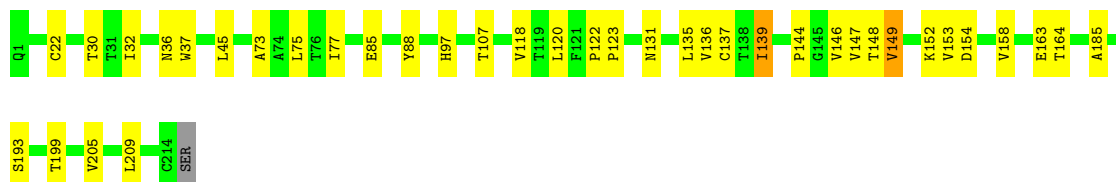
- Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain h:  81% 17% .

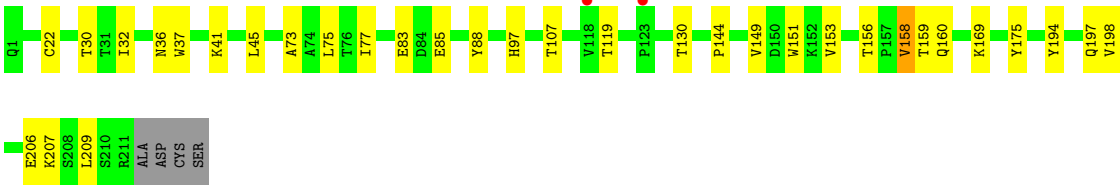
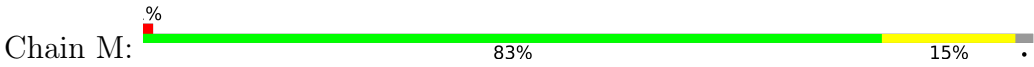


- Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain i:  82% 17% .



- Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	455.81Å 195.68Å 196.18Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	58.44 – 3.60 58.44 – 3.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (58.44-3.60) 88.3 (58.44-3.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.261 , 0.283 0.264 , 0.284	Depositor DCC
R_{free} test set	8783 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	121.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 89.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	60408	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: FLC, CL, NAG, LMT

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	0.37	0/2767	0.76	2/3776 (0.1%)
1	B	0.36	0/2767	0.77	2/3776 (0.1%)
1	C	0.37	0/2767	0.79	2/3776 (0.1%)
1	D	0.36	0/2767	0.79	2/3776 (0.1%)
1	E	0.34	0/2767	0.75	0/3776
1	P	0.38	0/2767	0.78	0/3776
1	Q	0.38	0/2767	0.78	0/3776
1	R	0.39	0/2767	0.80	2/3776 (0.1%)
1	S	0.41	0/2767	0.81	4/3776 (0.1%)
1	T	0.40	0/2767	0.78	4/3776 (0.1%)
2	F	0.31	0/1739	0.79	3/2374 (0.1%)
2	G	0.32	0/1753	0.76	5/2393 (0.2%)
2	H	0.33	0/1747	0.78	1/2385 (0.0%)
2	I	0.31	0/1739	0.75	3/2374 (0.1%)
2	J	0.35	0/1747	0.80	2/2385 (0.1%)
2	U	0.30	0/1728	0.76	1/2360 (0.0%)
2	V	0.31	0/1753	0.76	1/2393 (0.0%)
2	W	0.33	0/1753	0.77	3/2393 (0.1%)
2	X	0.33	0/1753	0.76	3/2393 (0.1%)
2	Y	0.31	0/1728	0.80	5/2360 (0.2%)
3	K	0.32	0/1644	0.75	0/2247
3	L	0.37	0/1639	0.76	1/2240 (0.0%)
3	M	0.33	0/1639	0.77	3/2240 (0.1%)
3	N	0.31	0/1639	0.68	0/2240
3	O	0.31	0/1639	0.72	2/2240 (0.1%)
3	Z	0.33	0/1664	0.73	1/2274 (0.0%)
3	f	0.34	0/1658	0.74	3/2266 (0.1%)
3	g	0.31	0/1639	0.76	0/2240
3	h	0.33	0/1639	0.74	1/2240 (0.0%)
3	i	0.35	0/1658	0.75	1/2266 (0.0%)
All	All	0.35	0/61568	0.77	57/84063 (0.1%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	197	TRP	CA-C-N	-7.31	112.25	119.64
2	F	197	TRP	C-N-CA	-7.31	112.25	119.64
2	J	126	THR	CA-C-N	6.60	124.48	119.66
2	J	126	THR	C-N-CA	6.60	124.48	119.66
1	R	178	LEU	CA-C-N	6.54	125.98	118.85
1	R	178	LEU	C-N-CA	6.54	125.98	118.85
1	T	178	LEU	CA-C-N	6.51	125.95	118.85
1	T	178	LEU	C-N-CA	6.51	125.95	118.85
2	H	56	GLY	N-CA-C	-6.48	106.38	115.32
1	C	19	ARG	CA-C-N	6.46	124.38	119.66
1	C	19	ARG	C-N-CA	6.46	124.38	119.66
3	f	97	HIS	N-CA-C	6.27	118.60	109.07
2	X	56	GLY	N-CA-C	-6.03	107.00	115.32
1	D	19	ARG	CA-C-N	5.99	124.03	119.66
1	D	19	ARG	C-N-CA	5.99	124.03	119.66
3	Z	97	HIS	N-CA-C	5.94	118.10	109.07
2	F	56	GLY	N-CA-C	-5.89	107.19	115.32
2	G	56	GLY	N-CA-C	-5.86	107.24	115.32
1	S	178	LEU	CA-C-N	5.76	127.04	119.84
1	S	178	LEU	C-N-CA	5.76	127.04	119.84
2	I	56	GLY	N-CA-C	-5.76	107.37	115.32
2	G	52	ASN	CA-C-N	5.63	126.00	119.47
2	G	52	ASN	C-N-CA	5.63	126.00	119.47
1	A	19	ARG	CA-C-N	5.62	123.76	119.66
1	A	19	ARG	C-N-CA	5.62	123.76	119.66
2	G	126	THR	CA-C-N	5.52	123.64	119.66
2	G	126	THR	C-N-CA	5.52	123.64	119.66
1	B	19	ARG	CA-C-N	5.49	123.67	119.66
1	B	19	ARG	C-N-CA	5.49	123.67	119.66
2	Y	126	THR	CA-C-N	5.45	123.64	119.66
2	Y	126	THR	C-N-CA	5.45	123.64	119.66
3	i	97	HIS	N-CA-C	5.44	117.34	109.07
2	U	56	GLY	N-CA-C	-5.37	107.91	115.32
3	M	156	THR	CA-C-N	-5.31	114.13	120.13
3	M	156	THR	C-N-CA	-5.31	114.13	120.13
3	O	60	VAL	CA-C-N	5.30	125.29	119.89
3	O	60	VAL	C-N-CA	5.30	125.29	119.89
2	W	56	GLY	N-CA-C	-5.26	108.06	115.32
3	L	93	TRP	N-CA-C	5.25	117.22	107.99
2	Y	52	ASN	CA-C-N	5.24	125.54	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	52	ASN	C-N-CA	5.24	125.54	119.47
2	Y	56	GLY	N-CA-C	-5.19	108.16	115.32
1	S	19	ARG	CA-C-N	5.17	123.43	119.66
1	S	19	ARG	C-N-CA	5.17	123.43	119.66
3	h	97	HIS	N-CA-C	5.14	116.89	109.07
2	I	52	ASN	CA-C-N	5.14	125.44	119.47
2	I	52	ASN	C-N-CA	5.14	125.44	119.47
2	W	52	ASN	CA-C-N	5.11	125.39	119.47
2	W	52	ASN	C-N-CA	5.11	125.39	119.47
3	f	60	VAL	CA-C-N	5.07	125.06	119.89
3	f	60	VAL	C-N-CA	5.07	125.06	119.89
2	V	56	GLY	N-CA-C	-5.05	108.36	115.32
3	M	97	HIS	N-CA-C	5.04	116.73	109.07
1	T	19	ARG	CA-C-N	5.02	123.32	119.66
1	T	19	ARG	C-N-CA	5.02	123.32	119.66
2	X	52	ASN	CA-C-N	5.02	125.29	119.47
2	X	52	ASN	C-N-CA	5.02	125.29	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2695	0	2691	53	0
1	B	2695	0	2691	51	0
1	C	2695	0	2691	52	0
1	D	2695	0	2691	61	0
1	E	2695	0	2691	57	0
1	P	2695	0	2691	56	0
1	Q	2695	0	2691	58	0
1	R	2695	0	2691	54	0
1	S	2695	0	2691	53	0
1	T	2695	0	2691	54	0
2	F	1693	0	1645	32	0
2	G	1707	0	1654	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1701	0	1649	37	0
2	I	1693	0	1645	21	0
2	J	1701	0	1649	26	0
2	U	1682	0	1632	25	0
2	V	1707	0	1653	26	0
2	W	1707	0	1653	42	0
2	X	1707	0	1653	24	0
2	Y	1682	0	1632	24	0
3	K	1606	0	1560	22	0
3	L	1601	0	1555	30	0
3	M	1601	0	1555	17	0
3	N	1601	0	1555	27	0
3	O	1601	0	1555	21	0
3	Z	1626	0	1573	15	0
3	f	1620	0	1568	26	0
3	g	1601	0	1555	22	0
3	h	1601	0	1555	21	0
3	i	1620	0	1568	20	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	P	14	0	13	0	0
4	Q	14	0	13	0	0
4	R	14	0	13	1	0
4	S	14	0	13	0	0
4	T	14	0	13	0	0
5	A	23	0	21	0	0
5	B	23	0	21	1	0
5	C	23	0	21	0	0
5	D	23	0	21	0	0
5	E	23	0	21	0	0
5	P	23	0	21	0	0
5	Q	23	0	21	0	0
5	R	23	0	21	0	0
5	S	23	0	21	0	0
5	T	25	0	23	0	0
6	A	13	0	5	0	0
6	T	13	0	5	1	0
7	P	2	0	0	0	0
All	All	60408	0	59326	947	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 (947) 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)
3:g:120:LEU:HD11	3:g:196:CYS:HB3	1.60	0.81
3:M:107:THR:HG21	3:M:144:PRO:HB3	1.66	0.77
1:Q:138:PRO:HD2	1:Q:139:MET:HE3	1.69	0.75
1:P:254:LEU:HD11	1:Q:254:LEU:HD22	1.67	0.74
1:S:254:LEU:HD11	1:T:254:LEU:HD22	1.69	0.73
3:f:107:THR:HG21	3:f:144:PRO:HB3	1.70	0.73
2:Y:130:VAL:HB	2:Y:217:LYS:HG3	1.72	0.72
2:F:6:GLN:H	2:F:114:GLN:HE22	1.37	0.72
3:f:148:THR:HB	3:f:199:THR:HB	1.71	0.72
3:L:131:ASN:HA	3:L:185:ALA:HB2	1.72	0.72
2:H:144:MET:HG2	2:H:193:PRO:HA	1.69	0.72
1:R:254:LEU:HD11	1:S:254:LEU:HD22	1.72	0.71
1:A:254:LEU:HD22	1:E:254:LEU:HD11	1.72	0.70
1:B:254:LEU:HD11	1:C:254:LEU:HD22	1.73	0.70
2:G:101:ASP:HB3	2:G:104:ARG:HG3	1.74	0.70
1:T:33:ASN:HB2	1:T:163:LYS:HD2	1.74	0.70
1:A:37:ARG:HH21	1:A:123:ARG:CZ	2.04	0.69
3:K:122:PRO:HG3	3:K:209:LEU:HD13	1.73	0.68
1:P:254:LEU:HD22	1:T:254:LEU:HD11	1.75	0.68
1:D:170:LEU:HD23	1:D:174:LEU:HD22	1.75	0.68
2:V:6:GLN:H	2:V:114:GLN:HE22	1.41	0.68
1:D:33:ASN:HB2	1:D:163:LYS:HD2	1.76	0.68
1:T:138:PRO:HD2	1:T:139:MET:HE3	1.75	0.68
1:B:167:PRO:HB2	1:B:188:THR:HG21	1.76	0.67
1:C:33:ASN:HB2	1:C:163:LYS:HD2	1.76	0.67
2:Y:6:GLN:H	2:Y:114:GLN:HE22	1.42	0.67
3:i:153:VAL:HG12	3:i:158:VAL:HG22	1.75	0.67
1:E:36:LEU:HD13	1:E:168:LEU:HD11	1.76	0.67
1:A:254:LEU:HD11	1:B:254:LEU:HD22	1.77	0.67
2:I:6:GLN:H	2:I:114:GLN:HE22	1.41	0.66
1:Q:254:LEU:HD11	1:R:254:LEU:HD22	1.76	0.66
3:Z:107:THR:HG21	3:Z:144:PRO:HB3	1.77	0.66
1:P:136:TYR:O	1:P:140:ASP:HB3	1.96	0.66
1:A:194:VAL:HG22	1:A:199:ILE:HG23	1.78	0.65
1:B:250:VAL:HB	1:C:251:THR:HG21	1.77	0.65
1:E:170:LEU:HD23	1:E:174:LEU:HD22	1.76	0.65
1:P:138:PRO:HD2	1:P:139:MET:HE3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:136:TYR:O	1:T:140:ASP:HB3	1.96	0.65
2:V:177:ALA:HB2	2:V:186:LEU:HD23	1.79	0.65
2:X:6:GLN:H	2:X:114:GLN:HE22	1.42	0.65
1:A:33:ASN:HB2	1:A:163:LYS:HD2	1.78	0.65
2:J:6:GLN:H	2:J:114:GLN:HE22	1.45	0.64
1:C:254:LEU:HD11	1:D:254:LEU:HD22	1.79	0.64
1:C:194:VAL:HG22	1:C:199:ILE:HG23	1.80	0.64
3:N:141:ASP:HA	3:N:174:LYS:HB3	1.78	0.64
1:R:134:LEU:HD12	1:R:270:VAL:HG11	1.78	0.64
2:X:10:GLU:HG3	2:X:18:MET:HE3	1.79	0.64
2:J:101:ASP:HB3	2:J:104:ARG:HG3	1.79	0.64
1:R:136:TYR:O	1:R:140:ASP:HB3	1.98	0.63
1:R:170:LEU:HD23	1:R:174:LEU:HD22	1.80	0.63
1:Q:136:TYR:O	1:Q:140:ASP:HB3	1.98	0.63
2:X:108:TYR:HA	3:i:36:ASN:HD21	1.63	0.63
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.80	0.63
3:g:120:LEU:HD13	3:g:207:LYS:HB2	1.81	0.63
1:D:36:LEU:HD13	1:D:168:LEU:HD11	1.80	0.63
1:B:220:LEU:HG	1:B:263:ILE:HD12	1.81	0.63
3:L:148:THR:HB	3:L:199:THR:HB	1.81	0.62
1:D:254:LEU:HD11	1:E:254:LEU:HD22	1.81	0.62
1:E:136:TYR:O	1:E:140:ASP:HB3	2.00	0.62
1:S:136:TYR:O	1:S:140:ASP:HB3	1.99	0.62
1:A:136:TYR:O	1:A:140:ASP:HB3	1.99	0.62
1:B:194:VAL:HG22	1:B:199:ILE:HG23	1.81	0.62
1:P:167:PRO:HB2	1:P:188:THR:HG21	1.80	0.62
2:H:52:ASN:HD22	2:H:54:TYR:H	1.48	0.62
3:i:107:THR:HG21	3:i:144:PRO:HB3	1.82	0.62
1:B:136:TYR:O	1:B:140:ASP:HB3	1.99	0.61
2:G:6:GLN:H	2:G:114:GLN:HE22	1.47	0.61
2:V:101:ASP:HB3	2:V:104:ARG:HG3	1.82	0.61
1:T:167:PRO:HB2	1:T:188:THR:HG21	1.82	0.61
2:J:30:THR:HA	2:J:53:PRO:HB2	1.82	0.61
1:C:136:TYR:O	1:C:140:ASP:HB3	2.00	0.61
1:R:167:PRO:HB2	1:R:188:THR:HG21	1.81	0.61
3:i:149:VAL:HG11	3:i:164:THR:HG21	1.82	0.61
2:F:10:GLU:HG3	2:F:18:MET:HE3	1.82	0.61
2:W:147:LEU:HD22	2:W:219:ILE:HG21	1.82	0.61
3:i:131:ASN:HA	3:i:185:ALA:HB2	1.82	0.61
2:W:6:GLN:H	2:W:114:GLN:HE22	1.48	0.61
1:A:167:PRO:HB2	1:A:188:THR:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:TYR:O	1:D:140:ASP:HB3	2.01	0.61
2:X:101:ASP:HB3	2:X:104:ARG:HG3	1.82	0.61
2:H:101:ASP:HB3	2:H:104:ARG:HG3	1.82	0.61
3:i:148:THR:HB	3:i:199:THR:HB	1.82	0.60
2:J:10:GLU:HG3	2:J:18:MET:HE3	1.83	0.60
1:R:33:ASN:HB2	1:R:163:LYS:HD2	1.81	0.60
2:W:10:GLU:HG3	2:W:18:MET:HE3	1.83	0.60
3:f:189:GLU:O	3:f:211:ARG:NH2	2.34	0.60
2:J:197:TRP:HE1	2:J:202:VAL:HB	1.66	0.60
1:B:33:ASN:HB2	1:B:163:LYS:HD2	1.83	0.60
2:F:156:PRO:HD2	2:F:210:ALA:HB1	1.84	0.60
3:K:107:THR:HG21	3:K:144:PRO:HB3	1.84	0.60
3:M:194:TYR:HB2	3:M:209:LEU:HB3	1.83	0.60
1:B:39:ILE:HB	1:B:178:LEU:HD11	1.84	0.60
1:C:170:LEU:HD23	1:C:174:LEU:HD22	1.84	0.60
2:W:164:ASN:HD22	2:W:168:LEU:HD13	1.66	0.60
1:T:256:MET:HE2	1:T:283:CYS:HB2	1.84	0.60
2:Y:101:ASP:HB3	2:Y:104:ARG:HG3	1.84	0.60
2:F:141:THR:HG22	2:F:143:SER:H	1.66	0.59
2:Y:98:ARG:NH2	2:Y:110:ASP:OD2	2.32	0.59
1:T:36:LEU:HD13	1:T:168:LEU:HD11	1.83	0.59
3:h:149:VAL:HB	3:h:198:VAL:HG22	1.83	0.59
2:V:134:ALA:HB1	2:V:222:ARG:HB2	1.84	0.59
2:I:101:ASP:HB3	2:I:104:ARG:HG3	1.83	0.59
1:A:190:TYR:O	2:H:104:ARG:NH1	2.36	0.59
2:J:98:ARG:NH2	2:J:110:ASP:OD2	2.25	0.59
1:A:251:THR:HG21	1:E:250:VAL:HB	1.85	0.59
1:P:134:LEU:HD12	1:P:270:VAL:HG11	1.84	0.59
2:V:10:GLU:HG3	2:V:18:MET:HE3	1.84	0.59
2:I:10:GLU:HG3	2:I:18:MET:HE3	1.84	0.59
1:S:167:PRO:HB2	1:S:188:THR:HG21	1.84	0.58
3:K:22:CYS:HB3	3:K:73:ALA:HB3	1.85	0.58
6:T:403:FLC:OA1	6:T:403:FLC:OHB	2.20	0.58
1:C:190:TYR:O	2:G:104:ARG:NH1	2.36	0.58
1:S:138:PRO:HD2	1:S:139:MET:HE3	1.84	0.58
1:A:170:LEU:HD23	1:A:174:LEU:HD22	1.85	0.58
1:E:167:PRO:HB2	1:E:188:THR:HG21	1.83	0.58
1:C:207:ILE:HD12	1:C:209:LEU:HD21	1.85	0.58
3:h:135:LEU:HB2	3:h:181:LEU:HB3	1.85	0.58
1:C:134:LEU:HD12	1:C:270:VAL:HG11	1.85	0.58
3:L:85:GLU:HG3	3:L:107:THR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:153:VAL:HG12	3:N:158:VAL:HG22	1.86	0.58
2:G:146:THR:HB	3:K:119:THR:HG21	1.85	0.58
1:Q:95:GLU:HA	1:Q:128:LEU:HD23	1.85	0.58
1:T:134:LEU:HD12	1:T:270:VAL:HG11	1.84	0.58
3:M:194:TYR:N	3:M:209:LEU:O	2.35	0.58
1:A:79:LEU:HD11	1:A:83:HIS:HB2	1.86	0.58
1:D:250:VAL:HB	1:E:251:THR:HG21	1.86	0.58
2:Y:177:ALA:HB2	2:Y:186:LEU:HD23	1.85	0.57
3:i:37:TRP:CE2	3:i:75:LEU:HB2	2.39	0.57
1:Q:134:LEU:HD12	1:Q:270:VAL:HG11	1.85	0.57
2:Y:197:TRP:HE1	2:Y:219:ILE:HG12	1.68	0.57
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.86	0.57
1:B:170:LEU:HD23	1:B:174:LEU:HD22	1.84	0.57
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.40	0.57
1:B:207:ILE:HD12	1:B:209:LEU:HD21	1.86	0.57
1:D:154:THR:OG1	1:D:155:THR:N	2.38	0.57
2:G:10:GLU:HG3	2:G:18:MET:HE3	1.87	0.57
1:P:170:LEU:HD23	1:P:174:LEU:HD22	1.87	0.57
1:E:39:ILE:HB	1:E:178:LEU:HD11	1.86	0.57
1:Q:170:LEU:HD23	1:Q:174:LEU:HD22	1.87	0.57
3:i:22:CYS:HB3	3:i:73:ALA:HB3	1.85	0.57
1:Q:39:ILE:HB	1:Q:178:LEU:HD11	1.85	0.57
1:Q:167:PRO:HB2	1:Q:188:THR:HG21	1.87	0.57
1:Q:36:LEU:HD13	1:Q:168:LEU:HD11	1.86	0.56
1:T:170:LEU:HD23	1:T:174:LEU:HD22	1.87	0.56
1:E:134:LEU:HD12	1:E:270:VAL:HG11	1.86	0.56
1:S:33:ASN:HB2	1:S:163:LYS:HD2	1.87	0.56
2:U:6:GLN:H	2:U:114:GLN:HE22	1.52	0.56
1:Q:220:LEU:HG	1:Q:263:ILE:HD12	1.86	0.56
3:M:22:CYS:HB3	3:M:73:ALA:HB3	1.86	0.56
2:Y:10:GLU:HG3	2:Y:18:MET:HE3	1.86	0.56
1:D:138:PRO:HD2	1:D:139:MET:HE3	1.88	0.56
1:R:46:ASN:ND2	1:S:41:LYS:HE2	2.19	0.56
2:U:130:VAL:HG22	2:U:151:VAL:HG22	1.87	0.56
1:P:194:VAL:O	2:W:55:ASN:ND2	2.38	0.56
2:J:52:ASN:ND2	2:J:55:ASN:HD22	2.04	0.56
1:C:36:LEU:HD13	1:C:168:LEU:HD11	1.88	0.56
3:K:134:THR:HG22	3:K:182:THR:HA	1.87	0.56
1:P:36:LEU:HD13	1:P:168:LEU:HD11	1.87	0.56
2:W:128:PRO:HD3	2:W:208:HIS:HD1	1.71	0.56
2:W:161:VAL:HG22	2:W:206:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:101:ASP:HB3	2:F:104:ARG:HG3	1.86	0.56
2:H:6:GLN:H	2:H:114:GLN:HE22	1.53	0.56
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.41	0.56
1:P:33:ASN:HB2	1:P:163:LYS:HD2	1.87	0.56
2:U:10:GLU:HG3	2:U:18:MET:HE3	1.87	0.56
1:E:138:PRO:HD2	1:E:139:MET:HE3	1.87	0.56
1:T:154:THR:OG1	1:T:155:THR:N	2.37	0.56
3:h:170:GLN:HG2	3:h:171:SER:H	1.70	0.56
1:D:39:ILE:HB	1:D:178:LEU:HD11	1.88	0.55
1:D:134:LEU:HD12	1:D:270:VAL:HG11	1.88	0.55
1:E:154:THR:OG1	1:E:155:THR:N	2.35	0.55
2:J:173:HIS:HB2	2:J:189:SER:HB2	1.88	0.55
2:J:208:HIS:N	2:J:213:THR:O	2.26	0.55
1:B:134:LEU:HD12	1:B:270:VAL:HG11	1.89	0.55
2:H:108:TYR:HA	3:L:36:ASN:HD21	1.72	0.55
2:W:101:ASP:HB3	2:W:104:ARG:HG3	1.89	0.55
3:g:200:HIS:O	3:g:201:GLU:HG2	2.07	0.55
1:C:37:ARG:HE	1:C:123:ARG:HD3	1.72	0.55
3:L:116:PRO:HB3	3:L:142:PHE:HB3	1.88	0.55
1:P:39:ILE:HB	1:P:178:LEU:HD11	1.88	0.55
1:P:274:LYS:HZ2	1:Q:215:PHE:HE1	1.55	0.55
2:U:132:PRO:O	3:h:124:SER:OG	2.22	0.55
2:X:205:ASN:ND2	2:X:216:ASP:OD1	2.40	0.55
1:B:252:THR:HG22	1:B:287:ILE:HD13	1.89	0.55
1:C:167:PRO:HB2	1:C:188:THR:HG21	1.88	0.55
1:E:95:GLU:HA	1:E:128:LEU:HD23	1.89	0.55
1:R:79:LEU:HD11	1:R:83:HIS:HB2	1.88	0.54
1:T:194:VAL:HG22	1:T:199:ILE:HG23	1.89	0.54
3:N:145:GLY:HA3	3:N:175:TYR:HD2	1.71	0.54
2:W:108:TYR:HA	3:f:36:ASN:HD21	1.72	0.54
3:h:107:THR:HG21	3:h:144:PRO:HB3	1.88	0.54
3:M:85:GLU:HG3	3:M:107:THR:HA	1.88	0.54
1:B:95:GLU:HA	1:B:128:LEU:HD23	1.89	0.54
1:P:249:GLY:HA3	1:P:291:LEU:HD13	1.90	0.54
1:B:138:PRO:HD2	1:B:139:MET:HE3	1.90	0.54
1:S:95:GLU:HA	1:S:128:LEU:HD23	1.90	0.54
1:P:41:LYS:HE2	1:T:46:ASN:ND2	2.23	0.54
1:R:36:LEU:HD13	1:R:168:LEU:HD11	1.88	0.54
1:R:194:VAL:HG22	1:R:199:ILE:HG23	1.90	0.54
1:E:34:MET:SD	1:E:205:THR:HG21	2.47	0.54
2:F:61:ASN:OD1	2:F:62:GLN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:249:GLY:HA3	1:S:291:LEU:HD13	1.89	0.54
1:T:37:ARG:HH21	1:T:123:ARG:CZ	2.21	0.54
3:g:154:ASP:HA	3:g:193:SER:HB3	1.90	0.54
3:O:122:PRO:HB3	3:O:209:LEU:HD21	1.90	0.54
3:O:165:THR:HB	2:I:176:PRO:HG2	1.90	0.54
1:B:154:THR:OG1	1:B:155:THR:N	2.41	0.54
2:H:133:LEU:HD11	2:H:150:LEU:HB2	1.88	0.54
2:U:101:ASP:HB3	2:U:104:ARG:HG3	1.88	0.54
2:J:108:TYR:HA	3:M:36:ASN:HD21	1.72	0.54
3:N:199:THR:HG23	3:N:204:THR:HB	1.90	0.54
1:Q:217:LEU:O	1:Q:222:ILE:HG12	2.07	0.54
1:A:134:LEU:HD12	1:A:270:VAL:HG11	1.89	0.53
1:A:256:MET:HE2	1:A:283:CYS:HB2	1.90	0.53
1:T:220:LEU:HG	1:T:263:ILE:HD12	1.90	0.53
1:C:252:THR:HG22	1:C:287:ILE:HD13	1.91	0.53
1:E:33:ASN:HB2	1:E:163:LYS:HD2	1.89	0.53
1:Q:224:SER:HB2	1:Q:279:TRP:CZ3	2.43	0.53
2:X:60:TYR:HE1	2:X:70:LEU:HG	1.73	0.53
2:I:172:VAL:HA	2:I:190:VAL:HG22	1.90	0.53
3:L:94:TYR:O	3:L:96:ASN:N	2.38	0.53
1:R:39:ILE:HB	1:R:178:LEU:HD11	1.90	0.53
3:N:169:LYS:HA	3:N:175:TYR:HD1	1.74	0.53
1:T:194:VAL:O	2:Y:55:ASN:ND2	2.42	0.53
2:V:156:PRO:HD2	2:V:210:ALA:HB1	1.91	0.53
1:C:194:VAL:O	2:G:55:ASN:ND2	2.41	0.53
1:S:134:LEU:HD12	1:S:270:VAL:HG11	1.90	0.53
1:T:230:VAL:O	1:T:233:VAL:HG22	2.09	0.53
3:M:149:VAL:HG22	3:M:198:VAL:HG12	1.90	0.53
1:D:249:GLY:HA3	1:D:291:LEU:HD13	1.91	0.53
1:D:254:LEU:HD12	1:E:251:THR:HG23	1.91	0.53
1:Q:168:LEU:HD23	1:Q:186:THR:HB	1.90	0.53
1:C:256:MET:HE2	1:C:283:CYS:HB2	1.90	0.53
1:E:168:LEU:HD23	1:E:186:THR:HB	1.91	0.53
1:E:207:ILE:HD12	1:E:209:LEU:HD21	1.90	0.53
3:g:37:TRP:CE2	3:g:75:LEU:HB2	2.44	0.53
2:W:128:PRO:HD3	2:W:208:HIS:ND1	2.24	0.53
2:F:48:ILE:HG12	2:F:64:PHE:CE2	2.44	0.52
2:H:148:GLY:HA2	2:H:163:TRP:HH2	1.73	0.52
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.44	0.52
1:R:252:THR:HG22	1:R:287:ILE:HD13	1.90	0.52
1:T:39:ILE:HB	1:T:178:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:177:ALA:HB2	2:I:186:LEU:HB2	1.90	0.52
2:G:108:TYR:HA	3:K:36:ASN:HD21	1.75	0.52
1:P:194:VAL:HG22	1:P:199:ILE:HG23	1.92	0.52
1:T:190:TYR:O	2:Y:104:ARG:NH1	2.42	0.52
2:H:10:GLU:HG3	2:H:18:MET:HE3	1.90	0.52
1:D:220:LEU:HG	1:D:263:ILE:HD12	1.91	0.52
3:K:85:GLU:HG3	3:K:107:THR:HA	1.90	0.52
1:P:154:THR:OG1	1:P:155:THR:N	2.43	0.52
1:P:250:VAL:HB	1:Q:251:THR:HG21	1.91	0.52
1:R:37:ARG:HH21	1:R:123:ARG:CZ	2.23	0.52
1:C:254:LEU:HD12	1:D:251:THR:HG23	1.92	0.52
2:X:60:TYR:CE1	2:X:70:LEU:HG	2.44	0.52
2:X:211:SER:HG	2:X:213:THR:HG1	1.50	0.52
3:Z:37:TRP:CE2	3:Z:75:LEU:HB2	2.45	0.52
2:I:61:ASN:OD1	2:I:62:GLN:N	2.42	0.52
1:A:138:PRO:HD2	1:A:139:MET:HE3	1.92	0.52
1:R:224:SER:HB2	1:R:279:TRP:CZ3	2.45	0.52
1:C:95:GLU:HA	1:C:128:LEU:HD23	1.92	0.52
3:N:127:GLU:O	3:N:130:THR:OG1	2.27	0.52
1:D:37:ARG:HH21	1:D:123:ARG:CZ	2.23	0.52
3:h:37:TRP:CE2	3:h:75:LEU:HB2	2.45	0.52
1:T:34:MET:SD	1:T:205:THR:HG21	2.50	0.52
1:S:168:LEU:HD23	1:S:186:THR:HB	1.92	0.51
3:Z:30:THR:OG1	3:Z:32:ILE:HG12	2.10	0.51
1:A:95:GLU:HA	1:A:128:LEU:HD23	1.92	0.51
3:K:151:TRP:O	3:K:157:PRO:HA	2.10	0.51
1:S:224:SER:HB2	1:S:279:TRP:CZ3	2.45	0.51
3:f:37:TRP:CE2	3:f:75:LEU:HB2	2.46	0.51
1:C:79:LEU:HD11	1:C:83:HIS:HB2	1.92	0.51
1:D:207:ILE:HD12	1:D:209:LEU:HD21	1.91	0.51
1:P:95:GLU:HA	1:P:128:LEU:HD23	1.92	0.51
1:S:274:LYS:NZ	1:T:215:PHE:HE1	2.09	0.51
3:L:22:CYS:HB3	3:L:73:ALA:HB3	1.93	0.51
2:V:140:GLN:C	2:V:142:ASN:H	2.19	0.51
1:Q:249:GLY:HA3	1:Q:291:LEU:HD13	1.91	0.51
1:R:168:LEU:HD23	1:R:186:THR:HB	1.93	0.51
2:X:141:THR:OG1	2:X:142:ASN:N	2.44	0.51
2:I:6:GLN:N	2:I:114:GLN:HE22	2.07	0.51
1:B:249:GLY:HA3	1:B:291:LEU:HD13	1.92	0.51
1:E:249:GLY:HA3	1:E:291:LEU:HD13	1.93	0.51
1:R:230:VAL:O	1:R:233:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:124:LYS:HG2	2:Y:125:THR:H	1.76	0.51
3:h:120:LEU:HB2	3:h:207:LYS:HB3	1.92	0.51
3:i:122:PRO:HB3	3:i:209:LEU:HD21	1.93	0.51
3:L:153:VAL:HG12	3:L:158:VAL:HG22	1.92	0.51
3:f:153:VAL:HG12	3:f:158:VAL:HG22	1.92	0.51
3:h:142:PHE:HE1	3:h:145:GLY:HA2	1.75	0.51
1:C:168:LEU:HD23	1:C:186:THR:HB	1.93	0.51
1:Q:33:ASN:HB2	1:Q:163:LYS:HD2	1.93	0.51
2:Y:163:TRP:HB2	2:Y:168:LEU:HB2	1.92	0.51
1:B:79:LEU:HD11	1:B:83:HIS:HB2	1.93	0.50
2:H:148:GLY:HA2	2:H:163:TRP:CH2	2.46	0.50
2:H:163:TRP:CZ3	2:H:204:CYS:HB3	2.46	0.50
3:N:85:GLU:HG3	3:N:107:THR:HA	1.94	0.50
1:R:138:PRO:HD2	1:R:139:MET:HE3	1.94	0.50
2:W:36:TRP:CZ3	2:W:96:CYS:HB3	2.46	0.50
1:A:220:LEU:HG	1:A:263:ILE:HD12	1.93	0.50
1:T:37:ARG:HE	1:T:123:ARG:HD3	1.76	0.50
1:T:168:LEU:HD23	1:T:186:THR:HB	1.91	0.50
1:P:230:VAL:O	1:P:233:VAL:HG22	2.12	0.50
1:P:274:LYS:NZ	1:Q:215:PHE:HE1	2.08	0.50
2:V:61:ASN:OD1	2:V:62:GLN:N	2.45	0.50
2:X:6:GLN:N	2:X:114:GLN:HE22	2.08	0.50
3:i:154:ASP:HA	3:i:193:SER:HB3	1.93	0.50
1:A:34:MET:SD	1:A:205:THR:HG21	2.51	0.50
1:B:168:LEU:HD23	1:B:186:THR:HB	1.92	0.50
1:E:252:THR:HG22	1:E:287:ILE:HD13	1.92	0.50
1:P:215:PHE:HE1	1:T:274:LYS:NZ	2.10	0.50
1:S:220:LEU:HG	1:S:263:ILE:HD12	1.93	0.50
1:T:170:LEU:O	2:X:54:TYR:OH	2.28	0.50
1:D:256:MET:HE2	1:D:283:CYS:HB2	1.94	0.50
2:F:152:LYS:NZ	3:N:127:GLU:OE1	2.43	0.50
1:Q:46:ASN:ND2	1:R:41:LYS:HE2	2.26	0.50
1:C:37:ARG:HH21	1:C:123:ARG:CZ	2.24	0.50
1:C:170:LEU:O	2:F:54:TYR:OH	2.23	0.50
1:D:167:PRO:HB2	1:D:188:THR:HG21	1.93	0.50
1:P:252:THR:HG22	1:P:287:ILE:HD13	1.93	0.50
1:Q:274:LYS:NZ	1:R:215:PHE:HE1	2.09	0.50
1:S:181:PHE:HB3	1:S:209:LEU:HB3	1.94	0.50
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.47	0.50
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.76	0.50
1:T:252:THR:HG22	1:T:287:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:124:SER:OG	3:g:127:GLU:HB2	2.12	0.50
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.77	0.49
3:L:143:TYR:HB2	3:L:174:LYS:HG3	1.93	0.49
1:Q:256:MET:HE2	1:Q:283:CYS:HB2	1.93	0.49
1:R:9:LEU:HD21	1:R:66:TYR:HB3	1.92	0.49
1:S:36:LEU:HD13	1:S:168:LEU:HD11	1.94	0.49
2:U:98:ARG:NH2	2:U:110:ASP:OD2	2.38	0.49
2:U:147:LEU:HD13	2:U:219:ILE:HG21	1.94	0.49
2:U:147:LEU:HD11	2:U:197:TRP:CD1	2.47	0.49
2:U:164:ASN:HB2	2:U:202:VAL:HG13	1.93	0.49
2:J:38:LYS:HG3	2:J:94:TYR:HE1	1.77	0.49
1:A:85:ILE:HD11	1:A:112:ILE:HD11	1.95	0.49
2:H:61:ASN:OD1	2:H:62:GLN:N	2.45	0.49
1:R:220:LEU:HG	1:R:263:ILE:HD12	1.94	0.49
2:X:2:VAL:HG21	2:X:111:TYR:CD2	2.47	0.49
2:J:2:VAL:HG21	2:J:111:TYR:CD2	2.46	0.49
1:A:39:ILE:HB	1:A:178:LEU:HD11	1.94	0.49
1:C:9:LEU:HD21	1:C:66:TYR:HB3	1.95	0.49
3:O:118:VAL:HG13	3:O:207:LYS:HD3	1.95	0.49
2:V:2:VAL:HG21	2:V:111:TYR:CD2	2.48	0.49
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.47	0.49
1:S:39:ILE:HB	1:S:178:LEU:HD11	1.92	0.49
3:Z:123:PRO:HB3	3:Z:134:THR:H	1.77	0.49
1:E:194:VAL:HG22	1:E:199:ILE:HG23	1.95	0.49
3:K:120:LEU:HG	3:K:209:LEU:HD12	1.94	0.49
1:P:273:ILE:HG12	1:Q:215:PHE:HA	1.94	0.49
1:T:207:ILE:HD12	1:T:209:LEU:HD21	1.93	0.49
2:W:2:VAL:HG21	2:W:111:TYR:CD2	2.47	0.49
3:i:118:VAL:HB	3:i:139:ILE:HG23	1.94	0.49
1:A:37:ARG:NH1	1:E:93:PRO:O	2.46	0.49
1:Q:230:VAL:O	1:Q:233:VAL:HG22	2.13	0.49
1:A:27:PRO:HG2	3:L:32:ILE:HD12	1.94	0.49
1:C:267:LEU:HD13	1:C:274:LYS:HE3	1.94	0.49
3:f:164:THR:HG23	3:f:179:SER:HB2	1.95	0.49
2:J:197:TRP:CH2	2:J:221:PRO:HB3	2.48	0.49
1:B:36:LEU:HD23	1:B:39:ILE:HD11	1.94	0.49
1:C:228:VAL:O	1:C:231:SER:OG	2.30	0.49
2:H:60:TYR:HE1	2:H:70:LEU:HG	1.77	0.49
1:S:186:THR:HG22	1:S:207:ILE:HG22	1.95	0.49
1:T:224:SER:HB2	1:T:279:TRP:CZ3	2.47	0.49
2:X:61:ASN:OD1	2:X:62:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:HD21	1:B:146:ILE:HA	1.78	0.49
3:O:36:ASN:HD21	2:I:108:TYR:HA	1.77	0.49
1:Q:228:VAL:O	1:Q:231:SER:OG	2.27	0.49
1:Q:254:LEU:HD12	1:R:251:THR:HG23	1.93	0.49
1:R:154:THR:OG1	1:R:155:THR:N	2.39	0.49
2:W:174:THR:HG23	2:W:188:SER:HB2	1.95	0.49
1:Q:219:GLN:HB3	1:Q:220:LEU:HD12	1.94	0.49
1:D:219:GLN:HB3	1:D:220:LEU:HD12	1.95	0.48
1:E:154:THR:HG23	1:E:156:LYS:H	1.78	0.48
3:N:122:PRO:HB3	3:N:209:LEU:HD21	1.95	0.48
3:f:85:GLU:HG3	3:f:107:THR:HA	1.95	0.48
1:C:39:ILE:HB	1:C:178:LEU:HD11	1.95	0.48
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.95	0.48
1:C:138:PRO:HD2	1:C:139:MET:HE3	1.95	0.48
1:C:249:GLY:HA3	1:C:291:LEU:HD13	1.95	0.48
1:P:19:ARG:HH11	1:P:157:ASP:HA	1.78	0.48
1:R:37:ARG:HE	1:R:123:ARG:HD3	1.79	0.48
3:i:30:THR:OG1	3:i:32:ILE:HG12	2.13	0.48
2:J:177:ALA:HB2	2:J:186:LEU:HD23	1.94	0.48
1:E:219:GLN:HB3	1:E:220:LEU:HD12	1.95	0.48
3:N:169:LYS:HA	3:N:175:TYR:CD1	2.48	0.48
1:P:224:SER:HB2	1:P:279:TRP:CZ3	2.49	0.48
1:T:19:ARG:HH11	1:T:157:ASP:HA	1.78	0.48
2:V:6:GLN:N	2:V:114:GLN:HE22	2.09	0.48
2:W:130:VAL:HG22	2:W:151:VAL:HG22	1.95	0.48
2:Y:61:ASN:OD1	2:Y:62:GLN:N	2.47	0.48
3:g:162:MET:HB3	3:g:181:LEU:HD12	1.95	0.48
2:Y:30:THR:HA	2:Y:53:PRO:HB2	1.94	0.48
2:Y:205:ASN:N	2:Y:205:ASN:HD22	2.10	0.48
3:Z:85:GLU:HG3	3:Z:107:THR:HA	1.95	0.48
2:H:2:VAL:HG21	2:H:111:TYR:CD2	2.48	0.48
3:L:118:VAL:HG11	3:L:198:VAL:HG21	1.95	0.48
1:C:34:MET:SD	1:C:205:THR:HG21	2.54	0.48
3:g:152:LYS:HB2	3:g:195:SER:HB3	1.95	0.48
1:A:168:LEU:HD23	1:A:186:THR:HB	1.95	0.48
1:B:273:ILE:HG12	1:C:215:PHE:HA	1.96	0.48
1:C:230:VAL:O	1:C:233:VAL:HG22	2.14	0.48
1:E:37:ARG:HH21	1:E:123:ARG:CZ	2.27	0.48
2:H:147:LEU:HD13	2:H:219:ILE:HG21	1.95	0.48
3:N:135:LEU:HB2	3:N:181:LEU:HB3	1.96	0.48
1:Q:252:THR:HG22	1:Q:287:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:98:ARG:NH2	2:X:110:ASP:OD2	2.33	0.48
2:J:207:ALA:HA	2:J:214:LYS:HA	1.94	0.48
2:H:50:LEU:CD2	2:H:59:SER:HB3	2.44	0.48
2:H:147:LEU:HA	3:L:121:PHE:CZ	2.48	0.48
1:S:154:THR:OG1	1:S:155:THR:N	2.45	0.48
2:W:132:PRO:HG3	2:W:217:LYS:HB3	1.94	0.48
2:W:163:TRP:CZ3	2:W:204:CYS:HB3	2.49	0.48
2:G:128:PRO:HB3	2:G:154:TYR:HB3	1.95	0.48
1:P:168:LEU:HD23	1:P:186:THR:HB	1.95	0.48
1:S:19:ARG:HG2	1:S:20:PRO:HD2	1.95	0.48
1:A:249:GLY:HA3	1:A:291:LEU:HD13	1.96	0.48
1:D:95:GLU:HA	1:D:128:LEU:HD23	1.96	0.48
2:G:130:VAL:HG12	2:G:151:VAL:HG22	1.96	0.48
2:X:6:GLN:H	2:X:114:GLN:NE2	2.10	0.48
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.49	0.47
2:G:2:VAL:HG21	2:G:111:TYR:CD2	2.50	0.47
2:G:61:ASN:OD1	2:G:62:GLN:N	2.47	0.47
1:Q:34:MET:SD	1:Q:205:THR:HG21	2.53	0.47
1:T:249:GLY:HA3	1:T:291:LEU:HD13	1.95	0.47
3:K:211:ARG:O	3:K:211:ARG:NH1	2.48	0.47
1:R:219:GLN:HB3	1:R:220:LEU:HD12	1.95	0.47
2:U:156:PRO:HD2	2:U:210:ALA:HB1	1.95	0.47
2:W:164:ASN:HD21	2:W:202:VAL:HG12	1.79	0.47
3:g:107:THR:HG21	3:g:144:PRO:HB3	1.95	0.47
1:D:194:VAL:HG22	1:D:199:ILE:HG23	1.96	0.47
1:E:79:LEU:HD11	1:E:83:HIS:HB2	1.95	0.47
2:H:145:VAL:HG23	2:H:194:SER:HB3	1.97	0.47
2:U:164:ASN:HB3	2:U:167:SER:HB2	1.95	0.47
2:W:144:MET:HA	2:W:193:PRO:HA	1.96	0.47
3:g:85:GLU:HG3	3:g:107:THR:HA	1.97	0.47
1:A:254:LEU:HD12	1:B:251:THR:HG23	1.95	0.47
1:D:137:TYR:H	1:D:275:ALA:HB3	1.79	0.47
1:E:220:LEU:HG	1:E:263:ILE:HD12	1.96	0.47
1:S:170:LEU:HD23	1:S:174:LEU:HD22	1.95	0.47
2:X:30:THR:HA	2:X:53:PRO:HB2	1.96	0.47
2:Y:6:GLN:N	2:Y:114:GLN:HE22	2.09	0.47
3:f:139:ILE:HG12	3:f:198:VAL:HG21	1.96	0.47
2:J:6:GLN:N	2:J:114:GLN:HE22	2.11	0.47
3:M:169:LYS:HA	3:M:175:TYR:HD1	1.78	0.47
1:A:192:THR:HG23	1:A:200:TYR:O	2.14	0.47
1:B:137:TYR:O	1:B:275:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:LEU:HD21	1:E:66:TYR:HB3	1.97	0.47
2:G:6:GLN:N	2:G:114:GLN:HE22	2.12	0.47
1:Q:37:ARG:HH21	1:Q:123:ARG:CZ	2.28	0.47
3:g:127:GLU:HG2	3:g:133:ALA:HA	1.97	0.47
3:g:131:ASN:O	3:g:185:ALA:N	2.47	0.47
1:D:36:LEU:HD23	1:D:39:ILE:HD11	1.96	0.47
2:F:133:LEU:HD11	2:F:150:LEU:HB2	1.96	0.47
1:Q:224:SER:HB2	1:Q:279:TRP:CH2	2.50	0.47
1:S:194:VAL:HG22	1:S:199:ILE:HG23	1.96	0.47
1:T:161:LEU:HD11	3:g:32:ILE:HG22	1.96	0.47
1:T:213:PHE:HE2	1:T:217:LEU:HD22	1.80	0.47
3:Z:22:CYS:HB3	3:Z:73:ALA:HB3	1.96	0.47
3:i:154:ASP:OD1	3:i:193:SER:N	2.43	0.47
1:A:207:ILE:HD12	1:A:209:LEU:HD21	1.96	0.47
1:B:37:ARG:HH21	1:B:123:ARG:CZ	2.28	0.47
1:D:321:ALA:C	1:D:324:PRO:HD2	2.40	0.47
2:F:6:GLN:N	2:F:114:GLN:HE22	2.07	0.47
3:L:30:THR:OG1	3:L:32:ILE:HG12	2.14	0.47
1:P:85:ILE:HD11	1:P:112:ILE:HD11	1.96	0.47
1:Q:79:LEU:HD11	1:Q:83:HIS:HB2	1.96	0.47
1:R:250:VAL:HB	1:S:251:THR:HG21	1.97	0.47
2:X:164:ASN:HB2	2:X:168:LEU:HD13	1.96	0.47
3:g:22:CYS:HB3	3:g:73:ALA:HB3	1.96	0.47
1:B:27:PRO:HG2	3:N:32:ILE:HD12	1.96	0.47
1:D:85:ILE:HD11	1:D:112:ILE:HD11	1.96	0.47
1:S:271:SER:O	1:T:212:GLU:HB2	2.15	0.47
1:T:328:PHE:CE2	1:T:332:ILE:HD11	2.50	0.47
2:W:52:ASN:HB3	2:W:55:ASN:HB2	1.96	0.47
2:W:61:ASN:OD1	2:W:62:GLN:N	2.47	0.47
3:M:197:GLN:HB3	3:M:206:GLU:HG2	1.97	0.47
1:A:215:PHE:HA	1:E:273:ILE:HG12	1.97	0.47
2:F:155:PHE:HA	2:F:156:PRO:HA	1.72	0.47
2:V:208:HIS:CE1	2:V:210:ALA:HB3	2.49	0.47
2:Y:121:SER:OG	2:Y:182:ASP:OD1	2.33	0.47
1:C:154:THR:OG1	1:C:155:THR:N	2.47	0.47
1:C:220:LEU:HG	1:C:263:ILE:HD12	1.96	0.47
2:F:48:ILE:HG23	2:F:64:PHE:CD2	2.50	0.47
3:L:118:VAL:HG12	3:L:139:ILE:HD12	1.97	0.47
1:S:256:MET:HE2	1:S:283:CYS:HB2	1.97	0.47
2:U:30:THR:HA	2:U:53:PRO:HB2	1.97	0.47
1:C:137:TYR:H	1:C:275:ALA:HB3	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:120:LEU:HD12	3:N:209:LEU:HB2	1.97	0.46
3:O:22:CYS:HB3	3:O:73:ALA:HB3	1.98	0.46
1:Q:274:LYS:HZ2	1:R:215:PHE:HE1	1.62	0.46
1:D:252:THR:HG22	1:D:287:ILE:HD13	1.96	0.46
2:F:38:LYS:HG3	2:F:94:TYR:HE1	1.80	0.46
1:S:252:THR:HG22	1:S:287:ILE:HD13	1.95	0.46
3:i:85:GLU:HG3	3:i:107:THR:HA	1.96	0.46
2:I:6:GLN:H	2:I:114:GLN:NE2	2.12	0.46
1:B:267:LEU:HD13	1:B:274:LYS:HE3	1.97	0.46
1:P:79:LEU:HD11	1:P:83:HIS:HB2	1.98	0.46
1:Q:194:VAL:HG22	1:Q:199:ILE:HG23	1.96	0.46
3:h:120:LEU:HD13	3:h:209:LEU:HD22	1.96	0.46
2:I:2:VAL:HG21	2:I:111:TYR:CD2	2.50	0.46
1:B:230:VAL:O	1:B:233:VAL:HG22	2.15	0.46
2:F:152:LYS:HZ2	3:N:134:THR:HG1	1.58	0.46
2:H:197:TRP:CD1	2:H:198:PRO:HA	2.50	0.46
1:S:79:LEU:HD11	1:S:83:HIS:HB2	1.97	0.46
1:A:274:LYS:NZ	1:B:215:PHE:HE1	2.13	0.46
1:A:279:TRP:HB2	1:A:334:TYR:CZ	2.51	0.46
2:F:98:ARG:NH2	2:F:110:ASP:OD2	2.35	0.46
3:L:159:THR:OG1	3:L:160:GLN:N	2.48	0.46
1:Q:94:ASN:OD1	1:Q:94:ASN:N	2.40	0.46
3:f:149:VAL:HG21	3:f:164:THR:HG21	1.96	0.46
3:g:77:ILE:HD11	3:g:88:TYR:HE2	1.80	0.46
1:E:95:GLU:OE2	1:E:100:LYS:NZ	2.46	0.46
2:H:30:THR:HA	2:H:53:PRO:HB2	1.97	0.46
1:P:220:LEU:HG	1:P:263:ILE:HD12	1.98	0.46
3:Z:170:GLN:HG2	3:Z:174:LYS:O	2.15	0.46
2:J:61:ASN:OD1	2:J:62:GLN:N	2.48	0.46
1:R:154:THR:HG23	1:R:156:LYS:H	1.81	0.46
1:T:321:ALA:C	1:T:324:PRO:HD2	2.41	0.46
3:g:30:THR:OG1	3:g:32:ILE:HG12	2.15	0.46
3:i:77:ILE:HD11	3:i:88:TYR:HE2	1.80	0.46
1:D:137:TYR:O	1:D:275:ALA:HB3	2.16	0.46
2:U:216:ASP:OD1	2:U:216:ASP:N	2.48	0.46
2:V:13:ARG:NH2	2:V:124:LYS:HD2	2.30	0.46
3:f:68:LEU:HD23	3:f:73:ALA:HA	1.97	0.46
1:A:94:ASN:OD1	1:A:94:ASN:N	2.42	0.46
1:B:224:SER:HB2	1:B:279:TRP:CZ3	2.51	0.46
3:K:123:PRO:HD3	3:K:135:LEU:HG	1.98	0.46
1:Q:154:THR:HG23	1:Q:156:LYS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:168:LEU:HG	2:U:170:SER:H	1.80	0.46
2:V:98:ARG:NH2	2:V:110:ASP:OD2	2.36	0.46
2:V:213:THR:HG22	2:V:215:VAL:HG23	1.98	0.46
2:Y:143:SER:OG	2:Y:144:MET:N	2.49	0.46
3:g:116:PRO:HA	3:g:142:PHE:HB3	1.98	0.46
2:I:18:MET:HE2	2:I:18:MET:HB2	1.85	0.46
1:A:230:VAL:O	1:A:233:VAL:HG22	2.16	0.46
5:B:402:LMT:H3B	5:B:402:LMT:H6D	1.96	0.46
3:K:132:LYS:HA	3:K:184:THR:HA	1.98	0.46
2:U:38:LYS:HG3	2:U:94:TYR:HE1	1.81	0.46
2:V:172:VAL:HG22	2:V:190:VAL:HB	1.97	0.46
3:M:119:THR:HA	3:M:207:LYS:HE2	1.97	0.46
1:E:230:VAL:O	1:E:233:VAL:HG22	2.16	0.45
1:R:249:GLY:HA3	1:R:291:LEU:HD13	1.98	0.45
3:Z:152:LYS:HG3	3:Z:157:PRO:HD3	1.99	0.45
1:A:219:GLN:HB3	1:A:220:LEU:HD12	1.97	0.45
3:N:115:SER:HA	3:N:116:PRO:HD3	1.84	0.45
3:N:152:LYS:HB2	3:N:195:SER:HB2	1.96	0.45
1:A:319:SER:HA	1:A:322:LEU:HB3	1.98	0.45
3:K:91:ALA:HB2	3:K:100:PHE:CD2	2.50	0.45
3:O:137:CYS:HB2	3:O:151:TRP:CH2	2.51	0.45
1:R:42:ILE:HG22	1:R:132:MET:HE1	1.98	0.45
1:R:207:ILE:HD12	1:R:209:LEU:HD21	1.97	0.45
1:S:96:LYS:O	1:S:127:VAL:HB	2.16	0.45
1:E:33:ASN:OD1	1:E:56:ARG:NH1	2.48	0.45
3:M:30:THR:OG1	3:M:32:ILE:HG12	2.17	0.45
2:Y:155:PHE:HB2	2:Y:183:LEU:HD23	1.99	0.45
1:D:230:VAL:O	1:D:233:VAL:HG22	2.16	0.45
3:K:37:TRP:CD2	3:K:75:LEU:HB2	2.51	0.45
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.98	0.45
1:S:254:LEU:HD12	1:T:251:THR:HG23	1.98	0.45
2:V:60:TYR:HE1	2:V:70:LEU:HG	1.80	0.45
1:A:252:THR:HG22	1:A:287:ILE:HD13	1.97	0.45
1:C:94:ASN:OD1	1:C:94:ASN:N	2.47	0.45
3:K:128:LEU:HD11	3:K:188:TRP:HZ3	1.81	0.45
1:R:308:TRP:CE3	1:R:311:ILE:HD12	2.52	0.45
3:i:37:TRP:CD2	3:i:75:LEU:HB2	2.52	0.45
1:B:19:ARG:HG2	1:B:20:PRO:HD2	1.99	0.45
2:U:2:VAL:HG21	2:U:111:TYR:CD2	2.51	0.45
2:U:18:MET:HE2	2:U:18:MET:HB2	1.90	0.45
1:B:85:ILE:HD11	1:B:112:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:LEU:O	2:I:54:TYR:OH	2.32	0.45
3:L:151:TRP:CZ3	3:L:196:CYS:HB2	2.52	0.45
2:W:60:TYR:HE1	2:W:70:LEU:HG	1.82	0.45
1:D:267:LEU:HD13	1:D:274:LYS:HE3	1.99	0.45
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.82	0.45
1:E:194:VAL:O	2:J:55:ASN:ND2	2.49	0.45
3:K:188:TRP:HD1	3:K:194:TYR:OH	2.00	0.45
1:S:19:ARG:HH11	1:S:157:ASP:HA	1.82	0.45
1:S:20:PRO:HD3	1:S:86:TRP:CD2	2.51	0.45
1:T:194:VAL:HB	2:Y:52:ASN:HD22	1.82	0.45
1:C:224:SER:HB2	1:C:279:TRP:CZ3	2.51	0.44
1:S:230:VAL:O	1:S:233:VAL:HG22	2.16	0.44
2:W:144:MET:HG2	2:W:193:PRO:HA	1.99	0.44
1:D:168:LEU:HD23	1:D:186:THR:HB	1.99	0.44
2:H:60:TYR:CE1	2:H:70:LEU:HG	2.52	0.44
3:O:159:THR:OG1	3:O:160:GLN:N	2.50	0.44
1:Q:137:TYR:O	1:Q:275:ALA:HB3	2.17	0.44
2:X:150:LEU:HD13	3:i:136:VAL:HG21	1.99	0.44
2:I:197:TRP:CD2	2:I:198:PRO:HA	2.52	0.44
1:S:273:ILE:HG12	1:T:215:PHE:HA	1.99	0.44
1:T:95:GLU:HA	1:T:128:LEU:HD23	1.99	0.44
2:U:61:ASN:OD1	2:U:62:GLN:N	2.50	0.44
2:W:45:LEU:O	3:f:100:PHE:HB2	2.16	0.44
3:f:143:TYR:CD1	3:f:144:PRO:HA	2.53	0.44
3:h:85:GLU:HG3	3:h:107:THR:HA	1.99	0.44
1:A:26:GLY:HA2	3:L:95:SER:OG	2.18	0.44
1:B:137:TYR:H	1:B:275:ALA:HB3	1.82	0.44
1:D:20:PRO:HA	1:D:21:PRO:HD3	1.81	0.44
3:L:152:LYS:HB2	3:L:195:SER:HB3	1.98	0.44
1:S:217:LEU:HD12	1:S:221:TYR:HB2	1.99	0.44
2:U:155:PHE:HA	2:U:156:PRO:HA	1.79	0.44
2:W:50:LEU:CD2	2:W:59:SER:HB3	2.47	0.44
2:J:51:ILE:HB	2:J:58:THR:HG22	1.99	0.44
1:D:37:ARG:HE	1:D:123:ARG:HD3	1.83	0.44
1:E:96:LYS:O	1:E:127:VAL:HB	2.18	0.44
1:P:9:LEU:HD21	1:P:66:TYR:HB3	2.00	0.44
1:P:96:LYS:O	1:P:127:VAL:HB	2.18	0.44
1:S:207:ILE:HD12	1:S:209:LEU:HD21	1.99	0.44
2:X:168:LEU:HD23	2:X:190:VAL:HG21	1.99	0.44
3:f:30:THR:OG1	3:f:32:ILE:HG12	2.17	0.44
1:A:9:LEU:HD21	1:A:66:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:68:LEU:HD23	3:L:73:ALA:HA	1.99	0.44
1:P:36:LEU:HD23	1:P:39:ILE:HD11	1.99	0.44
1:Q:37:ARG:HE	1:Q:123:ARG:HD3	1.82	0.44
1:Q:154:THR:OG1	1:Q:155:THR:N	2.45	0.44
1:T:154:THR:HG23	1:T:156:LYS:H	1.83	0.44
2:X:38:LYS:HG3	2:X:94:TYR:HE1	1.82	0.44
3:f:152:LYS:HG2	3:f:157:PRO:HA	1.99	0.44
1:A:215:PHE:HE1	1:E:274:LYS:HZ2	1.63	0.44
1:B:217:LEU:O	1:B:222:ILE:HG12	2.17	0.44
1:E:256:MET:HE2	1:E:283:CYS:HB2	1.99	0.44
2:F:195:SER:C	2:F:198:PRO:HD2	2.42	0.44
1:Q:139:MET:H	1:Q:139:MET:HG2	1.64	0.44
2:V:181:SER:OG	2:V:182:ASP:N	2.48	0.44
2:W:140:GLN:HG3	2:W:145:VAL:HG23	1.99	0.44
2:I:14:PRO:HG2	2:I:122:SER:HB3	1.98	0.44
1:B:219:GLN:HB3	1:B:220:LEU:HD12	2.00	0.44
1:D:19:ARG:HG2	1:D:20:PRO:HD2	2.00	0.44
1:P:217:LEU:O	1:P:222:ILE:HG12	2.17	0.44
3:f:39:GLN:HG3	3:f:88:TYR:HE1	1.83	0.44
3:g:91:ALA:HB2	3:g:100:PHE:CD2	2.53	0.44
3:h:39:GLN:OE1	3:h:41:LYS:HE3	2.18	0.44
1:A:215:PHE:HE1	1:E:274:LYS:NZ	2.15	0.44
1:C:250:VAL:HG21	1:D:247:THR:HG22	2.00	0.44
1:D:181:PHE:HB3	1:D:209:LEU:HB3	2.00	0.44
3:O:41:LYS:HB2	3:O:45:LEU:HB2	2.00	0.44
1:P:137:TYR:HA	1:P:138:PRO:HA	1.77	0.44
1:P:219:GLN:HB3	1:P:220:LEU:HD12	2.00	0.44
1:R:194:VAL:HG23	2:V:105:TYR:HB2	1.99	0.44
1:S:37:ARG:HH21	1:S:123:ARG:CZ	2.31	0.44
3:L:135:LEU:HB2	3:L:181:LEU:HB3	2.00	0.43
3:L:154:ASP:OD2	3:L:191:HIS:ND1	2.36	0.43
1:S:85:ILE:HD11	1:S:112:ILE:HD11	2.00	0.43
1:E:137:TYR:CB	1:E:274:LYS:HB3	2.48	0.43
1:E:239:ARG:HD2	1:E:301:ALA:HB1	2.00	0.43
3:O:85:GLU:HG3	3:O:107:THR:HA	1.99	0.43
1:R:185:ASN:OD1	4:R:401:NAG:N2	2.50	0.43
2:V:60:TYR:CE1	2:V:70:LEU:HG	2.54	0.43
1:E:224:SER:HB2	1:E:279:TRP:CZ3	2.53	0.43
1:P:319:SER:HA	1:P:322:LEU:HB3	2.00	0.43
1:R:224:SER:HB2	1:R:279:TRP:CH2	2.54	0.43
1:R:232:TRP:CH2	1:R:324:PRO:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:THR:HA	2:F:53:PRO:HD3	2.01	0.43
1:A:33:ASN:HB3	1:A:56:ARG:HB2	1.99	0.43
1:B:256:MET:HE2	1:B:283:CYS:HB2	2.01	0.43
1:B:319:SER:HA	1:B:322:LEU:HB3	1.99	0.43
1:C:31:SER:HB2	1:C:58:SER:HB3	2.00	0.43
2:F:146:THR:HB	3:N:119:THR:HG21	2.00	0.43
2:H:154:TYR:OH	2:H:186:LEU:HD23	2.19	0.43
2:H:155:PHE:HA	2:H:156:PRO:HA	1.84	0.43
2:H:179:LEU:HD13	2:H:184:TYR:CD1	2.53	0.43
3:L:111:GLN:NE2	3:L:172:ASN:O	2.49	0.43
1:Q:20:PRO:HD3	1:Q:86:TRP:CD2	2.54	0.43
1:R:100:LYS:HA	1:R:100:LYS:HD3	1.78	0.43
1:T:36:LEU:HD23	1:T:39:ILE:HD11	2.00	0.43
2:W:30:THR:HA	2:W:53:PRO:HB2	2.00	0.43
1:A:96:LYS:O	1:A:127:VAL:HB	2.18	0.43
2:F:2:VAL:HG21	2:F:111:TYR:CD2	2.53	0.43
2:G:45:LEU:O	3:K:100:PHE:HB2	2.18	0.43
2:H:110:ASP:HB3	2:H:111:TYR:H	1.68	0.43
2:W:29:PHE:CD2	2:W:77:SER:HA	2.54	0.43
1:A:37:ARG:HE	1:A:123:ARG:HD3	1.83	0.43
2:G:202:VAL:O	2:G:218:LYS:HA	2.19	0.43
3:f:120:LEU:HD12	3:f:196:CYS:HB3	2.01	0.43
3:h:197:GLN:HB3	3:h:206:GLU:HG3	2.00	0.43
3:N:118:VAL:O	3:N:207:LYS:NZ	2.37	0.43
3:O:141:ASP:HA	3:O:174:LYS:HB3	2.01	0.43
1:P:321:ALA:C	1:P:324:PRO:HD2	2.44	0.43
1:A:224:SER:HB2	1:A:279:TRP:CZ3	2.54	0.43
1:D:273:ILE:HG12	1:E:215:PHE:HA	2.01	0.43
2:F:50:LEU:CD2	2:F:59:SER:HB3	2.49	0.43
3:K:77:ILE:HD11	3:K:88:TYR:HE2	1.84	0.43
1:S:250:VAL:HB	1:T:251:THR:HG21	1.99	0.43
1:S:328:PHE:CE2	1:S:332:ILE:HD11	2.54	0.43
1:D:174:LEU:CD2	1:D:183:LEU:HD13	2.48	0.43
1:D:217:LEU:O	1:D:222:ILE:HG12	2.18	0.43
1:E:137:TYR:H	1:E:275:ALA:HB3	1.83	0.43
1:E:267:LEU:HD13	1:E:274:LYS:HE3	1.99	0.43
3:L:107:THR:HG21	3:L:144:PRO:HB3	2.01	0.43
1:P:34:MET:SD	1:P:205:THR:HG21	2.58	0.43
1:Q:207:ILE:HD12	1:Q:209:LEU:HD21	2.01	0.43
2:W:11:LEU:HD12	2:W:119:THR:O	2.18	0.43
1:A:250:VAL:HB	1:B:251:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:CB	1:C:274:LYS:HB3	2.49	0.42
1:D:154:THR:HG23	1:D:156:LYS:H	1.84	0.42
1:D:317:LEU:HA	1:D:320:ARG:HD2	2.01	0.42
2:H:193:PRO:O	2:H:196:THR:OG1	2.31	0.42
2:H:197:TRP:CG	2:H:198:PRO:HA	2.53	0.42
3:N:37:TRP:CZ3	3:N:90:CYS:HB3	2.54	0.42
1:P:66:TYR:CE2	1:P:114:ASN:HA	2.54	0.42
1:R:137:TYR:O	1:R:275:ALA:HB3	2.19	0.42
1:T:311:ILE:O	1:T:315:VAL:HG23	2.19	0.42
2:Y:108:TYR:HA	3:g:36:ASN:HD21	1.85	0.42
3:f:188:TRP:CH2	3:f:211:ARG:HG3	2.54	0.42
3:M:77:ILE:HD11	3:M:88:TYR:HE2	1.84	0.42
3:M:151:TRP:O	3:M:158:VAL:HB	2.19	0.42
1:B:154:THR:HG23	1:B:156:LYS:H	1.84	0.42
1:D:9:LEU:HD21	1:D:66:TYR:HB3	2.01	0.42
1:E:171:LYS:HG2	1:E:172:VAL:H	1.84	0.42
2:F:152:LYS:NZ	3:N:134:THR:OG1	2.34	0.42
2:G:38:LYS:HG3	2:G:94:TYR:HE1	1.84	0.42
2:G:155:PHE:HA	2:G:156:PRO:HA	1.75	0.42
1:Q:49:TYR:CE1	1:Q:144:CYS:HB3	2.54	0.42
2:U:29:PHE:CD2	2:U:77:SER:HA	2.53	0.42
1:C:37:ARG:NE	1:C:123:ARG:HD3	2.32	0.42
1:D:279:TRP:HB2	1:D:334:TYR:CZ	2.55	0.42
1:E:161:LEU:HD11	3:M:32:ILE:HG22	2.00	0.42
2:G:60:TYR:CE1	2:G:70:LEU:HG	2.55	0.42
3:K:151:TRP:CE3	3:K:181:LEU:HD22	2.55	0.42
3:N:77:ILE:HD11	3:N:88:TYR:HE2	1.84	0.42
1:P:19:ARG:HG2	1:P:20:PRO:HD2	2.01	0.42
1:P:251:THR:HG23	1:T:254:LEU:HD12	2.02	0.42
1:Q:311:ILE:O	1:Q:315:VAL:HG23	2.19	0.42
2:W:38:LYS:HG3	2:W:94:TYR:HE1	1.84	0.42
2:W:208:HIS:NE2	2:W:210:ALA:HB3	2.34	0.42
2:Y:2:VAL:HG21	2:Y:111:TYR:CD2	2.54	0.42
1:A:109:LEU:HB3	1:A:121:SER:HB3	2.02	0.42
1:D:137:TYR:CB	1:D:274:LYS:HB3	2.49	0.42
1:E:259:GLN:O	1:E:263:ILE:HG12	2.20	0.42
1:P:58:SER:HA	1:P:118:VAL:O	2.20	0.42
1:Q:226:MET:O	1:Q:230:VAL:HG23	2.19	0.42
3:f:37:TRP:CD2	3:f:75:LEU:HB2	2.55	0.42
1:E:181:PHE:HB3	1:E:209:LEU:HB3	1.99	0.42
2:F:45:LEU:O	3:N:100:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:133:LEU:HB2	2:G:148:GLY:C	2.45	0.42
3:L:91:ALA:HB2	3:L:100:PHE:CD2	2.54	0.42
3:O:186:ARG:HD3	3:O:190:ARG:HH22	1.83	0.42
1:R:20:PRO:HA	1:R:21:PRO:HD3	1.83	0.42
1:T:109:LEU:HB3	1:T:121:SER:HB3	2.00	0.42
3:h:123:PRO:HD2	3:h:188:TRP:CH2	2.54	0.42
1:E:56:ARG:HA	1:E:120:TYR:O	2.20	0.42
1:P:227:LEU:HD21	1:P:255:THR:HG22	2.01	0.42
1:R:254:LEU:HD12	1:S:251:THR:HG23	2.01	0.42
1:S:20:PRO:HA	1:S:21:PRO:HD3	1.82	0.42
1:T:319:SER:HA	1:T:322:LEU:HB3	2.01	0.42
2:W:6:GLN:H	2:W:114:GLN:NE2	2.17	0.42
2:X:18:MET:HE2	2:X:18:MET:HB2	1.93	0.42
2:Y:60:TYR:HE1	2:Y:70:LEU:HG	1.84	0.42
3:Z:45:LEU:HD13	3:Z:45:LEU:HA	1.90	0.42
3:i:120:LEU:HD23	3:i:137:CYS:HB2	2.00	0.42
3:i:123:PRO:HD3	3:i:135:LEU:HD13	2.02	0.42
1:B:325:VAL:O	1:B:329:VAL:HG23	2.20	0.42
2:G:11:LEU:HD12	2:G:119:THR:O	2.18	0.42
3:O:30:THR:OG1	3:O:32:ILE:HG12	2.19	0.42
1:P:37:ARG:HE	1:P:123:ARG:HD3	1.85	0.42
1:P:154:THR:HG23	1:P:156:LYS:H	1.83	0.42
2:U:162:THR:O	2:U:204:CYS:HB2	2.20	0.42
2:V:133:LEU:HB2	2:V:148:GLY:HA3	2.01	0.42
3:f:116:PRO:HA	3:f:142:PHE:HB3	2.01	0.42
2:F:18:MET:HE2	2:F:18:MET:HB2	1.90	0.42
2:F:163:TRP:HZ2	2:F:188:SER:HB2	1.85	0.42
1:Q:33:ASN:HB3	1:Q:56:ARG:HB2	2.02	0.42
1:S:137:TYR:O	1:S:275:ALA:HB3	2.20	0.42
2:U:108:TYR:HA	3:h:36:ASN:HD21	1.84	0.42
2:Y:163:TRP:CE2	2:Y:190:VAL:HB	2.54	0.42
3:f:40:GLU:O	3:f:86:ALA:HB1	2.20	0.42
3:f:121:PHE:HB2	3:f:136:VAL:HB	2.02	0.42
2:F:197:TRP:CD2	2:F:198:PRO:HD3	2.54	0.42
2:H:143:SER:O	2:H:194:SER:OG	2.28	0.42
3:N:37:TRP:CD2	3:N:75:LEU:HB2	2.54	0.42
1:Q:138:PRO:HD2	1:Q:139:MET:CE	2.44	0.42
1:Q:250:VAL:HB	1:R:251:THR:HG21	2.02	0.42
1:R:328:PHE:CE2	1:R:332:ILE:HD11	2.55	0.42
2:U:175:PHE:HE1	3:h:176:MET:HB2	1.84	0.42
1:A:217:LEU:O	1:A:222:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HA	1:B:120:TYR:O	2.19	0.42
1:B:96:LYS:O	1:B:127:VAL:HB	2.19	0.42
1:D:22:THR:HG22	1:D:24:ASN:H	1.85	0.42
2:F:11:LEU:HD12	2:F:119:THR:O	2.20	0.42
3:K:30:THR:OG1	3:K:32:ILE:HG12	2.20	0.42
3:O:37:TRP:CD2	3:O:75:LEU:HB2	2.54	0.42
3:O:60:VAL:HA	3:O:61:PRO:HD3	1.91	0.42
3:O:164:THR:HG23	3:O:179:SER:HB2	2.01	0.42
1:R:186:THR:HG22	1:R:207:ILE:HG22	2.01	0.42
1:R:259:GLN:O	1:R:263:ILE:HG12	2.20	0.42
1:S:267:LEU:HD13	1:S:274:LYS:HE3	2.02	0.42
1:T:79:LEU:HD11	1:T:83:HIS:HB2	2.01	0.42
2:X:155:PHE:HA	2:X:156:PRO:HA	1.81	0.42
2:I:29:PHE:CD2	2:I:77:SER:HA	2.55	0.42
1:A:194:VAL:HG23	2:H:105:TYR:HB2	2.02	0.41
1:B:228:VAL:O	1:B:231:SER:OG	2.33	0.41
1:C:319:SER:HA	1:C:322:LEU:HB3	2.02	0.41
1:D:56:ARG:HA	1:D:120:TYR:O	2.20	0.41
1:E:94:ASN:HD21	1:E:146:ILE:HA	1.85	0.41
1:E:194:VAL:HG21	2:J:50:LEU:HD11	2.02	0.41
2:F:30:THR:HA	2:F:53:PRO:HB2	2.01	0.41
2:H:146:THR:HG22	2:H:191:THR:HB	2.01	0.41
1:Q:161:LEU:HD11	3:h:32:ILE:HG22	2.02	0.41
2:Y:175:PHE:HE1	3:g:176:MET:HB2	1.85	0.41
3:h:22:CYS:HB3	3:h:73:ALA:HB3	2.01	0.41
1:A:181:PHE:HB3	1:A:209:LEU:HB3	2.03	0.41
1:B:111:ARG:HD2	1:B:119:LEU:HD23	2.00	0.41
1:D:79:LEU:HD11	1:D:83:HIS:HB2	2.02	0.41
1:D:95:GLU:OE2	1:D:100:LYS:NZ	2.52	0.41
1:Q:181:PHE:HB3	1:Q:209:LEU:HB3	2.01	0.41
1:R:213:PHE:HE2	1:R:217:LEU:HD22	1.86	0.41
2:V:36:TRP:CZ3	2:V:96:CYS:HB3	2.55	0.41
3:Z:120:LEU:HG	3:Z:209:LEU:HD21	2.02	0.41
3:f:77:ILE:HD11	3:f:88:TYR:HE2	1.85	0.41
2:J:30:THR:O	2:J:54:TYR:HB2	2.20	0.41
2:J:48:ILE:HG12	2:J:64:PHE:CE2	2.54	0.41
1:B:181:PHE:HB3	1:B:209:LEU:HB3	2.03	0.41
1:C:274:LYS:NZ	1:D:215:PHE:HE1	2.18	0.41
2:G:60:TYR:HE1	2:G:70:LEU:HG	1.85	0.41
2:H:6:GLN:N	2:H:114:GLN:HE22	2.16	0.41
2:H:222:ARG:HA	2:H:222:ARG:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:137:CYS:HB3	3:N:179:SER:HB3	2.02	0.41
1:P:88:PRO:O	1:P:90:THR:N	2.52	0.41
1:P:100:LYS:HD3	1:P:100:LYS:HA	1.77	0.41
1:P:161:LEU:HD11	3:f:32:ILE:HG22	2.01	0.41
2:V:100:GLY:HA3	2:V:108:TYR:CZ	2.56	0.41
2:W:208:HIS:HA	2:W:209:PRO:HD2	1.94	0.41
3:Z:41:LYS:HB2	3:Z:45:LEU:HB2	2.02	0.41
2:J:126:THR:HA	2:J:127:PRO:HD3	1.85	0.41
1:A:100:LYS:HA	1:A:100:LYS:HD3	1.79	0.41
1:C:250:VAL:HB	1:D:251:THR:HG21	2.02	0.41
2:H:132:PRO:O	3:L:124:SER:HB3	2.20	0.41
3:L:118:VAL:HG12	3:L:139:ILE:HG23	2.02	0.41
3:O:71:ASP:OD1	3:O:71:ASP:N	2.53	0.41
1:Q:19:ARG:HH11	1:Q:157:ASP:HA	1.86	0.41
1:R:37:ARG:NE	1:R:123:ARG:HD3	2.35	0.41
2:U:133:LEU:HD11	2:U:150:LEU:HB2	2.02	0.41
2:V:30:THR:HA	2:V:53:PRO:HB2	2.02	0.41
2:V:108:TYR:HA	3:Z:36:ASN:HD21	1.84	0.41
2:J:52:ASN:HB3	2:J:55:ASN:HB2	2.02	0.41
1:C:181:PHE:HB3	1:C:209:LEU:HB3	2.03	0.41
1:C:194:VAL:HG13	1:C:199:ILE:HG12	2.02	0.41
1:C:219:GLN:HB3	1:C:220:LEU:HD12	2.01	0.41
1:D:130:CYS:HA	1:D:131:PRO:HD2	1.89	0.41
1:Q:19:ARG:HG2	1:Q:20:PRO:HD2	2.02	0.41
1:R:95:GLU:HA	1:R:128:LEU:HD23	2.02	0.41
1:R:170:LEU:O	2:U:54:TYR:OH	2.34	0.41
1:R:181:PHE:HB3	1:R:209:LEU:HB3	2.03	0.41
1:T:130:CYS:HA	1:T:131:PRO:HD2	1.91	0.41
1:C:217:LEU:O	1:C:222:ILE:HG12	2.21	0.41
1:D:85:ILE:O	1:D:87:MET:HG3	2.20	0.41
2:F:163:TRP:CZ2	2:F:188:SER:HB2	2.56	0.41
3:K:41:LYS:HE2	3:K:83:GLU:O	2.21	0.41
1:P:135:GLN:OE1	1:P:135:GLN:N	2.53	0.41
1:S:219:GLN:HB3	1:S:220:LEU:HD12	2.02	0.41
1:T:95:GLU:OE2	1:T:100:LYS:NZ	2.51	0.41
1:T:219:GLN:HB3	1:T:220:LEU:HD12	2.02	0.41
3:h:142:PHE:CE1	3:h:145:GLY:HA2	2.54	0.41
1:B:137:TYR:CB	1:B:274:LYS:HB3	2.51	0.41
2:F:175:PHE:HA	2:F:176:PRO:HD3	1.87	0.41
3:L:186:ARG:O	3:L:190:ARG:HB2	2.21	0.41
1:R:242:ILE:HG21	1:S:244:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:274:LYS:HE2	1:S:274:LYS:HB2	1.90	0.41
1:T:37:ARG:NE	1:T:123:ARG:HD3	2.36	0.41
2:W:6:GLN:N	2:W:114:GLN:HE22	2.15	0.41
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.86	0.41
1:A:137:TYR:CB	1:A:274:LYS:HB3	2.51	0.41
1:A:250:VAL:HG21	1:B:247:THR:HG22	2.02	0.41
1:D:33:ASN:HB3	1:D:56:ARG:HB2	2.03	0.41
1:D:137:TYR:HB3	1:D:274:LYS:HB3	2.03	0.41
2:G:50:LEU:CD2	2:G:59:SER:HB3	2.51	0.41
3:O:68:LEU:HD23	3:O:73:ALA:HA	2.03	0.41
1:T:138:PRO:HD2	1:T:139:MET:CE	2.46	0.41
3:Z:37:TRP:CD2	3:Z:75:LEU:HB2	2.55	0.41
1:E:137:TYR:O	1:E:275:ALA:HB3	2.20	0.41
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.55	0.41
2:H:162:THR:OG1	2:H:205:ASN:HB2	2.21	0.41
3:N:120:LEU:HD22	3:N:121:PHE:H	1.85	0.41
3:N:170:GLN:HG2	3:N:171:SER:H	1.85	0.41
1:P:37:ARG:HH21	1:P:123:ARG:CZ	2.33	0.41
1:Q:20:PRO:HA	1:Q:21:PRO:HD3	1.82	0.41
1:Q:109:LEU:HB3	1:Q:121:SER:HB3	2.02	0.41
1:R:274:LYS:NZ	1:S:215:PHE:HE1	2.18	0.41
1:S:137:TYR:H	1:S:275:ALA:HB3	1.86	0.41
1:S:137:TYR:HA	1:S:138:PRO:HA	1.77	0.41
1:T:275:ALA:HB1	1:T:338:PHE:CD2	2.55	0.41
2:W:27:TYR:CE2	2:W:29:PHE:HA	2.56	0.41
2:W:155:PHE:HA	2:W:156:PRO:HA	1.81	0.41
2:W:205:ASN:ND2	2:W:216:ASP:OD2	2.53	0.41
2:W:219:ILE:HD13	2:W:219:ILE:HA	1.91	0.41
2:J:177:ALA:HA	2:J:186:LEU:HB3	2.03	0.41
2:I:48:ILE:HG12	2:I:64:PHE:CE2	2.56	0.41
2:I:198:PRO:HB3	2:I:221:PRO:HG3	2.02	0.41
3:M:41:LYS:HE2	3:M:83:GLU:O	2.21	0.41
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.82	0.41
1:C:317:LEU:HA	1:C:320:ARG:HD2	2.03	0.41
1:D:27:PRO:HG2	3:O:32:ILE:HD12	2.03	0.41
2:H:48:ILE:HG23	2:H:64:PHE:CD2	2.56	0.41
1:P:33:ASN:HB3	1:P:56:ARG:HB2	2.02	0.41
1:R:162:TRP:CE2	1:R:203:LEU:HB3	2.56	0.41
2:V:124:LYS:HE3	2:V:124:LYS:HB3	1.89	0.41
2:X:178:VAL:HG11	3:i:163:GLU:HG2	2.03	0.41
2:J:179:LEU:HD22	2:J:184:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:159:THR:OG1	3:M:160:GLN:N	2.54	0.41
1:A:139:MET:H	1:A:139:MET:HG2	1.73	0.40
1:E:94:ASN:OD1	1:E:94:ASN:N	2.45	0.40
2:H:160:THR:OG1	2:H:207:ALA:HB3	2.21	0.40
1:P:207:ILE:HD12	1:P:209:LEU:HD21	2.03	0.40
1:T:217:LEU:HD12	1:T:221:TYR:HB2	2.03	0.40
2:V:149:CYS:HB2	2:V:163:TRP:CZ2	2.56	0.40
2:W:211:SER:OG	2:W:213:THR:OG1	2.20	0.40
3:h:154:ASP:OD1	3:h:193:SER:HB3	2.21	0.40
1:C:19:ARG:HA	1:C:20:PRO:HD3	1.92	0.40
1:C:100:LYS:HA	1:C:100:LYS:HD3	1.81	0.40
1:D:274:LYS:NZ	1:E:215:PHE:HE1	2.19	0.40
1:P:190:TYR:O	2:W:104:ARG:NH1	2.54	0.40
1:Q:95:GLU:OE2	1:Q:100:LYS:NZ	2.52	0.40
2:W:18:MET:HE2	2:W:18:MET:HB2	1.98	0.40
2:W:133:LEU:HB3	3:f:121:PHE:HD1	1.86	0.40
3:Z:60:VAL:HA	3:Z:61:PRO:HD3	1.95	0.40
3:g:21:THR:HB	3:g:72:LYS:HD2	2.03	0.40
3:g:45:LEU:HD13	3:g:45:LEU:HA	1.91	0.40
1:B:20:PRO:HD3	1:B:86:TRP:CD2	2.56	0.40
1:D:194:VAL:HG23	2:I:105:TYR:HB2	2.03	0.40
1:E:33:ASN:HB3	1:E:56:ARG:HB2	2.02	0.40
2:F:110:ASP:HB3	2:F:111:TYR:H	1.68	0.40
1:P:256:MET:HE2	1:P:283:CYS:HB2	2.02	0.40
1:Q:137:TYR:CB	1:Q:274:LYS:HB3	2.52	0.40
1:R:227:LEU:HD21	1:R:255:THR:HG22	2.03	0.40
1:S:211:ARG:HD3	1:S:216:TYR:CE2	2.56	0.40
3:f:37:TRP:CZ3	3:f:90:CYS:HB3	2.56	0.40
1:B:226:MET:O	1:B:230:VAL:HG23	2.21	0.40
1:E:31:SER:HB2	1:E:58:SER:HB3	2.03	0.40
3:L:121:PHE:HA	3:L:122:PRO:HD2	1.93	0.40
3:L:149:VAL:HG11	3:L:164:THR:HG21	2.03	0.40
3:O:170:GLN:OE1	3:O:176:MET:HB3	2.22	0.40
1:S:34:MET:SD	1:S:205:THR:HG21	2.62	0.40
2:X:163:TRP:HZ3	2:X:219:ILE:HD11	1.86	0.40
3:Z:135:LEU:HD13	3:Z:181:LEU:HD23	2.03	0.40
3:h:37:TRP:CZ3	3:h:90:CYS:HB3	2.56	0.40
2:I:127:PRO:HA	2:I:128:PRO:HD3	1.77	0.40
1:D:100:LYS:HA	1:D:100:LYS:HD3	1.81	0.40
1:D:190:TYR:O	2:I:104:ARG:NH1	2.55	0.40
2:G:34:MET:HE3	2:G:34:MET:HB3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:50:LEU:HD21	2:H:59:SER:HB3	2.03	0.40
1:P:42:ILE:HG22	1:P:132:MET:HE1	2.03	0.40
1:P:46:ASN:ND2	1:Q:41:LYS:HE2	2.37	0.40
1:Q:319:SER:HA	1:Q:322:LEU:HB3	2.04	0.40
1:S:139:MET:H	1:S:139:MET:HG2	1.68	0.40
1:S:232:TRP:CH2	1:S:324:PRO:HA	2.57	0.40
2:W:146:THR:HG22	2:W:191:THR:HB	2.02	0.40
3:h:77:ILE:HD11	3:h:88:TYR:HE2	1.86	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	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	36	65
1	B	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	36	65
1	C	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	36	65
1	D	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	36	65
1	E	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	36	65
1	P	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	36	65
1	Q	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	36	65
1	R	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	36	65
1	S	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	36	65
1	T	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	36	65
2	F	220/224 (98%)	204 (93%)	16 (7%)	0	100	100
2	G	222/224 (99%)	197 (89%)	25 (11%)	0	100	100
2	H	221/224 (99%)	198 (90%)	23 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	220/224 (98%)	204 (93%)	16 (7%)	0	100	100
2	J	221/224 (99%)	200 (90%)	21 (10%)	0	100	100
2	U	219/224 (98%)	195 (89%)	24 (11%)	0	100	100
2	V	222/224 (99%)	196 (88%)	25 (11%)	1 (0%)	24	57
2	W	222/224 (99%)	199 (90%)	23 (10%)	0	100	100
2	X	222/224 (99%)	201 (90%)	21 (10%)	0	100	100
2	Y	219/224 (98%)	192 (88%)	27 (12%)	0	100	100
3	K	210/215 (98%)	190 (90%)	20 (10%)	0	100	100
3	L	209/215 (97%)	195 (93%)	13 (6%)	1 (0%)	24	57
3	M	209/215 (97%)	190 (91%)	19 (9%)	0	100	100
3	N	209/215 (97%)	193 (92%)	15 (7%)	1 (0%)	24	57
3	O	209/215 (97%)	198 (95%)	11 (5%)	0	100	100
3	Z	213/215 (99%)	192 (90%)	20 (9%)	1 (0%)	24	57
3	f	212/215 (99%)	198 (93%)	14 (7%)	0	100	100
3	g	209/215 (97%)	185 (88%)	24 (12%)	0	100	100
3	h	209/215 (97%)	191 (91%)	18 (9%)	0	100	100
3	i	212/215 (99%)	192 (91%)	20 (9%)	0	100	100
All	All	7639/7860 (97%)	7122 (93%)	503 (7%)	14 (0%)	43	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
1	P	68	VAL
1	Q	68	VAL
1	R	68	VAL
1	S	68	VAL
1	T	68	VAL
2	V	172	VAL
3	Z	152	LYS
3	L	95	SER
3	N	167	PRO

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	305/316 (96%)	302 (99%)	3 (1%)	68	75
1	B	305/316 (96%)	303 (99%)	2 (1%)	76	78
1	C	305/316 (96%)	302 (99%)	3 (1%)	68	75
1	D	305/316 (96%)	303 (99%)	2 (1%)	76	78
1	E	305/316 (96%)	303 (99%)	2 (1%)	76	78
1	P	305/316 (96%)	303 (99%)	2 (1%)	76	78
1	Q	305/316 (96%)	302 (99%)	3 (1%)	68	75
1	R	305/316 (96%)	303 (99%)	2 (1%)	76	78
1	S	305/316 (96%)	302 (99%)	3 (1%)	68	75
1	T	305/316 (96%)	302 (99%)	3 (1%)	68	75
2	F	191/193 (99%)	188 (98%)	3 (2%)	55	69
2	G	193/193 (100%)	191 (99%)	2 (1%)	68	75
2	H	192/193 (100%)	189 (98%)	3 (2%)	55	69
2	I	191/193 (99%)	190 (100%)	1 (0%)	81	80
2	J	192/193 (100%)	191 (100%)	1 (0%)	81	80
2	U	190/193 (98%)	189 (100%)	1 (0%)	81	80
2	V	193/193 (100%)	193 (100%)	0	100	100
2	W	193/193 (100%)	193 (100%)	0	100	100
2	X	193/193 (100%)	190 (98%)	3 (2%)	55	69
2	Y	190/193 (98%)	188 (99%)	2 (1%)	65	74
3	K	179/182 (98%)	176 (98%)	3 (2%)	53	69
3	L	179/182 (98%)	176 (98%)	3 (2%)	53	69
3	M	179/182 (98%)	175 (98%)	4 (2%)	45	65
3	N	179/182 (98%)	178 (99%)	1 (1%)	78	79
3	O	179/182 (98%)	176 (98%)	3 (2%)	53	69
3	Z	182/182 (100%)	181 (100%)	1 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	f	181/182 (100%)	179 (99%)	2 (1%)	65	74
3	g	179/182 (98%)	176 (98%)	3 (2%)	53	69
3	h	179/182 (98%)	175 (98%)	4 (2%)	45	65
3	i	181/182 (100%)	174 (96%)	7 (4%)	28	54
All	All	6765/6910 (98%)	6693 (99%)	72 (1%)	65	74

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	158	ILE
1	A	242	ILE
1	B	42	ILE
1	B	158	ILE
1	C	42	ILE
1	C	158	ILE
1	C	242	ILE
1	D	42	ILE
1	D	158	ILE
1	E	42	ILE
1	E	158	ILE
2	F	159	VAL
2	F	190	VAL
2	F	220	VAL
2	G	159	VAL
2	G	215	VAL
2	H	52	ASN
2	H	149	CYS
2	H	172	VAL
3	K	45	LEU
3	K	119	THR
3	K	132	LYS
3	L	45	LEU
3	L	130	THR
3	L	149	VAL
3	N	45	LEU
3	O	45	LEU
3	O	130	THR
3	O	147	VAL
1	P	42	ILE
1	P	158	ILE

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Mol	Chain	Res	Type
1	Q	42	ILE
1	Q	158	ILE
1	Q	242	ILE
1	R	42	ILE
1	R	158	ILE
1	S	42	ILE
1	S	158	ILE
1	S	242	ILE
1	T	42	ILE
1	T	158	ILE
1	T	242	ILE
2	U	172	VAL
2	X	159	VAL
2	X	183	LEU
2	X	220	VAL
2	Y	205	ASN
2	Y	220	VAL
3	Z	45	LEU
3	f	45	LEU
3	f	130	THR
3	g	45	LEU
3	g	149	VAL
3	g	197	GLN
3	h	45	LEU
3	h	146	VAL
3	h	149	VAL
3	h	205	VAL
3	i	45	LEU
3	i	139	ILE
3	i	146	VAL
3	i	147	VAL
3	i	149	VAL
3	i	152	LYS
3	i	205	VAL
2	J	2	VAL
2	I	130	VAL
3	M	45	LEU
3	M	130	THR
3	M	153	VAL
3	M	158	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	83	HIS
1	B	8	HIS
1	B	24	ASN
1	B	298	ASN
1	C	8	HIS
1	C	219	GLN
1	D	8	HIS
1	D	83	HIS
1	D	298	ASN
1	E	8	HIS
1	E	219	GLN
2	G	173	HIS
2	G	180	GLN
2	H	52	ASN
3	K	36	ASN
3	K	97	HIS
3	L	36	ASN
3	L	170	GLN
3	N	36	ASN
3	N	131	ASN
3	N	200	HIS
3	O	36	ASN
1	P	8	HIS
1	P	24	ASN
1	P	83	HIS
1	P	298	ASN
1	Q	83	HIS
1	Q	219	GLN
1	Q	298	ASN
1	R	83	HIS
1	S	8	HIS
1	S	24	ASN
1	S	298	ASN
1	T	83	HIS
1	T	266	GLN
1	T	298	ASN
2	U	55	ASN
2	V	55	ASN
2	X	55	ASN
2	Y	205	ASN
3	Z	36	ASN
3	Z	96	ASN

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Mol	Chain	Res	Type
3	Z	170	GLN
3	Z	172	ASN
3	f	36	ASN
3	f	96	ASN
3	g	36	ASN
3	g	97	HIS
3	g	131	ASN
3	g	172	ASN
3	h	36	ASN
3	h	173	ASN
3	i	36	ASN
3	i	96	ASN
3	i	111	GLN
2	J	55	ASN
2	J	180	GLN
3	M	36	ASN
3	M	96	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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
4	NAG	E	401	1	14,14,15	0.34	0	17,19,21	0.55	0
5	LMT	T	402	-	26,26,36	1.13	2 (7%)	37,37,47	0.98	1 (2%)
4	NAG	A	401	1	14,14,15	0.27	0	17,19,21	0.52	0
5	LMT	D	402	-	24,24,36	1.04	2 (8%)	35,35,47	1.11	2 (5%)
4	NAG	B	401	1	14,14,15	0.71	0	17,19,21	1.10	1 (5%)
5	LMT	E	402	-	24,24,36	1.10	2 (8%)	35,35,47	1.12	2 (5%)
6	FLC	A	403	-	12,12,12	1.03	0	17,17,17	1.03	1 (5%)
5	LMT	A	402	-	24,24,36	1.10	2 (8%)	35,35,47	1.25	3 (8%)
5	LMT	S	402	-	24,24,36	1.07	2 (8%)	35,35,47	1.20	3 (8%)
4	NAG	Q	401	1	14,14,15	0.72	1 (7%)	17,19,21	0.81	0
4	NAG	R	401	1	14,14,15	0.49	0	17,19,21	0.59	0
5	LMT	P	402	-	24,24,36	1.07	2 (8%)	35,35,47	1.13	3 (8%)
4	NAG	P	401	1	14,14,15	0.55	0	17,19,21	1.57	2 (11%)
5	LMT	C	402	-	24,24,36	1.07	2 (8%)	35,35,47	1.32	6 (17%)
5	LMT	Q	402	-	24,24,36	1.06	2 (8%)	35,35,47	1.43	5 (14%)
4	NAG	D	401	1	14,14,15	0.47	0	17,19,21	1.06	1 (5%)
5	LMT	R	402	-	24,24,36	1.05	2 (8%)	35,35,47	1.02	1 (2%)
4	NAG	T	401	1	14,14,15	0.37	0	17,19,21	0.63	0
6	FLC	T	403	-	12,12,12	1.10	0	17,17,17	1.17	1 (5%)
4	NAG	C	401	1	14,14,15	0.59	0	17,19,21	1.92	5 (29%)
5	LMT	B	402	-	24,24,36	1.15	2 (8%)	35,35,47	1.28	5 (14%)
4	NAG	S	401	1	14,14,15	0.36	0	17,19,21	1.21	1 (5%)

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
4	NAG	E	401	1	-	4/6/23/26	0/1/1/1
5	LMT	T	402	-	-	4/11/51/61	0/2/2/2
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
5	LMT	D	402	-	-	5/8/48/61	0/2/2/2
4	NAG	B	401	1	-	6/6/23/26	0/1/1/1
5	LMT	E	402	-	-	2/8/48/61	0/2/2/2
6	FLC	A	403	-	-	0/16/16/16	-
5	LMT	A	402	-	-	5/8/48/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	S	402	-	-	5/8/48/61	0/2/2/2
4	NAG	Q	401	1	-	5/6/23/26	0/1/1/1
4	NAG	R	401	1	-	4/6/23/26	0/1/1/1
5	LMT	P	402	-	-	2/8/48/61	0/2/2/2
4	NAG	P	401	1	-	4/6/23/26	0/1/1/1
5	LMT	C	402	-	-	3/8/48/61	0/2/2/2
5	LMT	Q	402	-	-	4/8/48/61	0/2/2/2
4	NAG	D	401	1	-	4/6/23/26	0/1/1/1
5	LMT	R	402	-	-	4/8/48/61	0/2/2/2
4	NAG	T	401	1	-	4/6/23/26	0/1/1/1
6	FLC	T	403	-	-	3/16/16/16	-
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
5	LMT	B	402	-	-	3/8/48/61	0/2/2/2
4	NAG	S	401	1	-	3/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	LMT	O5B-C1B	3.17	1.50	1.41
5	E	402	LMT	O5B-C1B	2.99	1.49	1.41
5	Q	402	LMT	O5B-C1B	2.98	1.49	1.41
5	C	402	LMT	O5B-C1B	2.94	1.49	1.41
5	A	402	LMT	O5B-C1B	2.92	1.49	1.41
5	T	402	LMT	O5B-C1B	2.88	1.49	1.41
5	S	402	LMT	O5B-C1B	2.83	1.49	1.41
5	P	402	LMT	O5B-C1B	2.77	1.49	1.41
5	D	402	LMT	O5B-C1B	2.75	1.48	1.41
5	R	402	LMT	O5B-C1B	2.74	1.48	1.41
5	T	402	LMT	O5'-C1'	2.65	1.48	1.41
5	P	402	LMT	O5'-C1'	2.45	1.48	1.42
5	E	402	LMT	O5'-C1'	2.32	1.48	1.42
5	S	402	LMT	O5'-C1'	2.27	1.48	1.42
5	A	402	LMT	O5'-C1'	2.25	1.48	1.42
5	R	402	LMT	O5'-C1'	2.23	1.48	1.42
5	B	402	LMT	O5'-C1'	2.23	1.48	1.42
5	D	402	LMT	O5'-C1'	2.23	1.48	1.42
5	Q	402	LMT	O5'-C1'	2.21	1.48	1.42
4	Q	401	NAG	C1-C2	2.15	1.55	1.52
5	C	402	LMT	O5'-C1'	2.07	1.47	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	401	NAG	C1-O5-C5	5.16	119.10	112.19
4	C	401	NAG	C1-O5-C5	4.81	118.63	112.19
5	A	402	LMT	O5B-C5B-C4B	3.96	116.83	109.70
5	B	402	LMT	O5B-C5B-C4B	3.94	116.80	109.70
5	Q	402	LMT	C2'-C3'-C4'	3.87	118.45	109.68
4	C	401	NAG	C2-N2-C7	-3.82	117.78	122.90
5	C	402	LMT	O5'-C5'-C4'	3.80	117.58	109.72
4	S	401	NAG	C1-O5-C5	-3.69	107.25	112.19
5	Q	402	LMT	C1B-O1B-C4'	-3.48	109.72	117.98
4	P	401	NAG	O5-C1-C2	3.27	116.35	111.29
5	S	402	LMT	C2'-C3'-C4'	3.24	117.03	109.68
5	Q	402	LMT	C3'-C4'-C5'	3.16	117.94	110.93
5	B	402	LMT	C1B-O5B-C5B	3.16	119.89	113.72
4	D	401	NAG	C1-O5-C5	-3.08	108.06	112.19
6	A	403	FLC	OB2-CBC-CB	3.00	118.89	113.14
5	P	402	LMT	O5'-C1'-C2'	2.99	115.55	110.30
5	S	402	LMT	O5B-C5B-C4B	2.98	115.07	109.70
5	R	402	LMT	C1B-O1B-C4'	-2.98	110.92	117.98
5	E	402	LMT	C1B-O1B-C4'	-2.86	111.19	117.98
6	T	403	FLC	OB2-CBC-CB	2.84	118.59	113.14
5	C	402	LMT	C3'-C4'-C5'	2.80	117.13	110.93
5	P	402	LMT	C1B-O1B-C4'	-2.79	111.36	117.98
5	T	402	LMT	C1B-O1B-C4'	-2.77	111.42	117.98
4	C	401	NAG	C4-C3-C2	-2.74	107.00	111.02
5	C	402	LMT	C2'-C3'-C4'	2.69	115.79	109.68
4	B	401	NAG	O5-C1-C2	-2.64	107.21	111.29
5	Q	402	LMT	O5B-C1B-C2B	2.62	115.76	110.37
5	P	402	LMT	C1'-C2'-C3'	2.59	115.64	110.36
5	D	402	LMT	C1B-O1B-C4'	-2.58	111.86	117.98
5	Q	402	LMT	C1'-C2'-C3'	2.57	115.59	110.36
5	C	402	LMT	C1B-O1B-C4'	-2.49	112.07	117.98
5	D	402	LMT	C2'-C3'-C4'	2.49	115.33	109.68
5	C	402	LMT	C1B-C2B-C3B	2.36	114.98	110.01
4	C	401	NAG	O5-C1-C2	2.35	114.93	111.29
5	E	402	LMT	O5B-C1B-C2B	2.34	115.18	110.37
5	B	402	LMT	O5'-C5'-C4'	2.34	114.56	109.72
5	B	402	LMT	O5B-C1B-C2B	2.30	115.10	110.37
5	S	402	LMT	C1'-C2'-C3'	2.30	115.05	110.36
5	B	402	LMT	C6B-C5B-C4B	-2.26	107.46	113.02
5	A	402	LMT	C1B-O5B-C5B	2.17	117.95	113.72
4	C	401	NAG	C6-C5-C4	-2.13	107.79	113.02
5	A	402	LMT	C3B-C4B-C5B	2.09	114.01	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	402	LMT	O5B-C1B-C2B	2.02	114.53	110.37

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2
4	C	401	NAG	C8-C7-N2-C2
4	C	401	NAG	O7-C7-N2-C2
4	D	401	NAG	C8-C7-N2-C2
4	D	401	NAG	O7-C7-N2-C2
4	P	401	NAG	C8-C7-N2-C2
4	P	401	NAG	O7-C7-N2-C2
4	Q	401	NAG	O7-C7-N2-C2
4	R	401	NAG	C8-C7-N2-C2
4	R	401	NAG	O7-C7-N2-C2
4	S	401	NAG	C3-C2-N2-C7
4	S	401	NAG	C8-C7-N2-C2
4	S	401	NAG	O7-C7-N2-C2
5	A	402	LMT	O5B-C1B-O1B-C4'
5	B	402	LMT	O5B-C1B-O1B-C4'
5	Q	402	LMT	C4B-C5B-C6B-O6B
4	Q	401	NAG	C8-C7-N2-C2
4	Q	401	NAG	O5-C5-C6-O6
5	P	402	LMT	O5'-C5'-C6'-O6'
5	R	402	LMT	O5'-C5'-C6'-O6'
5	Q	402	LMT	O5'-C5'-C6'-O6'
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	B	401	NAG	O5-C5-C6-O6
5	D	402	LMT	O5'-C5'-C6'-O6'
5	T	402	LMT	O5B-C5B-C6B-O6B
5	C	402	LMT	C4'-C5'-C6'-O6'
5	T	402	LMT	C4'-C5'-C6'-O6'
5	T	402	LMT	O5'-C5'-C6'-O6'
4	Q	401	NAG	C4-C5-C6-O6
5	D	402	LMT	O5B-C5B-C6B-O6B
4	T	401	NAG	C8-C7-N2-C2
4	T	401	NAG	O7-C7-N2-C2
5	Q	402	LMT	O5B-C5B-C6B-O6B
4	B	401	NAG	C4-C5-C6-O6

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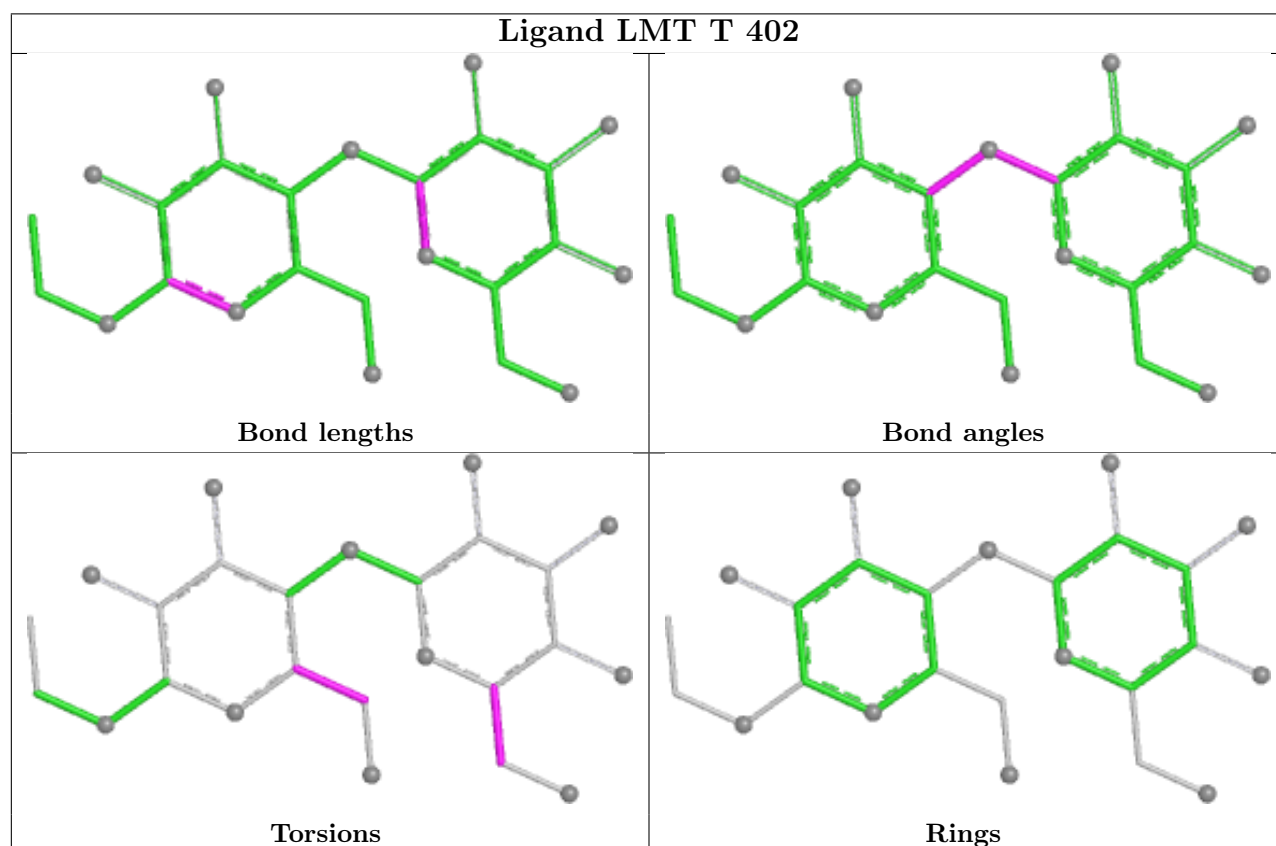
Mol	Chain	Res	Type	Atoms
5	P	402	LMT	C4'-C5'-C6'-O6'
5	S	402	LMT	O5B-C5B-C6B-O6B
5	Q	402	LMT	C4'-C5'-C6'-O6'
5	R	402	LMT	C4'-C5'-C6'-O6'
4	T	401	NAG	C4-C5-C6-O6
5	D	402	LMT	C4'-C5'-C6'-O6'
5	S	402	LMT	C4B-C5B-C6B-O6B
4	E	401	NAG	C8-C7-N2-C2
5	C	402	LMT	O5'-C5'-C6'-O6'
4	E	401	NAG	O7-C7-N2-C2
4	T	401	NAG	O5-C5-C6-O6
5	A	402	LMT	C4B-C5B-C6B-O6B
4	P	401	NAG	O5-C5-C6-O6
5	R	402	LMT	C4B-C5B-C6B-O6B
5	S	402	LMT	O5B-C1B-O1B-C4'
5	T	402	LMT	C4B-C5B-C6B-O6B
5	S	402	LMT	C2B-C1B-O1B-C4'
5	A	402	LMT	C4'-C5'-C6'-O6'
5	B	402	LMT	C4'-C5'-C6'-O6'
5	S	402	LMT	O5'-C5'-C6'-O6'
5	E	402	LMT	O5B-C1B-O1B-C4'
5	D	402	LMT	C4B-C5B-C6B-O6B
5	A	402	LMT	O5'-C5'-C6'-O6'
5	R	402	LMT	O5B-C5B-C6B-O6B
5	B	402	LMT	O5'-C5'-C6'-O6'
5	A	402	LMT	O5B-C5B-C6B-O6B
6	T	403	FLC	CAC-CA-CB-CBC
6	T	403	FLC	CAC-CA-CB-OHB
4	B	401	NAG	C3-C2-N2-C7
4	D	401	NAG	C3-C2-N2-C7
4	Q	401	NAG	C3-C2-N2-C7
4	R	401	NAG	C3-C2-N2-C7
4	P	401	NAG	C4-C5-C6-O6
5	E	402	LMT	C2B-C1B-O1B-C4'
4	E	401	NAG	C4-C5-C6-O6
4	B	401	NAG	C1-C2-N2-C7
4	D	401	NAG	C1-C2-N2-C7
4	E	401	NAG	C1-C2-N2-C7
4	R	401	NAG	C1-C2-N2-C7
5	C	402	LMT	C4B-C5B-C6B-O6B
5	D	402	LMT	C3'-C4'-O1B-C1B
6	T	403	FLC	CAC-CA-CB-CG

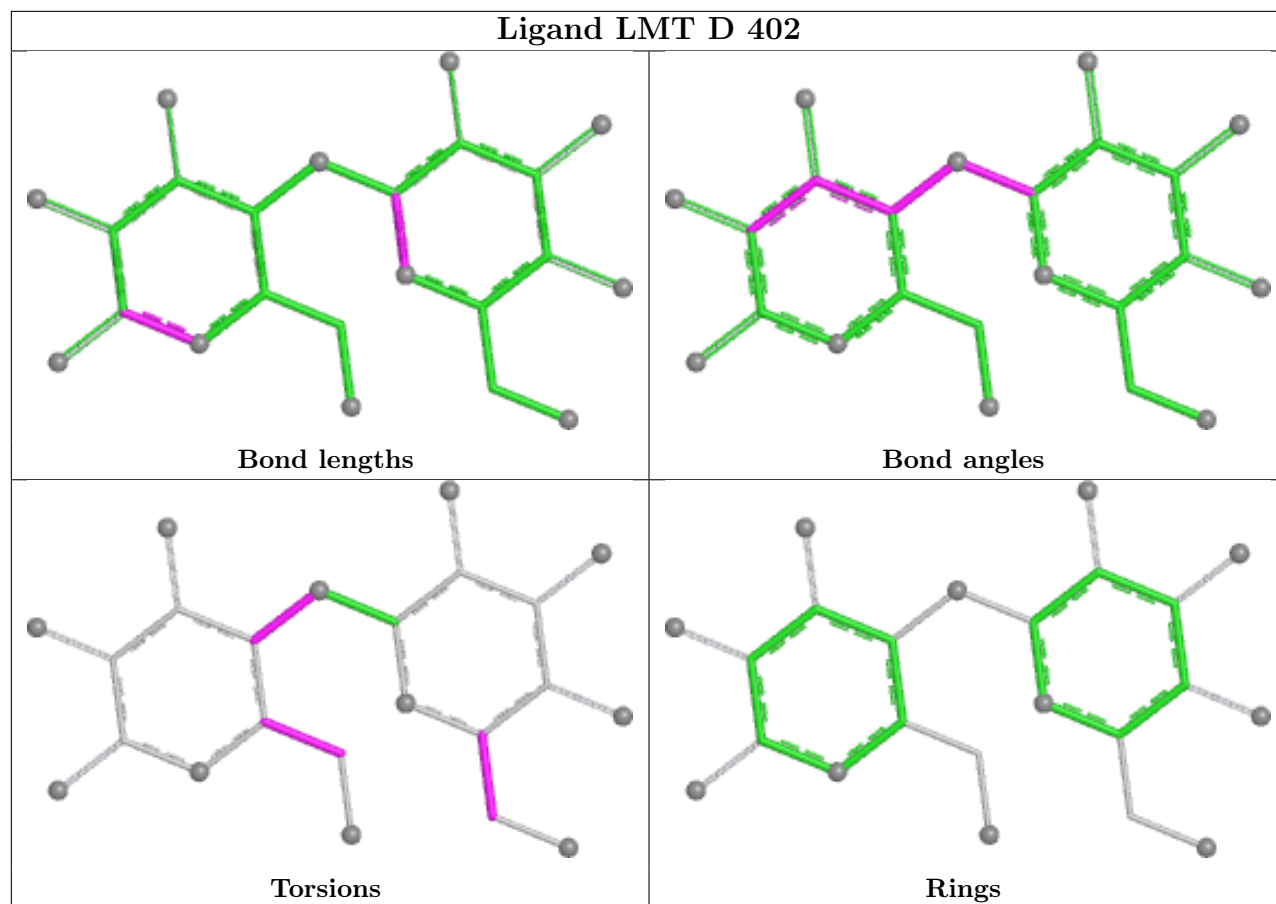
There are no ring outliers.

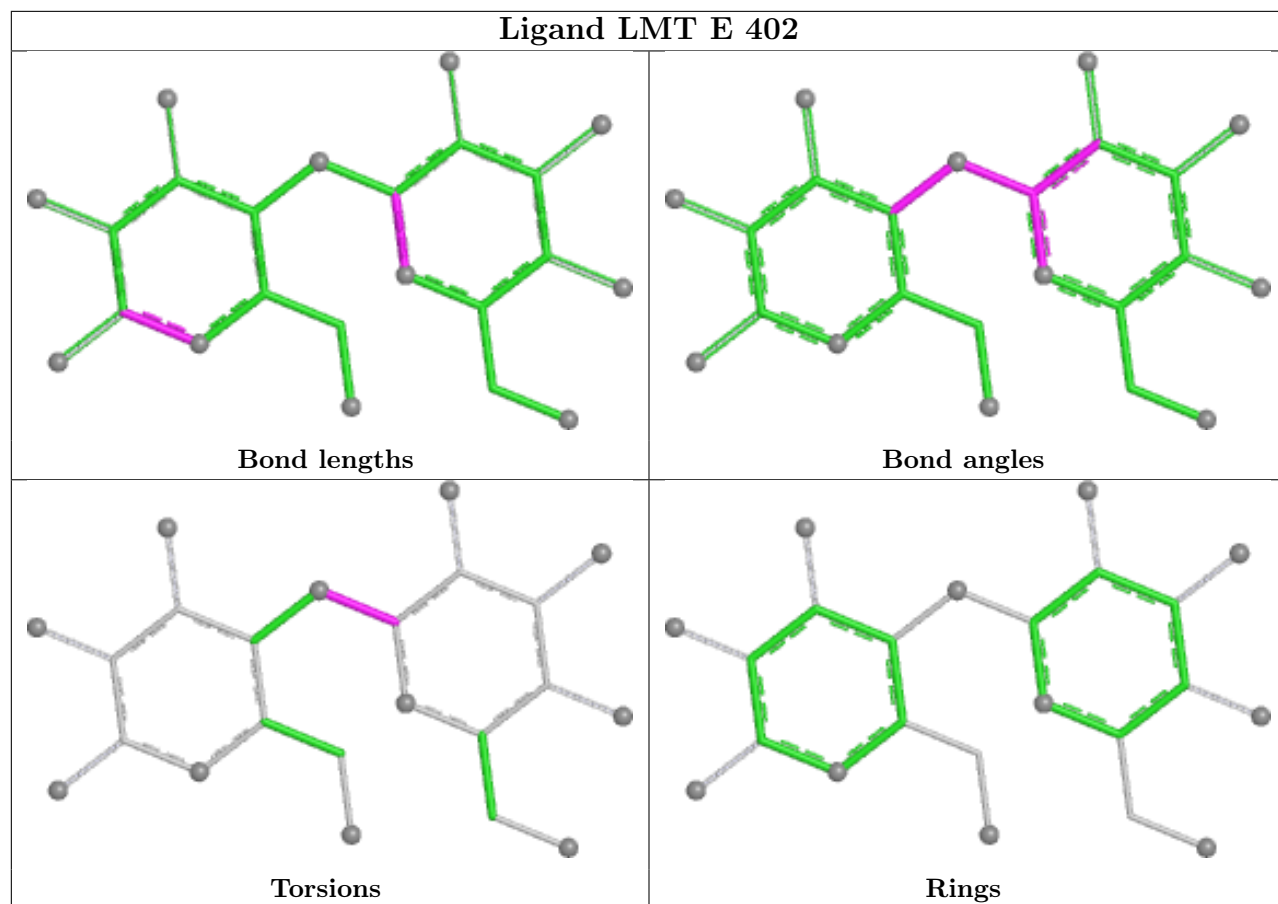
3 monomers are involved in 3 short contacts:

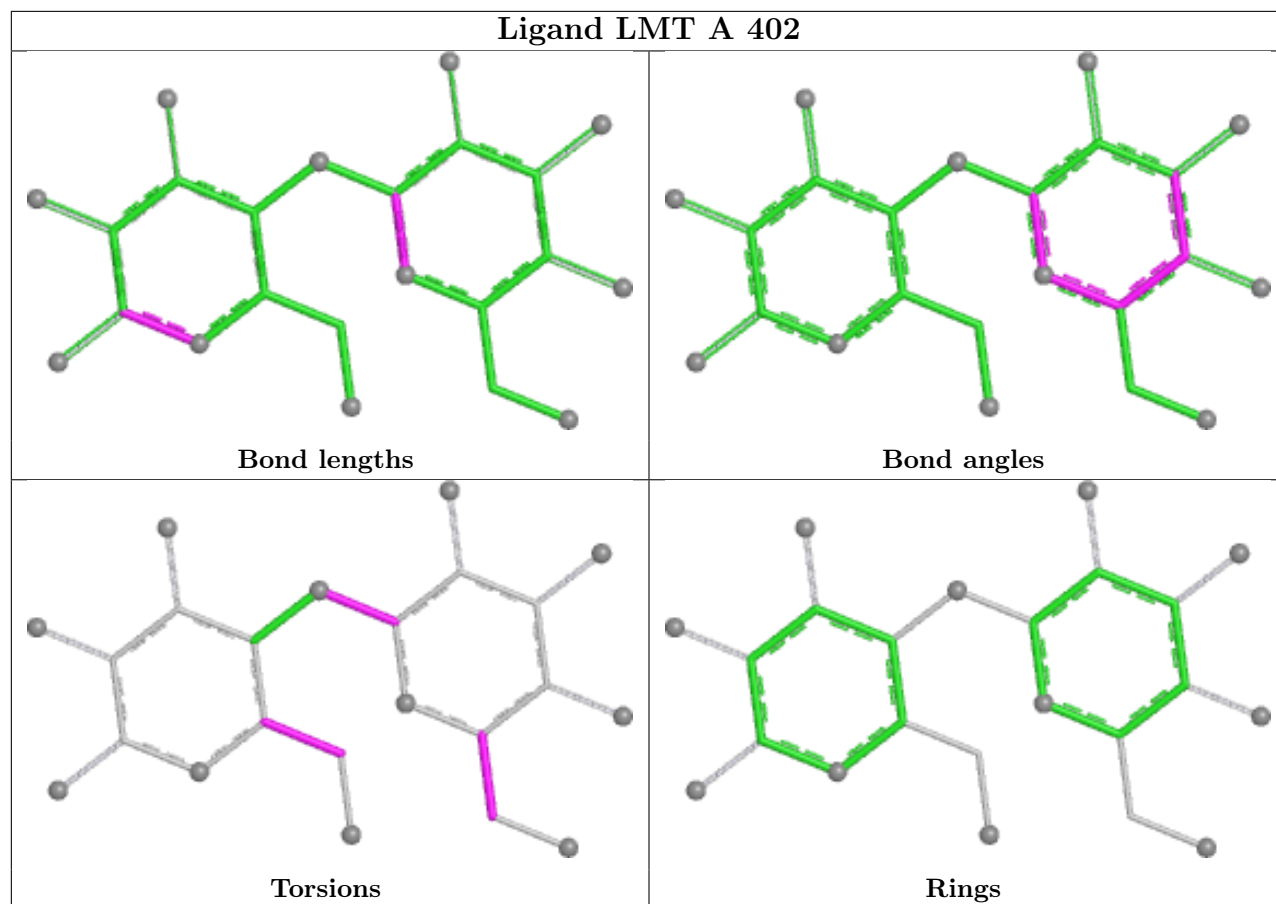
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	401	NAG	1	0
6	T	403	FLC	1	0
5	B	402	LMT	1	0

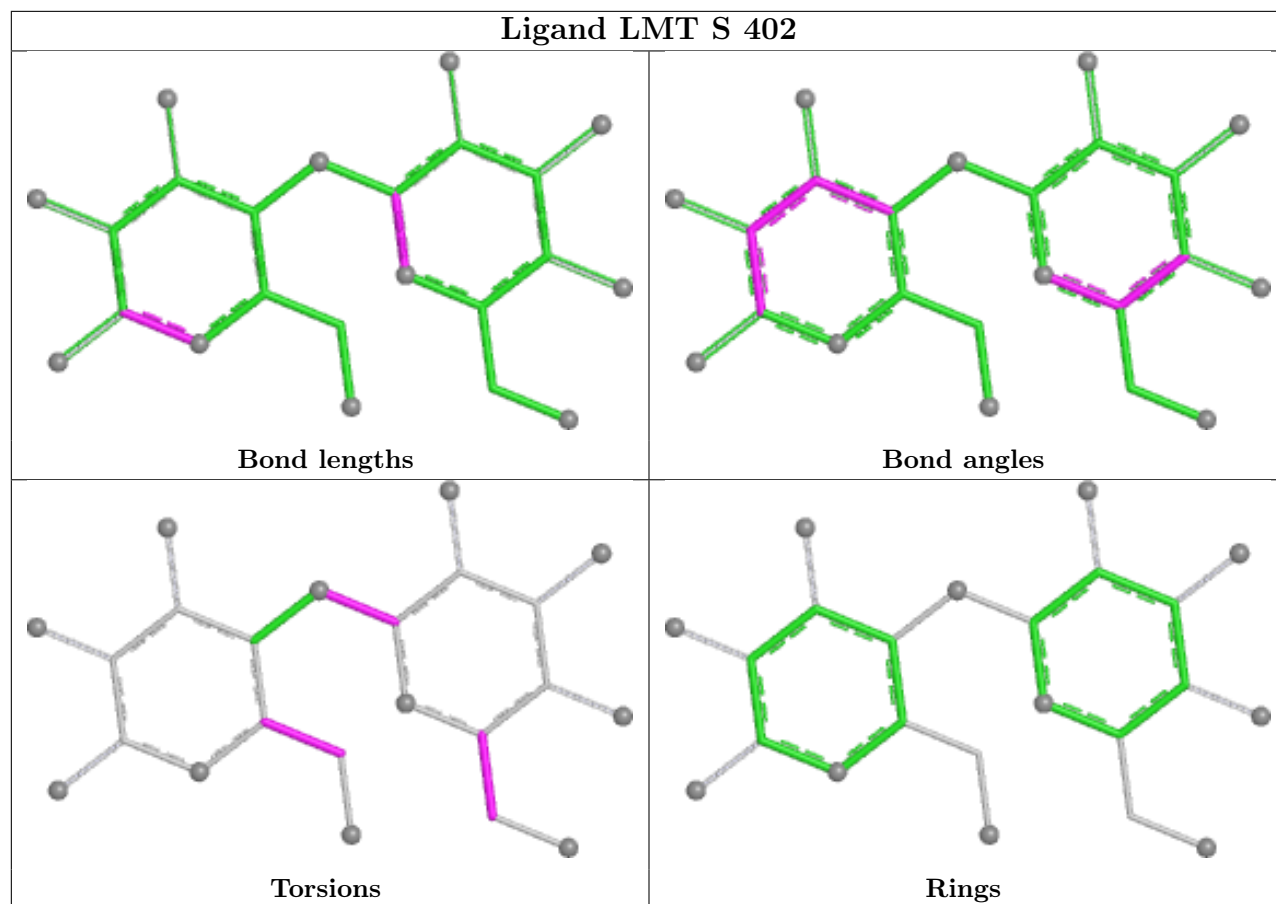
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

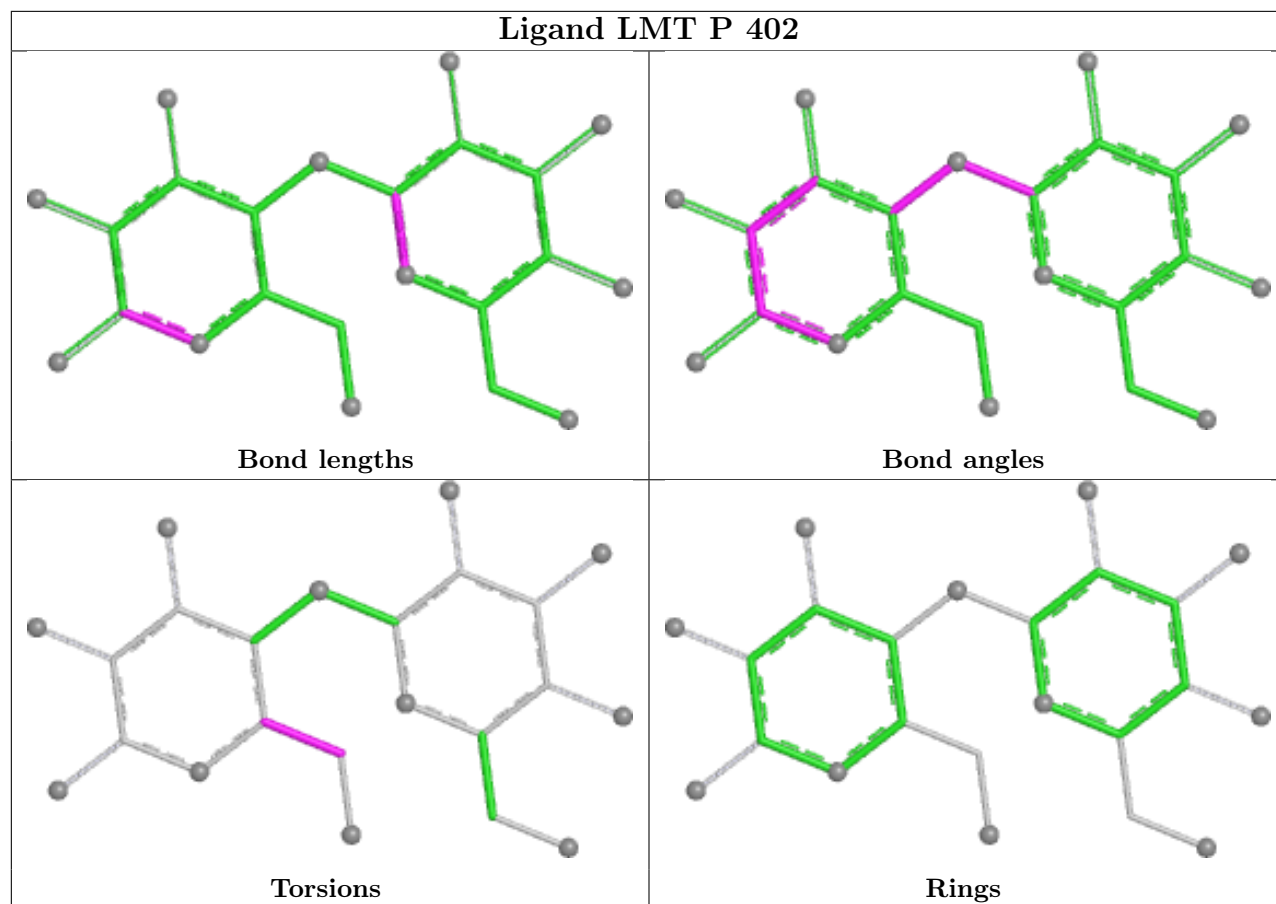


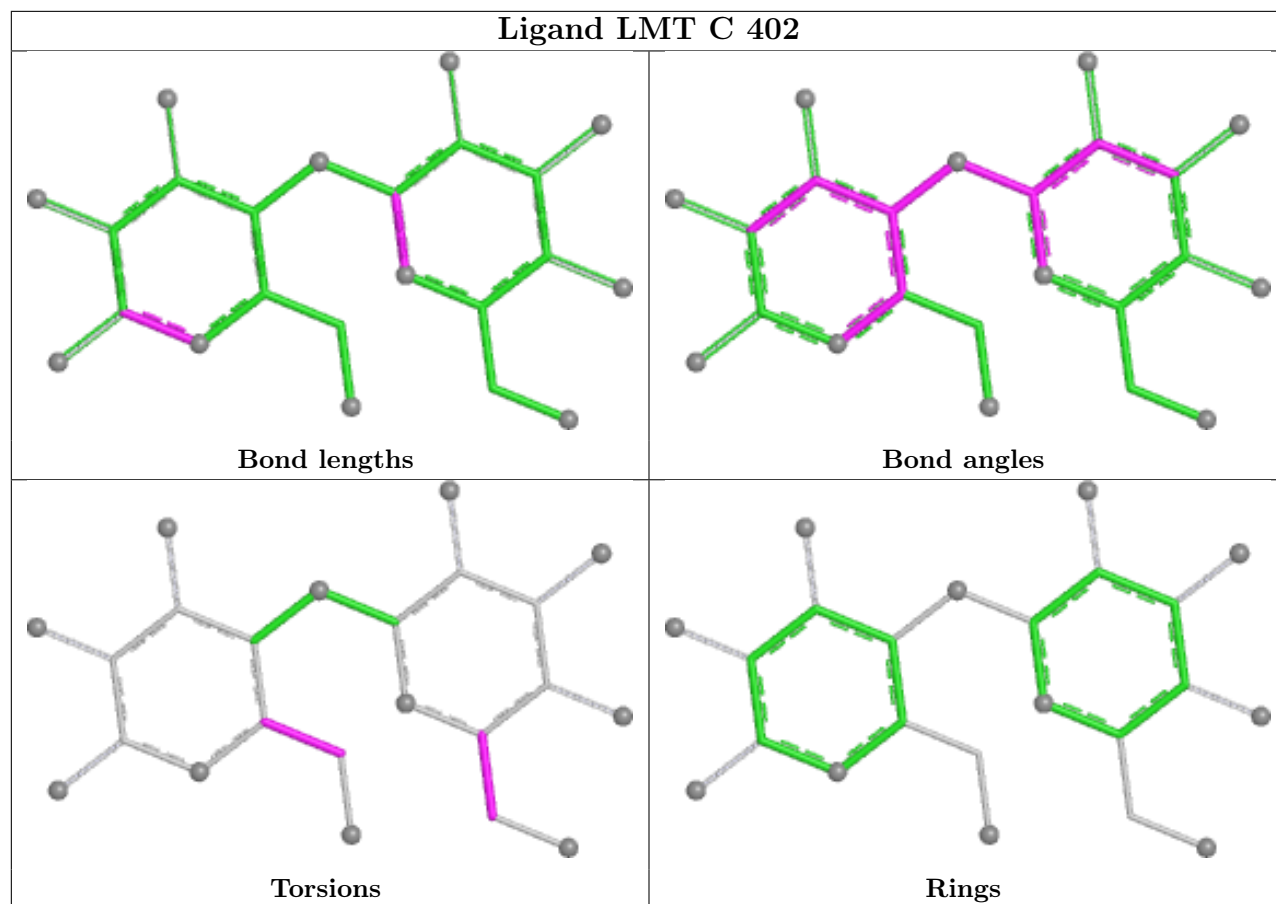


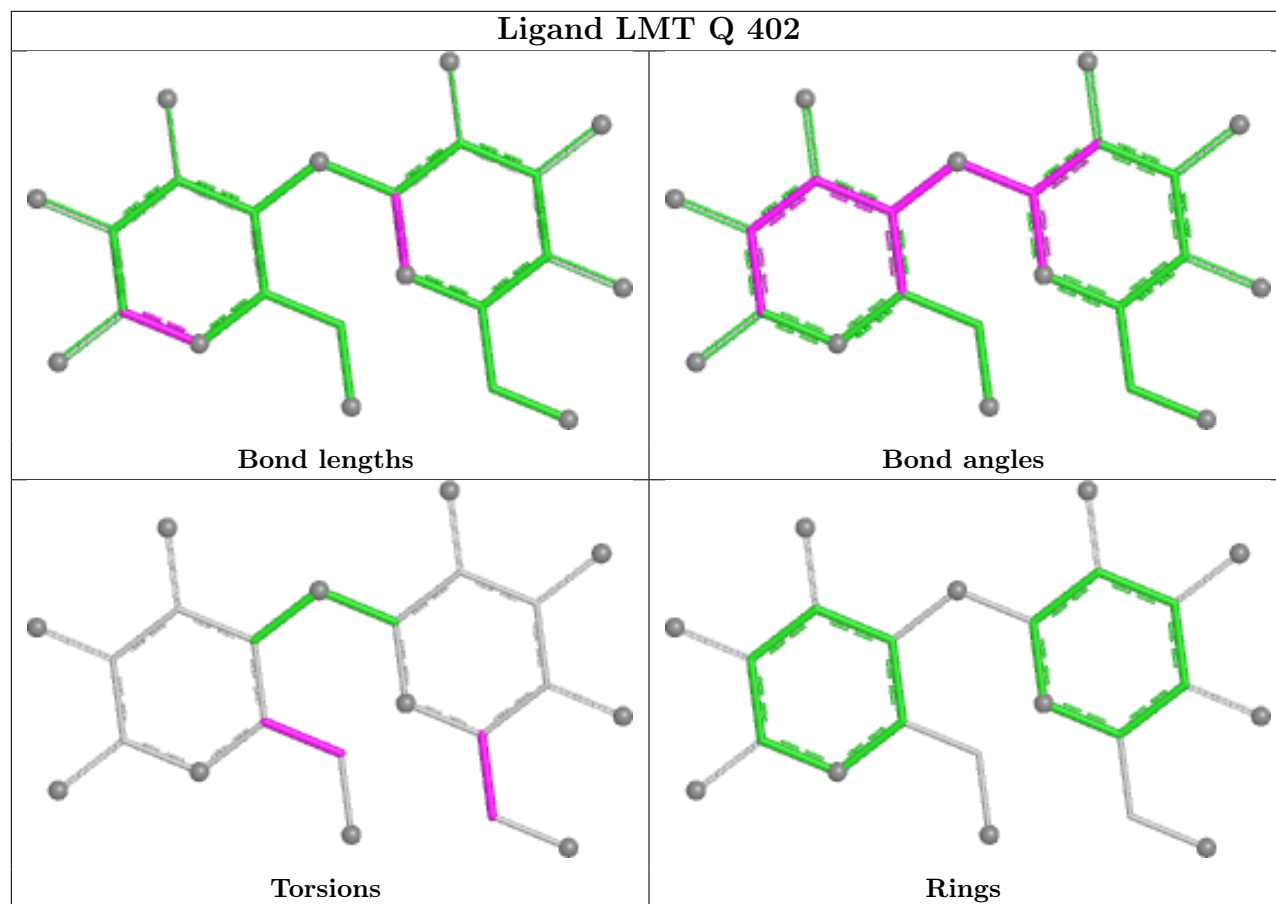


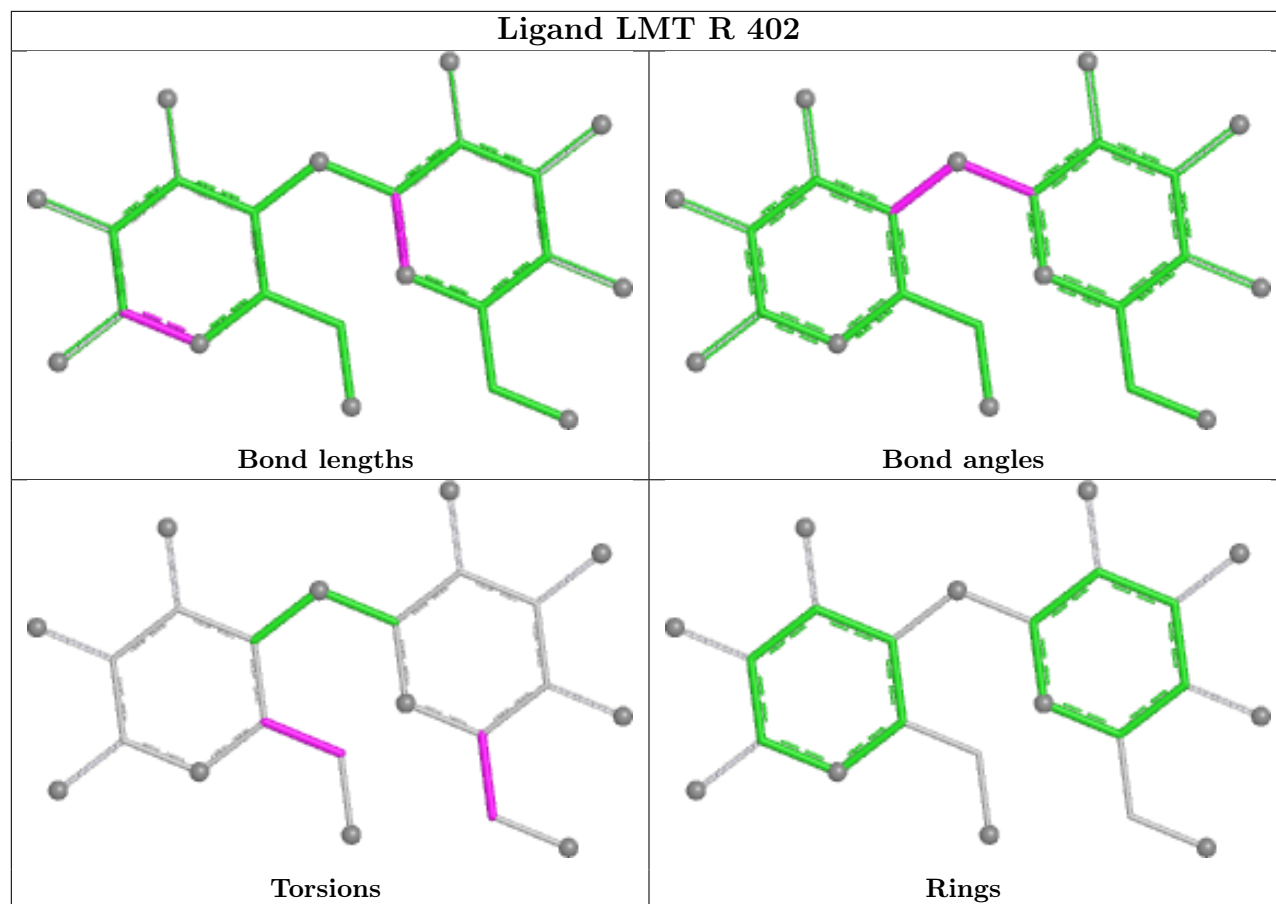


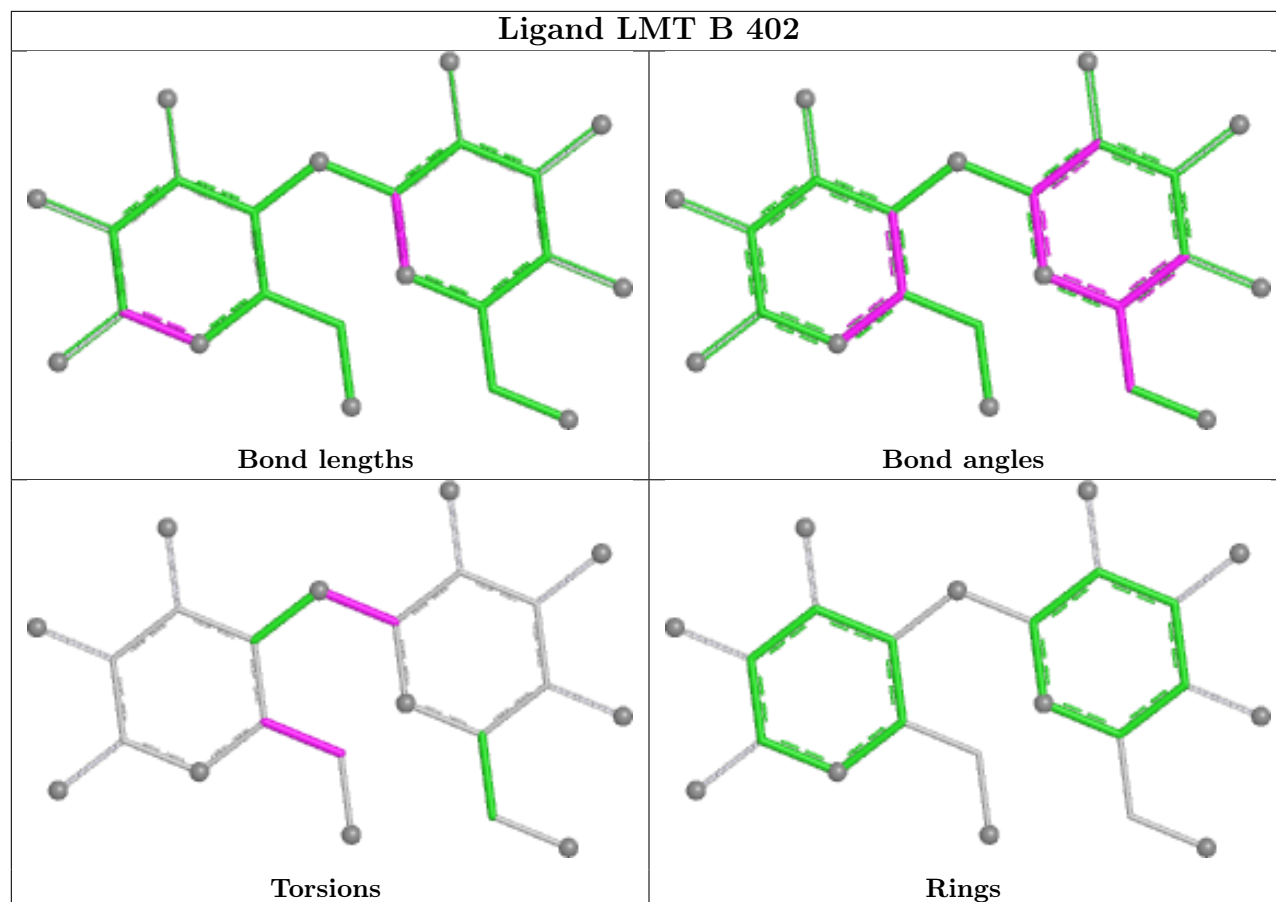












5.7 Other polymers [i](#)

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	337/347 (97%)	0.03	8 (2%) 59 34	91, 137, 216, 241	0
1	B	337/347 (97%)	0.08	12 (3%) 46 26	100, 143, 229, 269	0
1	C	337/347 (97%)	-0.05	5 (1%) 72 44	94, 140, 228, 260	0
1	D	337/347 (97%)	0.08	7 (2%) 63 37	103, 144, 219, 255	0
1	E	337/347 (97%)	-0.09	6 (1%) 67 40	99, 146, 221, 259	0
1	P	337/347 (97%)	0.04	6 (1%) 67 40	92, 110, 180, 204	0
1	Q	337/347 (97%)	-0.02	6 (1%) 67 40	88, 110, 175, 199	0
1	R	337/347 (97%)	0.13	11 (3%) 49 28	87, 105, 166, 183	0
1	S	337/347 (97%)	0.02	8 (2%) 59 34	82, 101, 171, 193	0
1	T	337/347 (97%)	-0.05	7 (2%) 63 37	84, 109, 173, 203	0
2	F	222/224 (99%)	-0.15	1 (0%) 87 66	112, 139, 215, 248	0
2	G	224/224 (100%)	-0.13	1 (0%) 88 70	103, 168, 199, 209	0
2	H	223/224 (99%)	-0.21	0 100 100	84, 121, 151, 224	0
2	I	222/224 (99%)	-0.28	3 (1%) 73 46	105, 133, 203, 223	0
2	J	223/224 (99%)	-0.02	5 (2%) 62 36	115, 162, 263, 278	0
2	U	221/224 (98%)	-0.07	2 (0%) 81 56	121, 172, 241, 253	0
2	V	224/224 (100%)	-0.27	1 (0%) 88 70	114, 154, 185, 261	0
2	W	224/224 (100%)	-0.45	0 100 100	102, 126, 145, 207	0
2	X	224/224 (100%)	-0.24	2 (0%) 81 56	98, 118, 137, 187	0
2	Y	221/224 (98%)	0.04	4 (1%) 67 40	139, 197, 278, 297	0
3	K	212/215 (98%)	-0.19	2 (0%) 81 56	104, 133, 187, 198	0
3	L	211/215 (98%)	-0.33	0 100 100	81, 109, 162, 172	0
3	M	211/215 (98%)	-0.15	2 (0%) 81 56	118, 151, 247, 254	0
3	N	211/215 (98%)	-0.28	3 (1%) 73 46	111, 150, 173, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	O	211/215 (98%)	-0.17	4 (1%) 66 39	104, 134, 153, 160	0
3	Z	215/215 (100%)	-0.24	1 (0%) 87 66	112, 161, 190, 244	0
3	f	214/215 (99%)	-0.34	0 100 100	101, 124, 138, 174	0
3	g	211/215 (98%)	0.05	3 (1%) 73 46	150, 223, 274, 281	0
3	h	211/215 (98%)	-0.14	2 (0%) 81 56	119, 178, 207, 217	0
3	i	214/215 (99%)	-0.40	0 100 100	99, 119, 138, 169	0
All	All	7719/7860 (98%)	-0.10	112 (1%) 72 44	81, 134, 233, 297	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	ALA	6.9
1	R	244	ALA	5.2
1	C	24	ASN	5.0
1	S	107	ASN	4.2
1	C	89	ASP	4.2
3	g	164	THR	4.2
1	P	64	LEU	4.0
1	T	107	ASN	4.0
1	S	264	ASN	3.9
1	A	244	ALA	3.8
1	R	277	ASP	3.6
2	J	161	VAL	3.6
3	K	183	LEU	3.5
1	B	81	VAL	3.5
1	B	89	ASP	3.4
1	B	147	ASP	3.3
1	R	89	ASP	3.3
1	D	131	PRO	3.2
2	J	176	PRO	3.2
1	E	277	ASP	3.2
1	S	147	ASP	3.2
1	R	98	ALA	3.1
1	S	6	LEU	3.1
1	Q	277	ASP	3.1
1	B	240	THR	2.9
1	B	251	THR	2.9
1	T	98	ALA	2.9
2	J	55	ASN	2.9
3	N	126	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	2.8
1	D	132	MET	2.8
1	R	249	GLY	2.8
1	B	99	TYR	2.8
2	I	130	VAL	2.8
1	B	98	ALA	2.7
1	P	98	ALA	2.7
3	O	62	ALA	2.7
2	F	62	GLN	2.7
1	D	277	ASP	2.6
3	g	84	ASP	2.6
1	E	178	LEU	2.6
1	S	277	ASP	2.5
3	Z	64	PHE	2.5
1	D	68	VAL	2.5
2	Y	132	PRO	2.4
1	E	240	THR	2.4
3	O	43	ASP	2.4
1	B	230	VAL	2.4
2	J	150	LEU	2.4
2	X	135	PRO	2.4
2	I	66	GLY	2.4
3	O	59	GLY	2.4
1	T	124	ILE	2.4
3	K	109	LEU	2.4
1	A	290	ALA	2.4
1	Q	244	ALA	2.4
1	A	99	TYR	2.3
1	A	291	LEU	2.3
1	T	210	LYS	2.3
1	P	112	ILE	2.3
2	J	47	TRP	2.3
1	D	244	ALA	2.3
1	S	106	PRO	2.3
3	M	123	PRO	2.3
2	V	174	THR	2.3
2	G	152	LYS	2.3
2	U	23	LYS	2.3
3	O	173	ASN	2.2
3	h	196	CYS	2.2
1	B	248	LEU	2.2
1	D	247	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	S	237	PHE	2.2
1	B	241	ALA	2.2
2	Y	149	CYS	2.2
1	T	290	ALA	2.2
1	R	231	SER	2.2
2	X	192	VAL	2.2
1	D	249	GLY	2.2
1	R	159	GLU	2.2
1	Q	179	PRO	2.2
1	Q	89	ASP	2.2
2	Y	161	VAL	2.2
1	E	98	ALA	2.1
3	h	135	LEU	2.2
1	A	89	ASP	2.1
1	C	99	TYR	2.1
3	M	118	VAL	2.1
2	I	109	PHE	2.1
1	P	159	GLU	2.1
1	R	240	THR	2.1
1	R	187	SER	2.1
1	C	23	ASP	2.1
2	Y	174	THR	2.1
3	N	50	ILE	2.1
1	Q	246	VAL	2.1
1	A	292	LEU	2.1
1	E	258	ALA	2.1
1	R	224	SER	2.1
1	R	271	SER	2.1
1	P	277	ASP	2.1
1	S	238	ASP	2.1
1	E	95	GLU	2.1
1	C	98	ALA	2.1
1	Q	98	ALA	2.1
3	N	96	ASN	2.1
1	T	89	ASP	2.1
1	T	262	GLY	2.1
2	U	128	PRO	2.1
1	A	245	ARG	2.1
3	g	165	THR	2.0
1	P	25	GLY	2.0
1	B	45	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 [i](#)

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

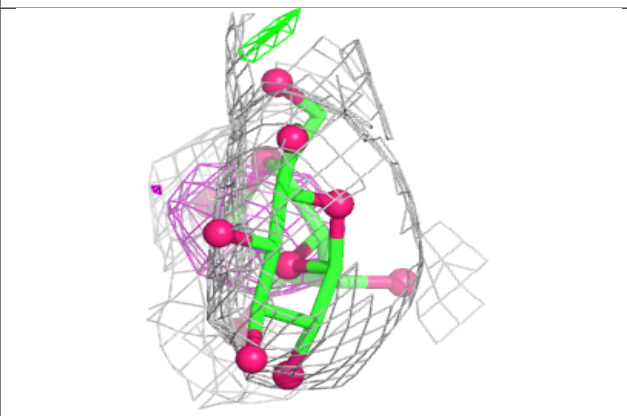
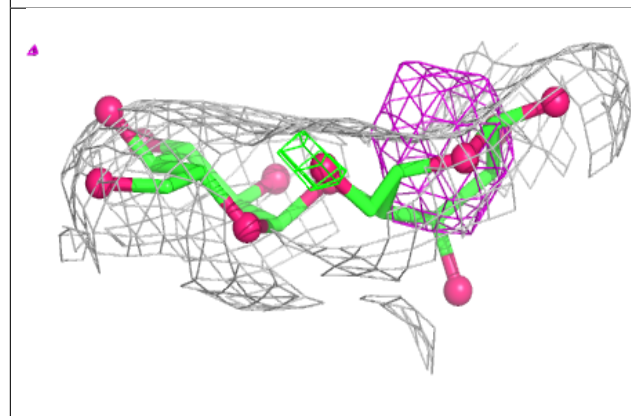
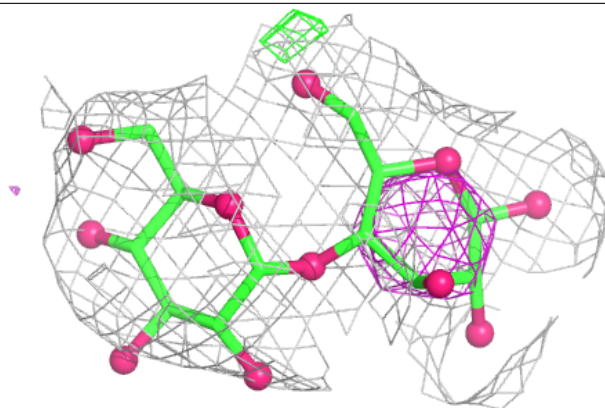
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	R	401	14/15	0.28	0.10	191,191,191,191	0
4	NAG	C	401	14/15	0.39	0.13	158,158,158,158	0
4	NAG	D	401	14/15	0.41	0.13	204,204,204,204	0
4	NAG	A	401	14/15	0.45	0.13	165,165,165,165	0
4	NAG	Q	401	14/15	0.52	0.10	176,176,176,176	0
4	NAG	E	401	14/15	0.52	0.11	170,170,170,170	0
4	NAG	T	401	14/15	0.58	0.13	182,182,182,182	0
4	NAG	S	401	14/15	0.59	0.09	218,218,218,218	0
5	LMT	Q	402	23/35	0.61	0.11	143,143,143,143	0
4	NAG	B	401	14/15	0.62	0.11	172,172,172,172	0
5	LMT	D	402	23/35	0.63	0.09	189,189,189,189	0
4	NAG	P	401	14/15	0.64	0.10	232,232,232,232	0
5	LMT	C	402	23/35	0.65	0.09	173,173,173,173	0
5	LMT	E	402	23/35	0.68	0.08	177,177,177,177	0
5	LMT	S	402	23/35	0.68	0.09	130,130,130,130	0
6	FLC	A	403	13/13	0.68	0.10	168,168,168,168	0
5	LMT	B	402	23/35	0.70	0.09	181,181,181,181	0
5	LMT	P	402	23/35	0.71	0.10	149,149,149,149	0
6	FLC	T	403	13/13	0.72	0.08	187,187,187,187	0
5	LMT	T	402	25/35	0.76	0.13	145,145,145,145	0
5	LMT	R	402	23/35	0.76	0.09	149,149,149,149	0
5	LMT	A	402	23/35	0.76	0.10	211,211,211,211	0
7	CL	P	404	1/1	0.87	0.31	115,115,115,115	0
7	CL	P	403	1/1	0.93	0.16	115,115,115,115	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.

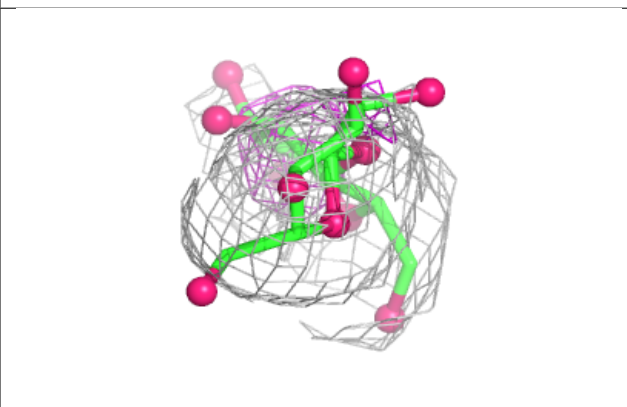
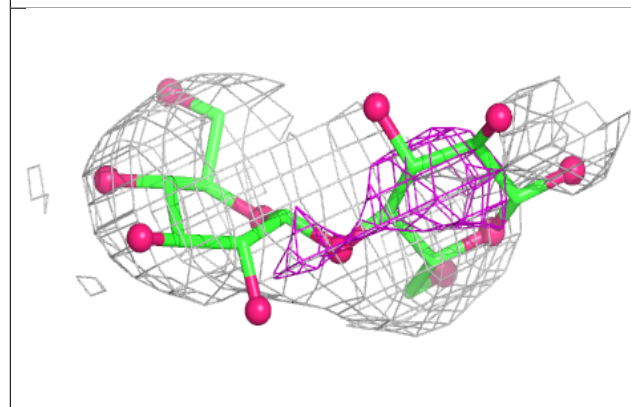
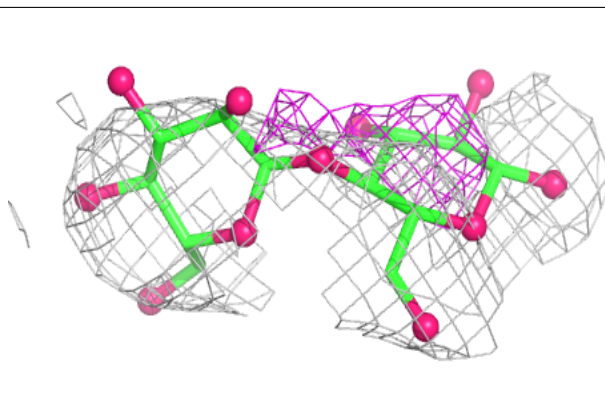
Electron density around LMT Q 402:

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



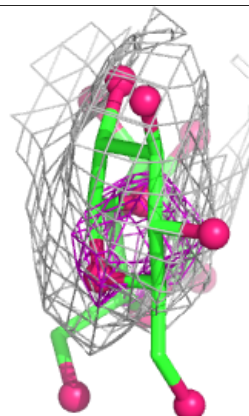
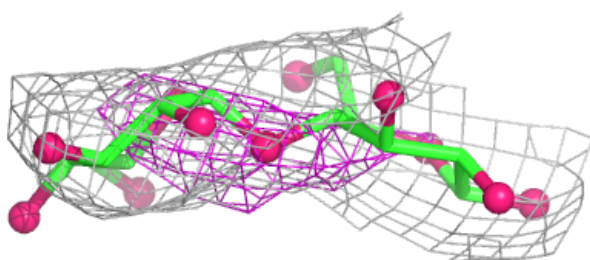
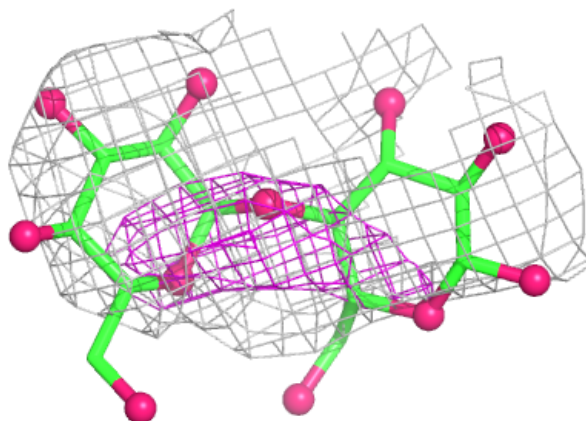
Electron density around LMT D 402:

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

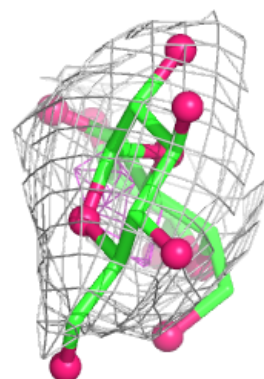
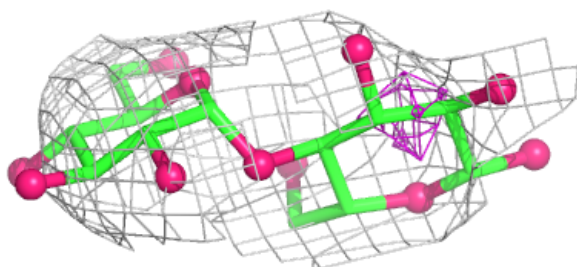
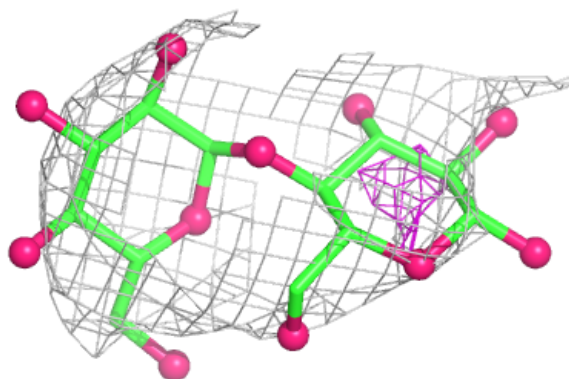


Electron density around LMT C 402:

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

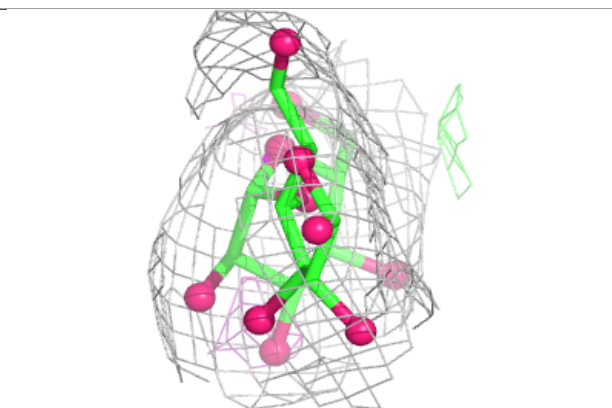
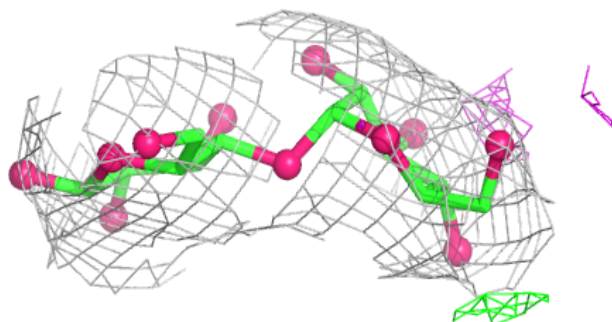
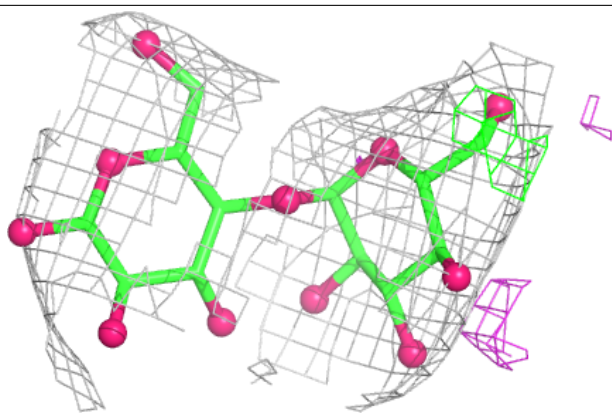
**Electron density around LMT E 402:**

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

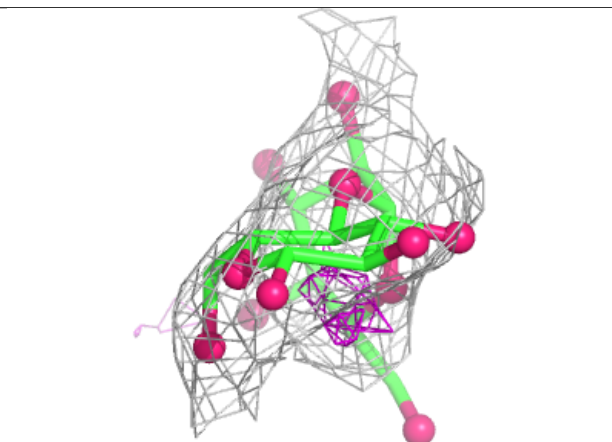
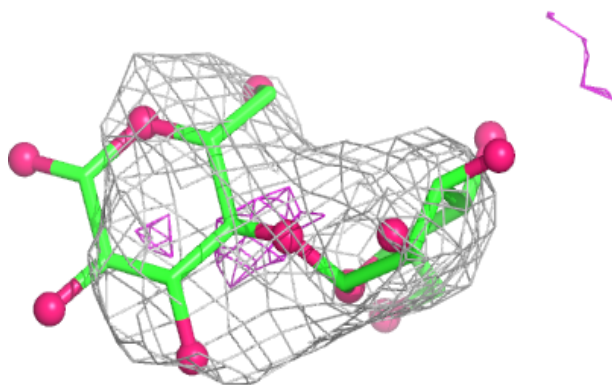
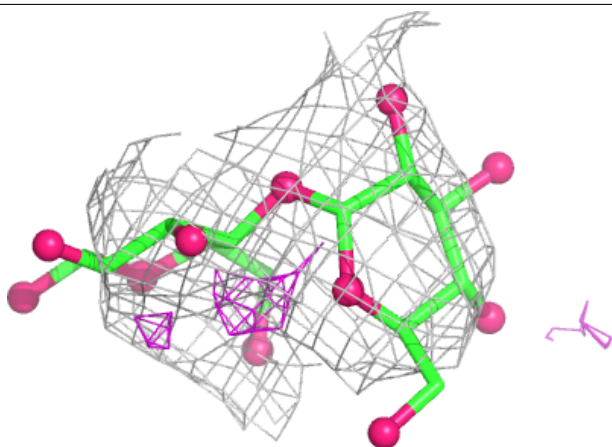


Electron density around LMT S 402:

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

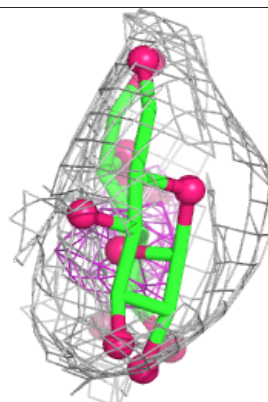
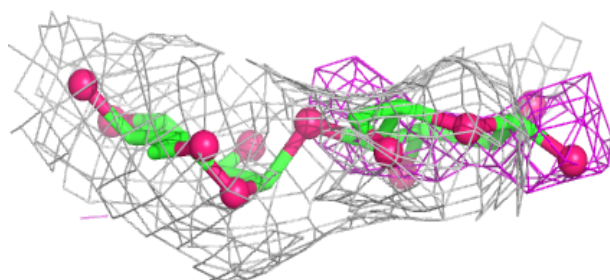
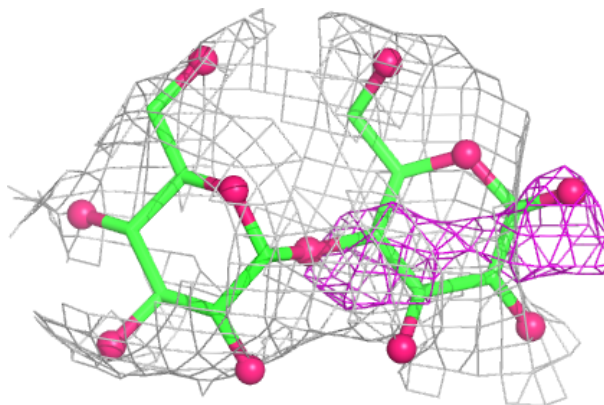
**Electron density around LMT B 402:**

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

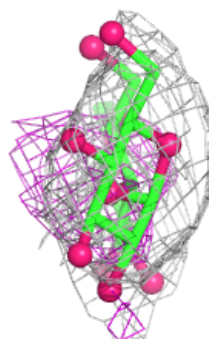
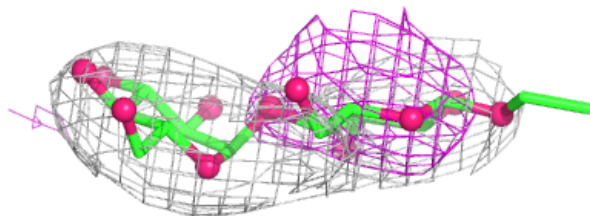
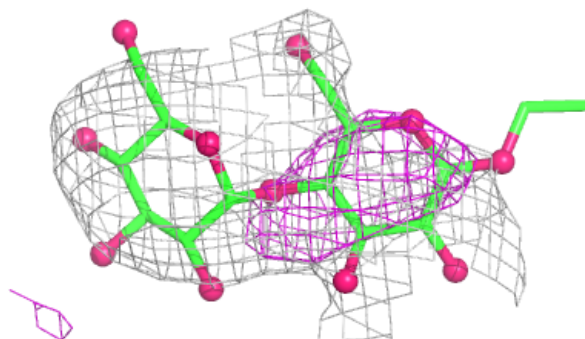


Electron density around LMT P 402:

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

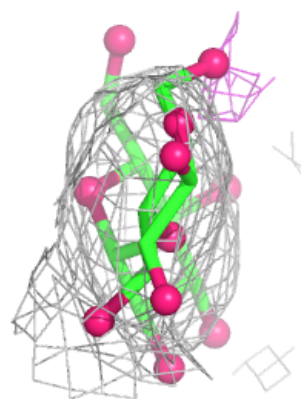
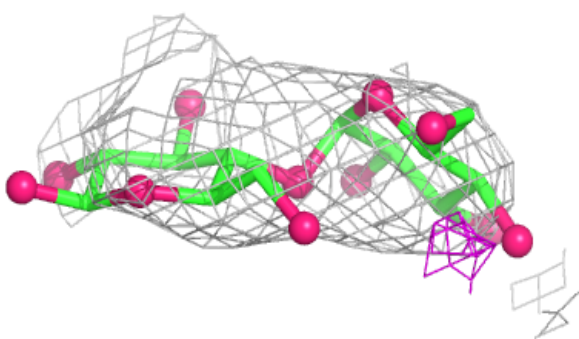
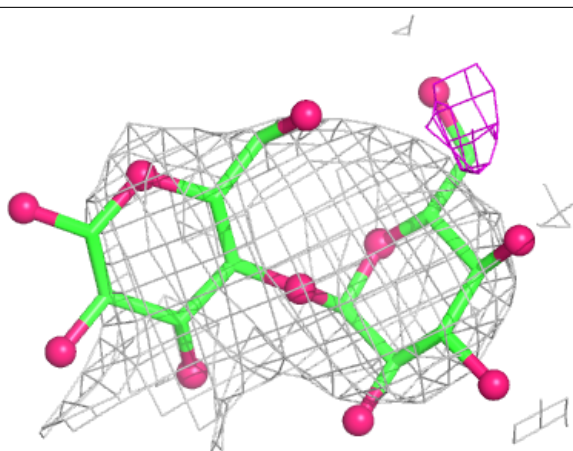
**Electron density around LMT T 402:**

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

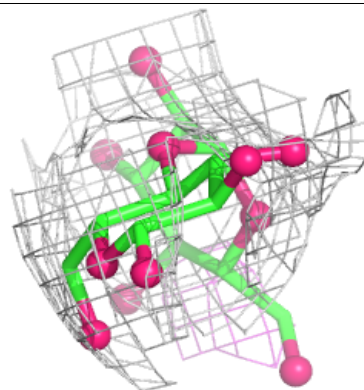
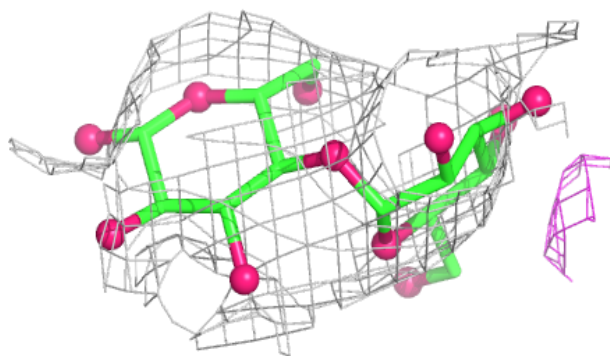
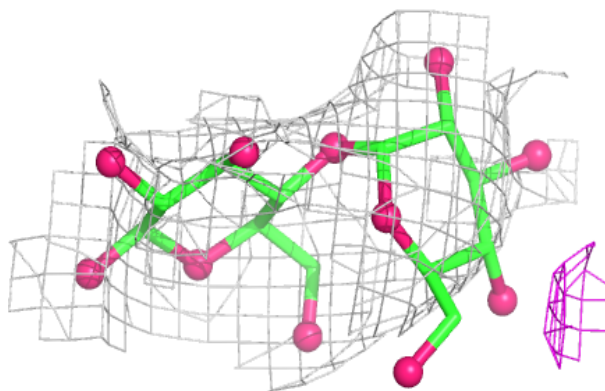


Electron density around LMT R 402:

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

**Electron density around LMT A 402:**

$2mF_o-DF_c$ (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.