



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:58 AM UTC

PDB ID : 4TNW / pdb_00004tnw
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab and POPC in a lipid-modulated conformation
Authors : Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.
Deposited on : 2014-06-05
Resolution : 3.20 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

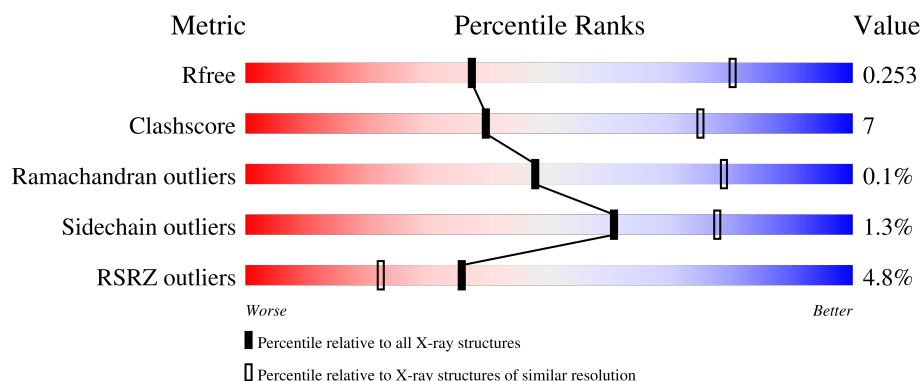
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	9% 78% 20% ..
1	B	347	4% 77% 21% ..
1	C	347	6% 76% 21% ..
1	D	347	5% 79% 18% ..
1	E	347	5% 78% 18% ..

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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 8 unique types of molecules in this entry. The entry contains 60818 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	342	Total	C	N	O	S	0	0	0
			2744	1786	449	494	15			
1	B	341	Total	C	N	O	S	0	0	0
			2734	1780	446	493	15			
1	C	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	D	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	P	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	Q	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	R	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	S	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	T	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	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

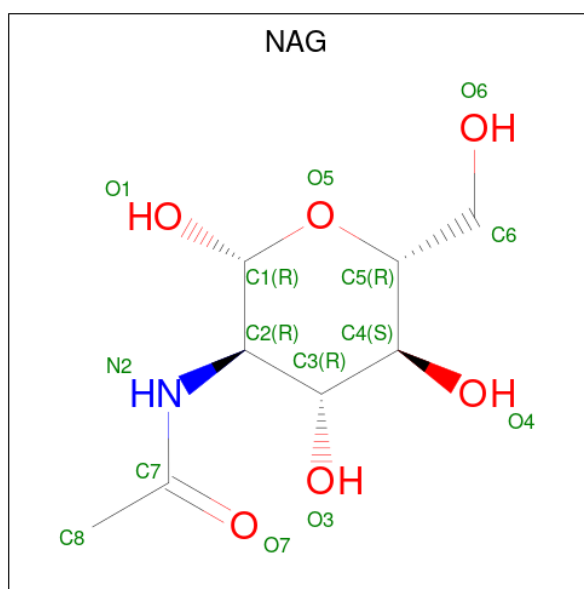
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	G	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			
2	H	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			
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	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.

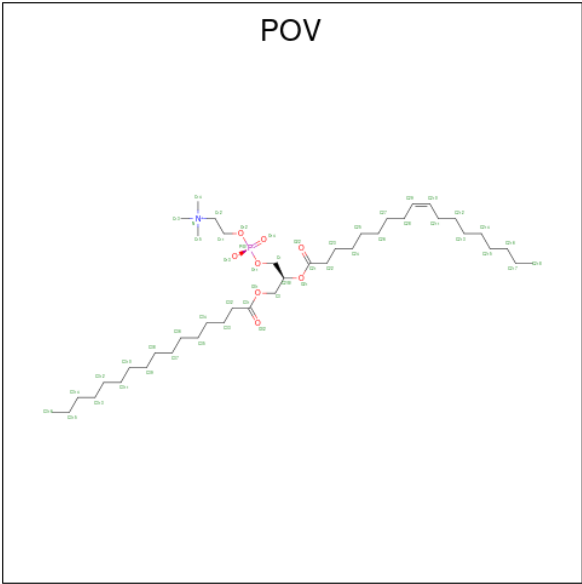
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	210	Total	C	N	O	S	0	0	0
			1590	999	266	319	6			
3	L	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	N	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	O	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	Z	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	7			
3	f	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	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	210	Total	C	N	O	S	0	0	0
			1590	999	266	319	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	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 (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 23	C 14	N 1	O 7	P 1	0	0
5	D	1	Total 26	C 16	N 1	O 8	P 1	0	0

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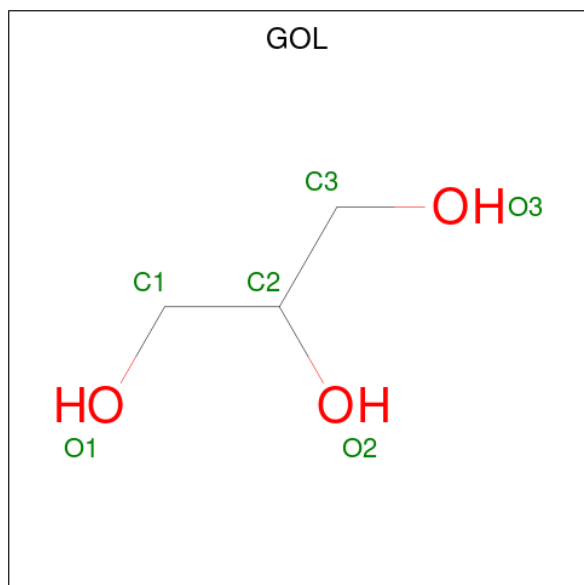
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	P	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
5	Q	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
5	R	1	Total	C	N	O	P	0	0
			34	24	1	8	1		
5	R	1	Total	C	O	P		0	0
			35	26	8	1			
5	T	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

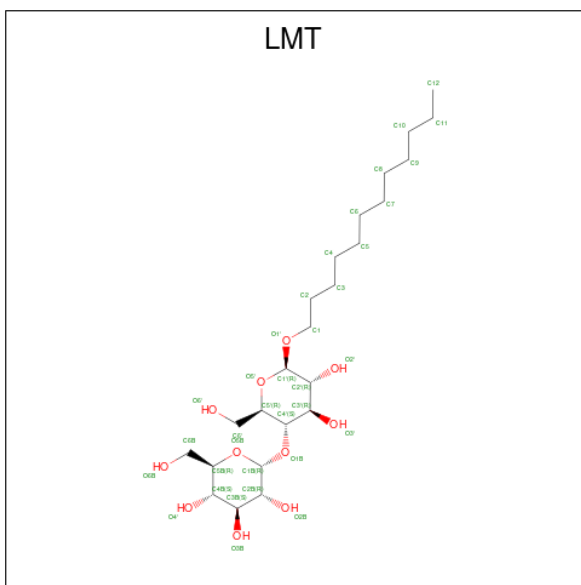
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	P	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

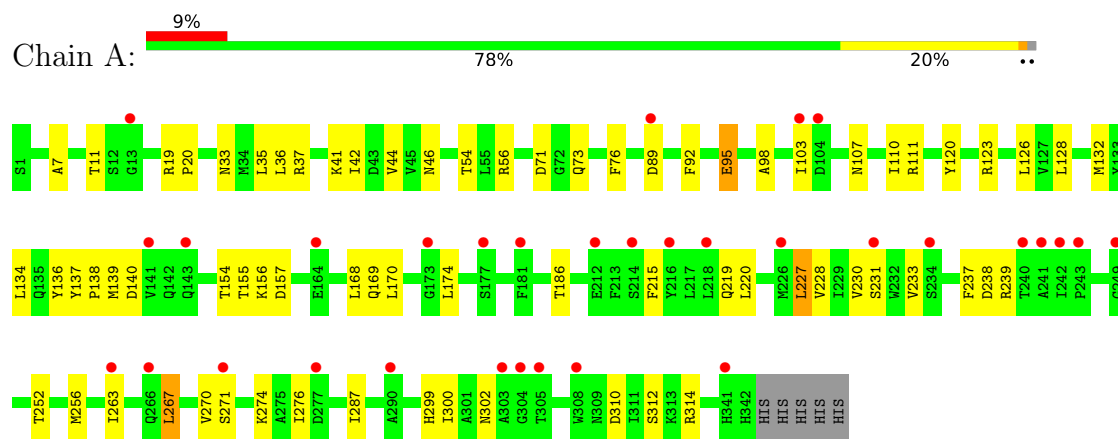


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 23	C 12	O 11	0	0
8	C	1	Total 23	C 12	O 11	0	0
8	D	1	Total 23	C 12	O 11	0	0
8	E	1	Total 23	C 12	O 11	0	0
8	P	1	Total 23	C 12	O 11	0	0
8	S	1	Total 23	C 12	O 11	0	0
8	T	1	Total 23	C 12	O 11	0	0

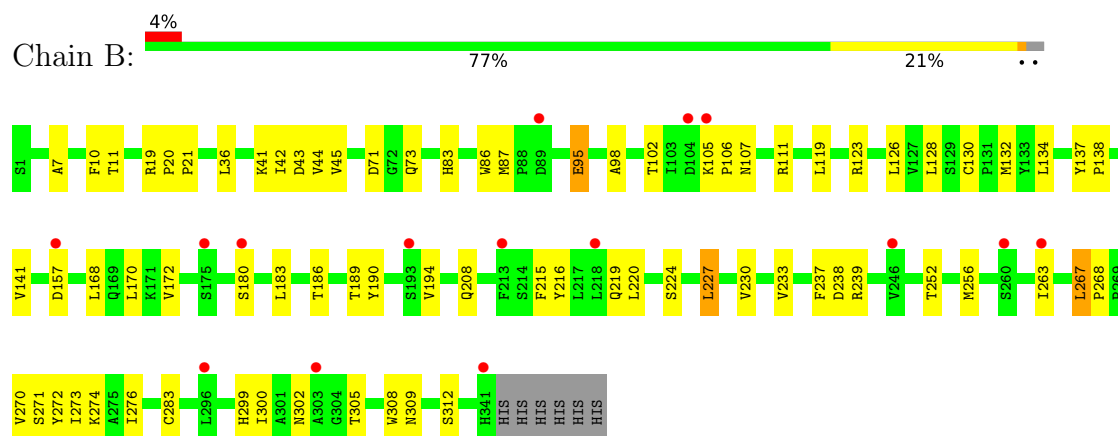
3 Residue-property plots [i](#)

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.

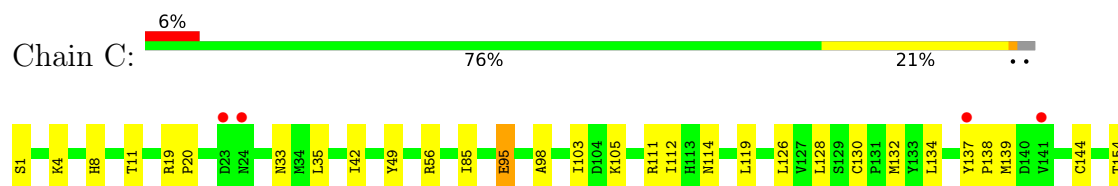
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

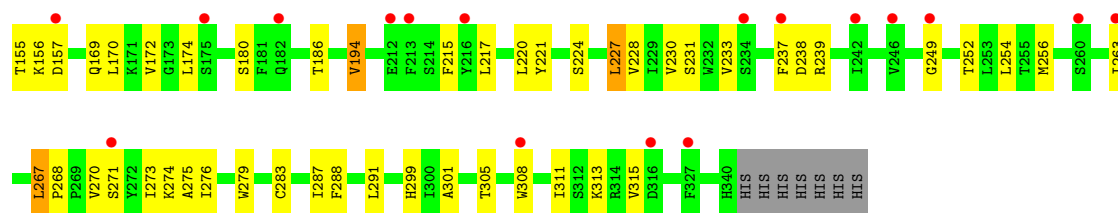


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

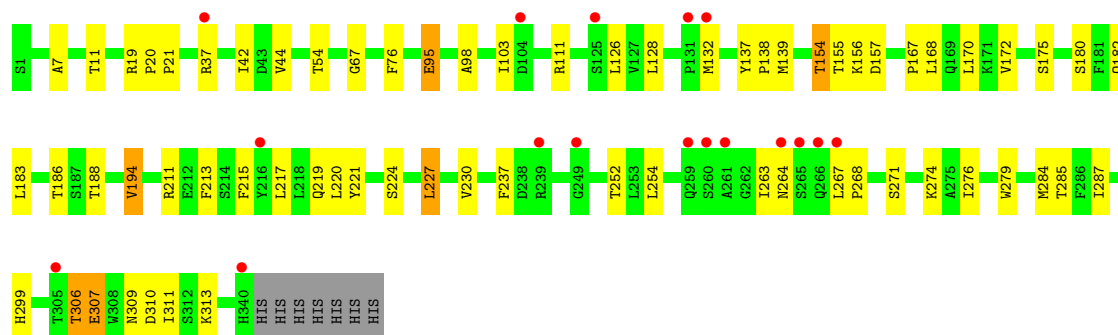
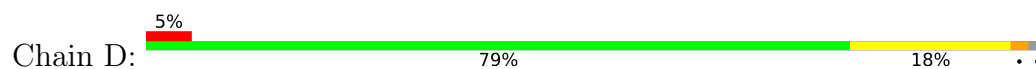


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

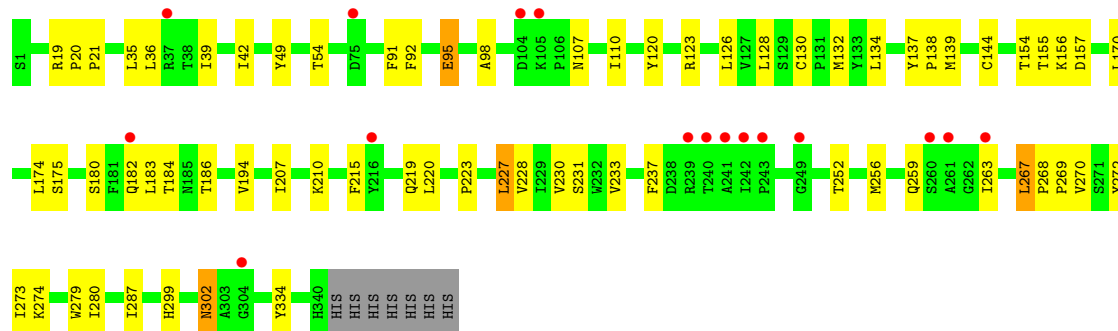
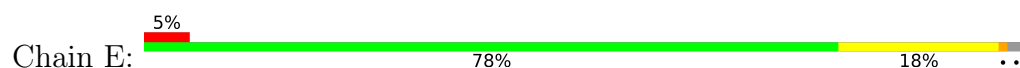




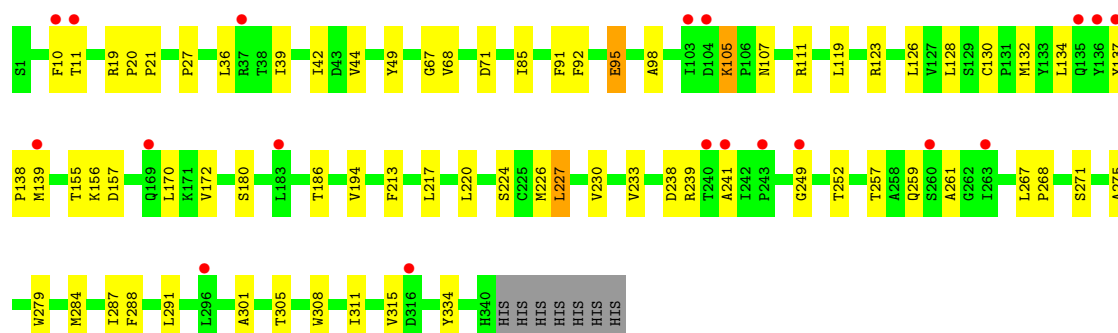
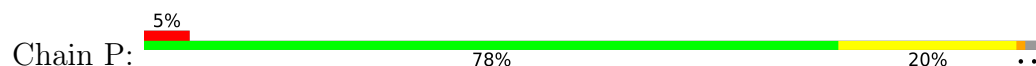
● Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



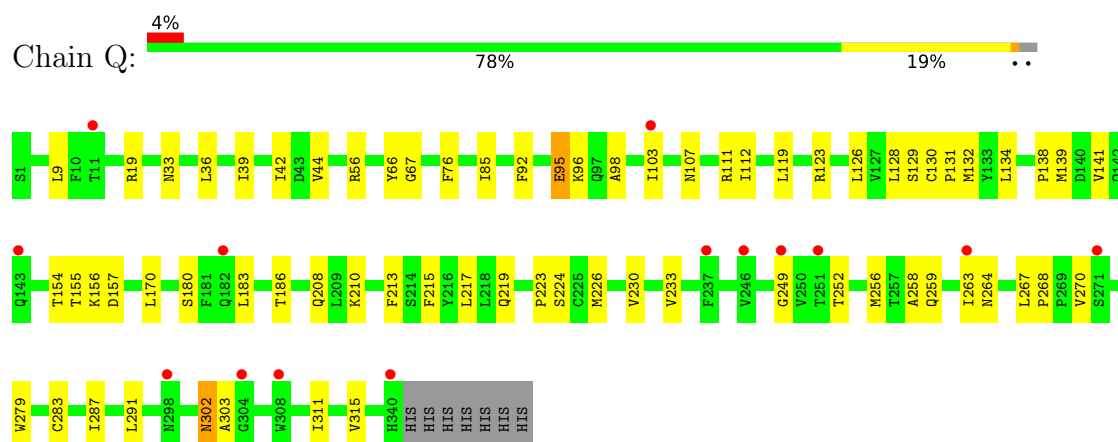
● Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



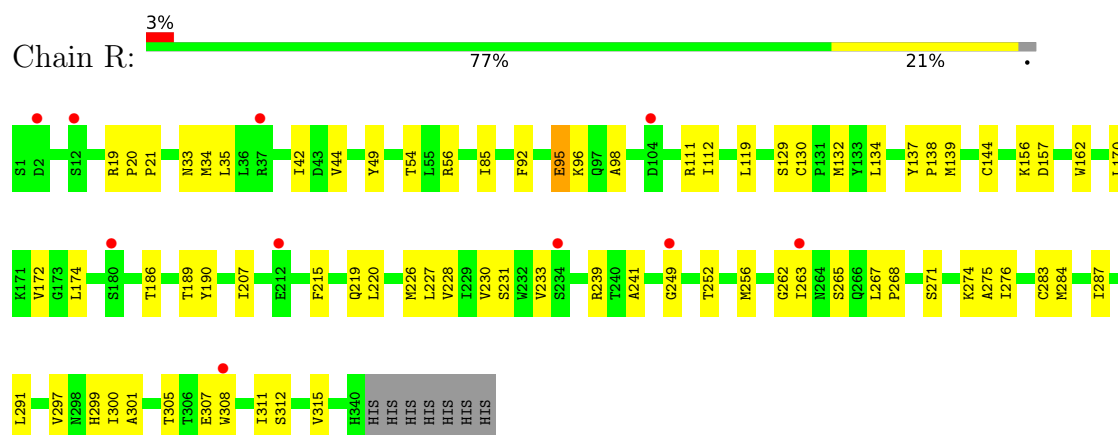
● Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



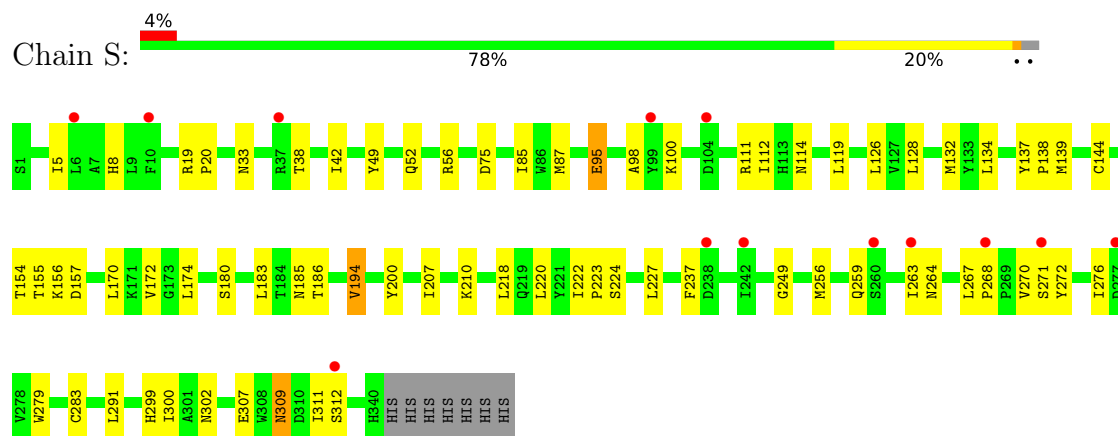
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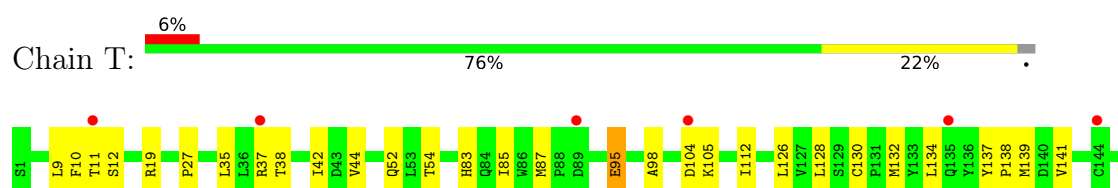
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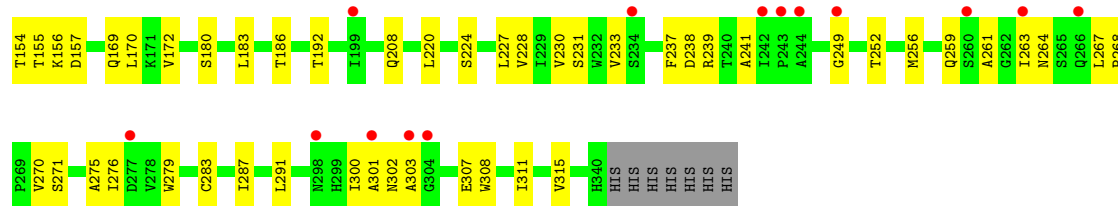


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

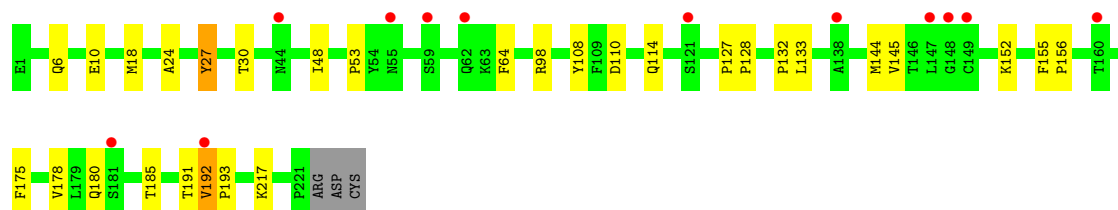
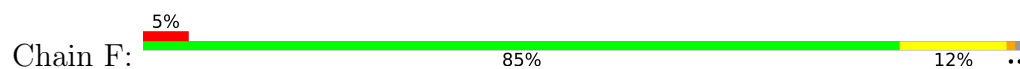


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

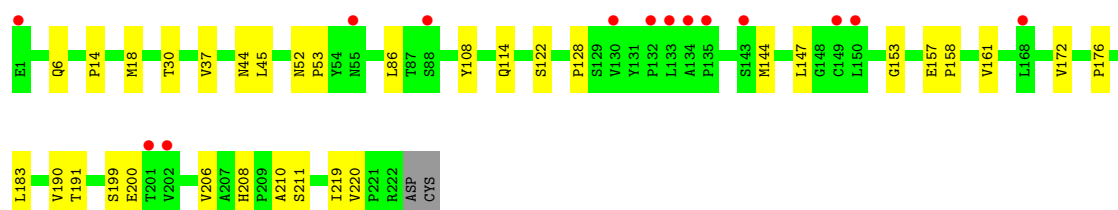
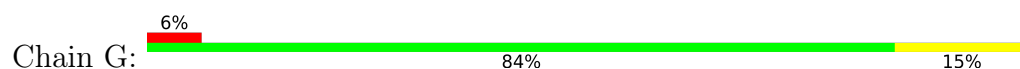




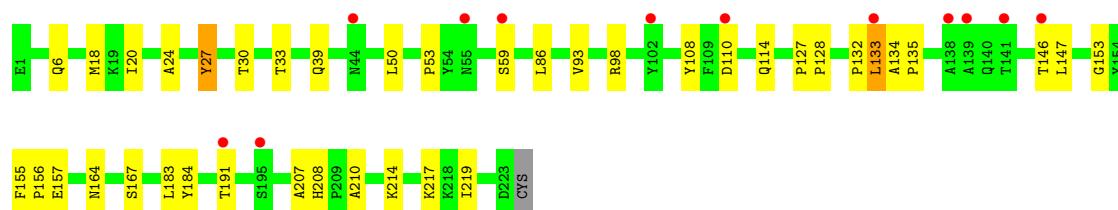
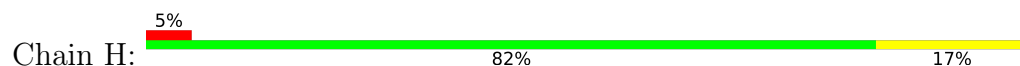
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



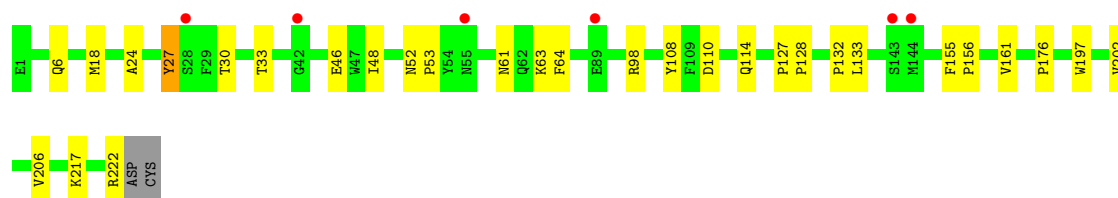
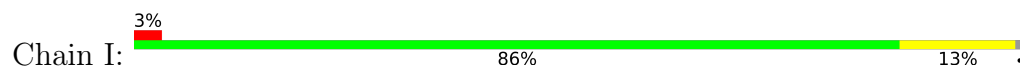
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



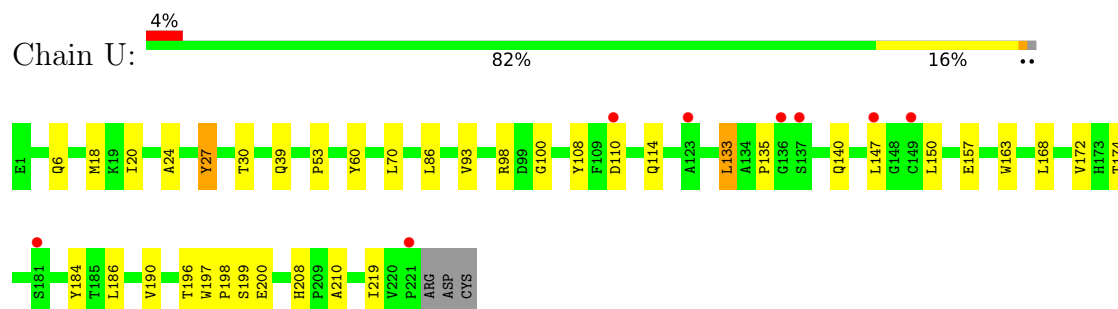
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



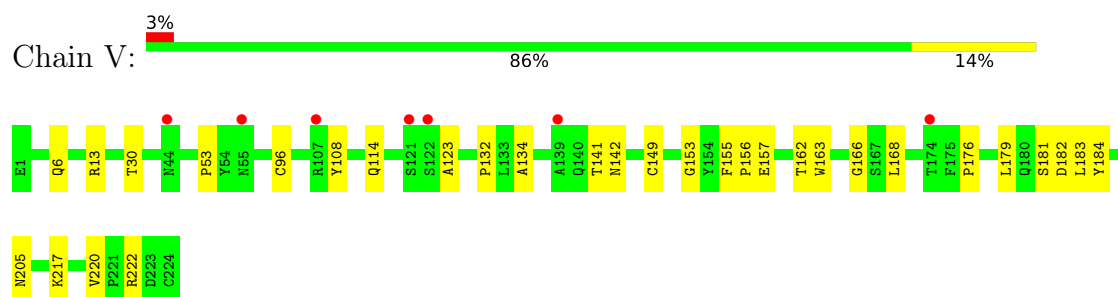
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



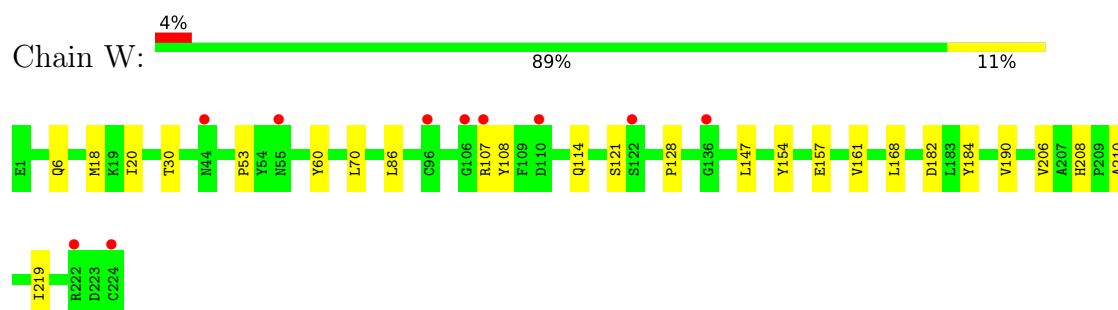
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



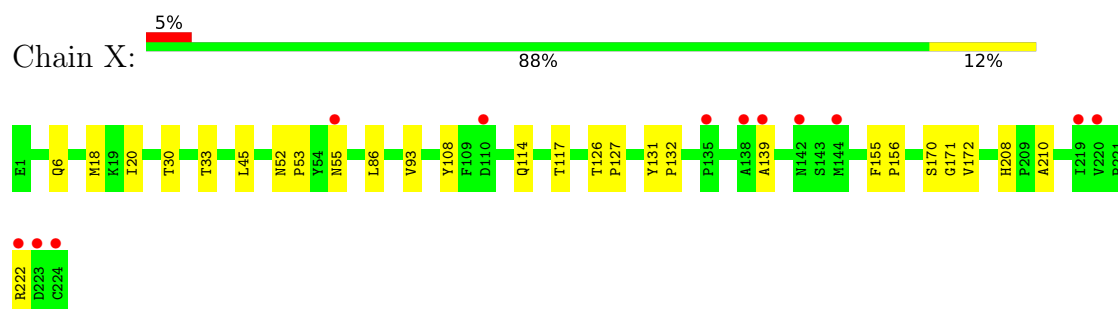
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



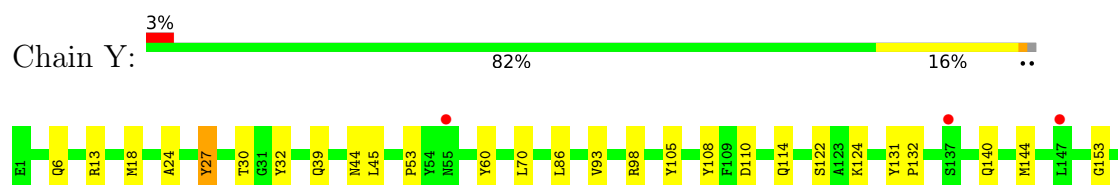
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

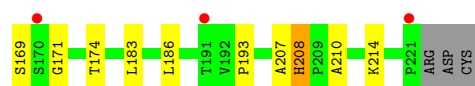


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

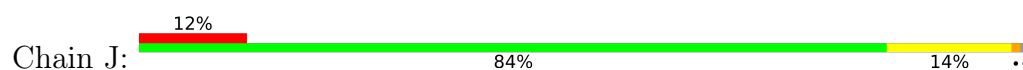


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

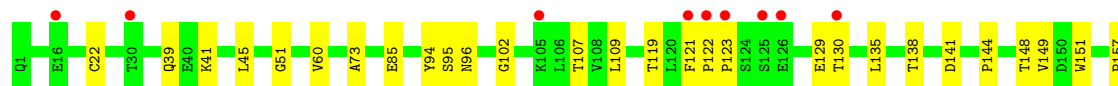
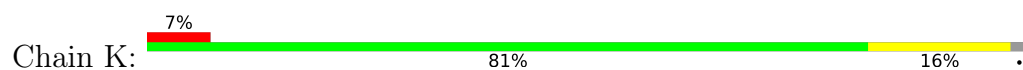




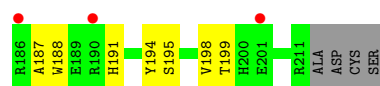
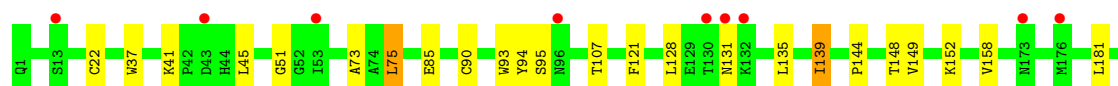
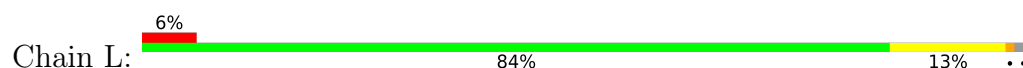
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



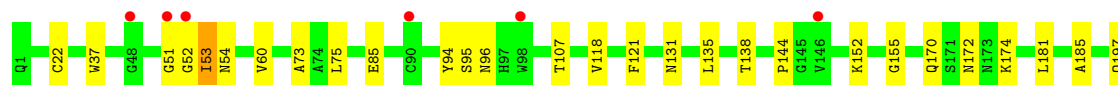
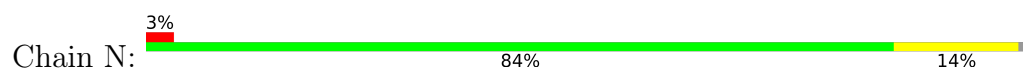
- Molecule 3: Mouse monoclonal Fab fragment, light chain



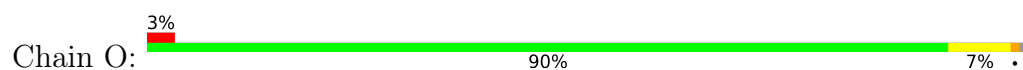
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain

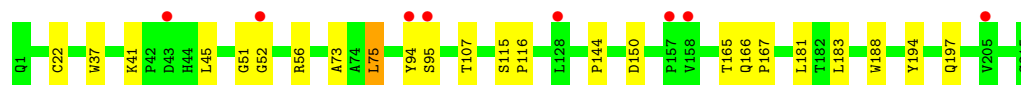
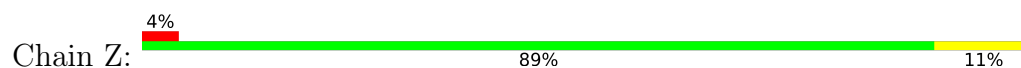


- Molecule 3: Mouse monoclonal Fab fragment, light chain

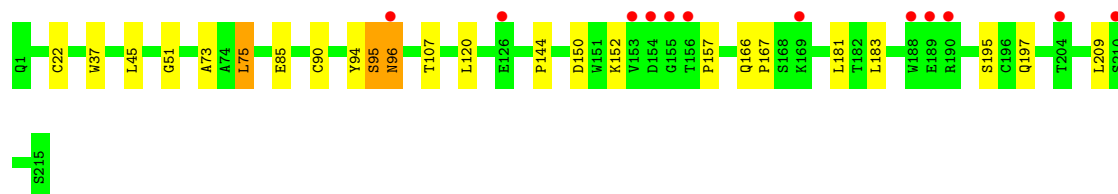
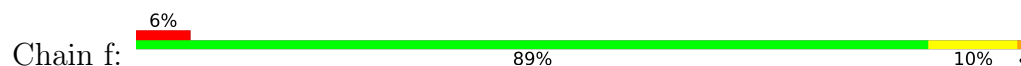




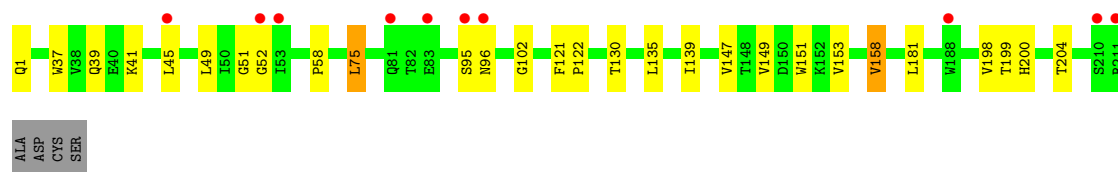
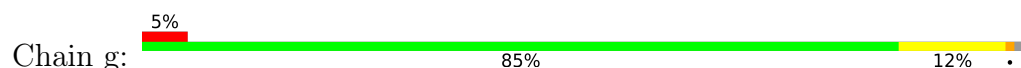
- Molecule 3: Mouse monoclonal Fab fragment, light chain



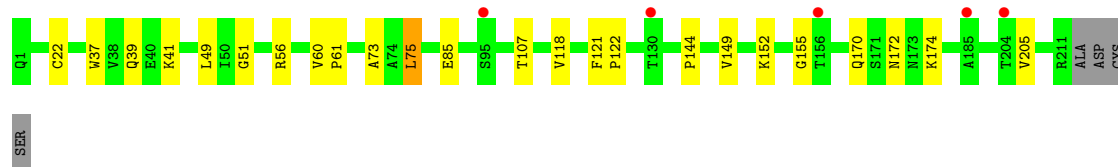
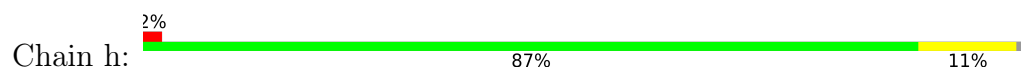
- Molecule 3: Mouse monoclonal Fab fragment, light chain



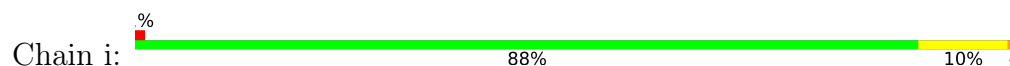
- Molecule 3: Mouse monoclonal Fab fragment, light chain



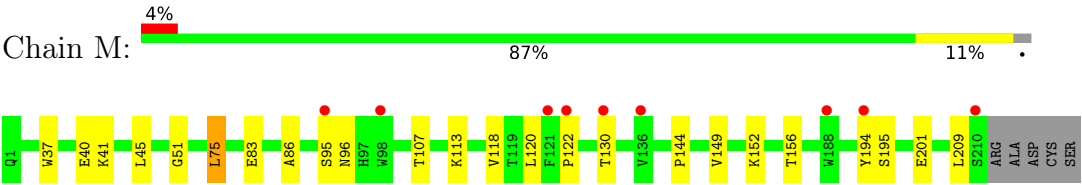
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	453.75Å 192.87Å 196.14Å 90.00° 92.27° 90.00°	Depositor
Resolution (Å)	58.70 – 3.20 58.70 – 3.20	Depositor EDS
% Data completeness (in resolution range)	77.6 (58.70-3.20) 92.3 (58.70-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.227 , 0.251 0.232 , 0.253	Depositor DCC
R_{free} test set	14870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	60818	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: LMT, POV, GOL, NAG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2819	0.78	3/3847 (0.1%)
1	B	0.31	0/2808	0.77	3/3832 (0.1%)
1	C	0.31	0/2797	0.78	2/3817 (0.1%)
1	D	0.33	0/2797	0.82	5/3817 (0.1%)
1	E	0.32	0/2797	0.79	5/3817 (0.1%)
1	P	0.32	0/2797	0.79	4/3817 (0.1%)
1	Q	0.32	0/2797	0.77	4/3817 (0.1%)
1	R	0.32	0/2797	0.77	3/3817 (0.1%)
1	S	0.32	0/2797	0.76	0/3817
1	T	0.32	0/2797	0.78	1/3817 (0.0%)
2	F	0.26	0/1728	0.71	2/2360 (0.1%)
2	G	0.29	0/1739	0.72	0/2374
2	H	0.26	0/1747	0.72	0/2385
2	I	0.25	0/1739	0.70	0/2374
2	J	0.30	0/1739	0.75	2/2374 (0.1%)
2	U	0.26	0/1728	0.69	0/2360
2	V	0.27	0/1753	0.72	1/2393 (0.0%)
2	W	0.26	0/1753	0.72	0/2393
2	X	0.26	0/1753	0.74	1/2393 (0.0%)
2	Y	0.26	0/1728	0.72	3/2360 (0.1%)
3	K	0.27	0/1628	0.71	2/2226 (0.1%)
3	L	0.28	0/1639	0.74	1/2240 (0.0%)
3	M	0.29	0/1628	0.77	4/2226 (0.2%)
3	N	0.29	0/1639	0.73	2/2240 (0.1%)
3	O	0.27	0/1639	0.70	0/2240
3	Z	0.28	0/1664	0.73	1/2274 (0.0%)
3	f	0.28	0/1664	0.71	0/2274
3	g	0.28	0/1639	0.72	0/2240
3	h	0.27	0/1639	0.70	0/2240
3	i	0.27	0/1658	0.71	0/2266
All	All	0.30	0/61847	0.75	49/84447 (0.1%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	11	THR	N-CA-C	-9.03	100.59	111.69
1	D	67	GLY	N-CA-C	7.89	123.66	110.56
1	T	11	THR	N-CA-C	-7.79	102.42	112.23
1	C	267	LEU	CA-C-N	6.80	124.56	119.66
1	C	267	LEU	C-N-CA	6.80	124.56	119.66
1	E	267	LEU	CA-C-N	6.76	124.53	119.66
1	E	267	LEU	C-N-CA	6.76	124.53	119.66
3	L	131	ASN	CB-CA-C	-6.33	109.26	116.54
1	D	307	GLU	N-CA-C	-6.19	103.46	111.02
1	B	302	ASN	N-CA-C	6.13	118.77	111.71
1	P	67	GLY	N-CA-C	5.84	122.18	110.97
2	Y	140	GLN	CB-CA-C	-5.68	109.50	117.23
3	M	95	SER	CB-CA-C	-5.66	110.03	116.54
3	M	156	THR	CA-C-N	-5.66	113.38	120.51
3	M	156	THR	C-N-CA	-5.66	113.38	120.51
2	X	139	ALA	CB-CA-C	-5.59	110.15	116.63
1	D	306	THR	N-CA-C	5.48	118.01	111.71
1	Q	302	ASN	N-CA-C	5.45	117.98	111.71
1	Q	92	PHE	CA-C-N	5.45	125.53	119.32
1	Q	92	PHE	C-N-CA	5.45	125.53	119.32
1	R	265	SER	N-CA-C	5.43	117.00	111.14
1	P	92	PHE	CA-C-N	5.35	125.42	119.32
1	P	92	PHE	C-N-CA	5.35	125.42	119.32
3	Z	94	TYR	N-CA-C	-5.28	102.93	110.59
1	E	302	ASN	N-CA-C	5.26	117.76	111.71
1	D	310	ASP	N-CA-C	5.22	117.87	111.82
3	N	60	VAL	CA-C-N	5.22	125.22	119.89
3	N	60	VAL	C-N-CA	5.22	125.22	119.89
3	K	60	VAL	CA-C-N	5.15	125.14	119.89
3	K	60	VAL	C-N-CA	5.15	125.14	119.89
1	A	302	ASN	N-CA-C	5.15	117.63	111.71
1	Q	67	GLY	N-CA-C	5.15	119.11	110.56
2	F	192	VAL	CA-C-N	5.15	125.15	119.90
2	F	192	VAL	C-N-CA	5.15	125.15	119.90
2	V	181	SER	CB-CA-C	-5.15	110.66	116.63
3	M	96	ASN	N-CA-C	5.14	118.65	112.38
1	R	92	PHE	CA-C-N	5.12	125.16	119.32
1	R	92	PHE	C-N-CA	5.12	125.16	119.32
1	B	267	LEU	CA-C-N	5.09	123.33	119.66
1	B	267	LEU	C-N-CA	5.09	123.33	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	208	HIS	CA-C-N	5.08	124.87	119.28
2	Y	208	HIS	C-N-CA	5.08	124.87	119.28
2	J	8	GLY	CA-C-N	5.06	124.99	119.78
2	J	8	GLY	C-N-CA	5.06	124.99	119.78
1	A	92	PHE	CA-C-N	5.03	125.05	119.32
1	A	92	PHE	C-N-CA	5.03	125.05	119.32
1	D	264	ASN	N-CA-C	5.00	116.73	111.28
1	E	92	PHE	CA-C-N	5.00	125.02	119.32
1	E	92	PHE	C-N-CA	5.00	125.02	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2744	0	2744	48	0
1	B	2734	0	2737	52	0
1	C	2724	0	2729	54	0
1	D	2724	0	2729	47	0
1	E	2724	0	2730	49	0
1	P	2724	0	2730	48	0
1	Q	2724	0	2730	44	0
1	R	2724	0	2731	48	0
1	S	2724	0	2730	54	0
1	T	2724	0	2730	56	0
2	F	1682	0	1632	26	0
2	G	1693	0	1645	23	0
2	H	1701	0	1649	27	0
2	I	1693	0	1645	24	0
2	J	1693	0	1645	23	0
2	U	1682	0	1632	23	0
2	V	1707	0	1653	20	0
2	W	1707	0	1653	16	0
2	X	1707	0	1653	17	0
2	Y	1682	0	1632	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1590	0	1542	25	0
3	L	1601	0	1555	19	0
3	M	1590	0	1542	12	0
3	N	1601	0	1555	21	0
3	O	1601	0	1555	17	0
3	Z	1626	0	1573	13	0
3	f	1626	0	1573	19	0
3	g	1601	0	1555	18	0
3	h	1601	0	1555	13	0
3	i	1620	0	1568	14	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	S	14	0	13	1	0
4	T	14	0	13	0	0
5	A	23	0	26	1	0
5	D	26	0	26	5	0
5	P	42	0	61	4	0
5	Q	46	0	67	6	0
5	R	69	0	83	6	0
5	T	43	0	63	3	0
6	A	1	0	0	0	0
6	P	1	0	0	0	0
7	B	6	0	8	0	0
8	B	23	0	21	0	0
8	C	23	0	21	0	0
8	D	23	0	21	1	0
8	E	23	0	21	0	0
8	P	23	0	21	0	0
8	S	23	0	21	1	0
8	T	23	0	21	1	0
All	All	60818	0	59930	812	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 7.

All (812) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:THR:HA	1:D:309:ASN:HB2	1.53	0.90
1:Q:302:ASN:HD22	1:R:241:ALA:HB2	1.36	0.89
1:T:37:ARG:NH2	1:T:54:THR:OG1	2.10	0.84
1:C:305:THR:HG22	1:C:308:TRP:HD1	1.43	0.83
1:R:156:LYS:HA	3:Z:95:SER:HB2	1.61	0.83
1:D:156:LYS:HA	3:O:95:SER:HB2	1.61	0.81
2:Y:13:ARG:HH22	2:Y:124:LYS:HD2	1.46	0.81
1:Q:302:ASN:ND2	1:R:241:ALA:HB2	1.96	0.81
1:D:37:ARG:NH1	1:D:54:THR:OG1	2.17	0.78
1:Q:141:VAL:HG22	1:Q:210:LYS:HG2	1.67	0.76
1:P:241:ALA:HB2	1:T:302:ASN:HD22	1.52	0.75
1:P:91:PHE:HA	1:Q:103:ILE:HD11	1.69	0.75
1:B:220:LEU:HD22	1:B:263:ILE:HG13	1.68	0.74
3:M:194:TYR:HB2	3:M:209:LEU:HB3	1.69	0.74
2:X:108:TYR:HB2	3:i:51:GLY:HA3	1.68	0.74
1:B:44:VAL:HG11	1:B:134:LEU:HD11	1.69	0.74
1:T:10:PHE:HE2	1:T:83:HIS:HB3	1.52	0.74
1:Q:44:VAL:HG11	1:Q:134:LEU:HD11	1.69	0.73
3:i:107:THR:HG21	3:i:144:PRO:HB3	1.72	0.71
2:Y:108:TYR:HB2	3:g:51:GLY:HA3	1.72	0.71
3:M:107:THR:HG21	3:M:144:PRO:HB3	1.73	0.71
1:Q:267:LEU:HD12	1:Q:268:PRO:HD2	1.72	0.70
1:S:156:LYS:HA	3:i:95:SER:HB2	1.72	0.70
1:B:71:ASP:OD2	1:B:73:GLN:NE2	2.23	0.70
2:X:222:ARG:NH1	3:i:123:PRO:O	2.24	0.70
2:X:18:MET:HE1	2:X:20:ILE:HG13	1.74	0.70
1:C:305:THR:HG22	1:C:308:TRP:CD1	2.25	0.70
1:P:267:LEU:HD12	1:P:268:PRO:HD2	1.73	0.69
3:f:152:LYS:HB2	3:f:195:SER:HB2	1.72	0.69
2:V:153:GLY:HA2	2:V:183:LEU:HB3	1.73	0.69
2:I:6:GLN:H	2:I:114:GLN:HE22	1.41	0.69
2:V:6:GLN:H	2:V:114:GLN:HE22	1.40	0.69
1:T:267:LEU:HD12	1:T:268:PRO:HD2	1.74	0.68
1:R:267:LEU:HD12	1:R:268:PRO:HD2	1.74	0.68
1:S:111:ARG:HD2	1:S:119:LEU:HD23	1.76	0.68
2:I:108:TYR:HB2	3:O:51:GLY:HA3	1.74	0.68
2:V:108:TYR:HB2	3:Z:51:GLY:HA3	1.76	0.68
1:A:238:ASP:OD1	1:A:239:ARG:N	2.27	0.68
1:T:10:PHE:CE2	1:T:83:HIS:HB3	2.28	0.68
2:U:108:TYR:HB2	3:h:51:GLY:HA3	1.76	0.67
2:J:219:ILE:HG22	2:J:221:PRO:HD3	1.76	0.67
2:W:6:GLN:H	2:W:114:GLN:HE22	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:210:LYS:NZ	8:S:402:LMT:O4'	2.27	0.67
2:W:108:TYR:HB2	3:f:51:GLY:HA3	1.77	0.67
2:G:108:TYR:HB2	3:K:51:GLY:HA3	1.77	0.67
3:K:107:THR:HG21	3:K:144:PRO:HB3	1.76	0.67
2:J:108:TYR:HB2	3:M:51:GLY:HA3	1.76	0.67
1:C:267:LEU:HD21	1:C:274:LYS:HE3	1.77	0.67
2:H:108:TYR:HB2	3:L:51:GLY:HA3	1.78	0.66
1:E:186:THR:HG22	1:E:207:ILE:HG22	1.78	0.66
1:D:267:LEU:HD11	1:D:274:LYS:HE3	1.78	0.66
5:D:401:POV:O13	1:E:259:GLN:NE2	2.28	0.66
1:A:37:ARG:NH1	1:A:54:THR:OG1	2.29	0.66
1:Q:249:GLY:HA3	1:Q:291:LEU:HD13	1.78	0.66
2:U:6:GLN:H	2:U:114:GLN:HE22	1.43	0.66
1:A:103:ILE:HG21	1:E:98:ALA:HB3	1.78	0.66
1:E:134:LEU:HD12	1:E:270:VAL:HG21	1.78	0.66
3:O:135:LEU:HD12	3:O:181:LEU:HD23	1.78	0.66
1:T:238:ASP:OD1	1:T:239:ARG:N	2.28	0.65
3:N:107:THR:HG21	3:N:144:PRO:HB3	1.78	0.65
2:J:173:HIS:HB2	2:J:189:SER:HB2	1.78	0.65
2:V:134:ALA:HB3	2:V:222:ARG:HG3	1.78	0.65
3:h:107:THR:HG21	3:h:144:PRO:HB3	1.76	0.65
2:W:30:THR:HA	2:W:53:PRO:HB2	1.78	0.65
1:B:267:LEU:HD21	1:B:274:LYS:HE3	1.78	0.65
3:K:41:LYS:HB2	3:K:45:LEU:HB3	1.77	0.65
1:Q:36:LEU:HD21	1:Q:39:ILE:HD11	1.78	0.65
1:R:44:VAL:HG11	1:R:134:LEU:HD11	1.78	0.65
2:J:18:MET:HE1	2:J:20:ILE:HG13	1.79	0.64
1:D:307:GLU:O	1:D:311:ILE:HG13	1.96	0.64
1:C:220:LEU:HD22	1:C:263:ILE:HG13	1.78	0.64
1:T:249:GLY:HA3	1:T:291:LEU:HD13	1.79	0.64
1:A:238:ASP:OD2	1:E:302:ASN:ND2	2.31	0.64
2:G:6:GLN:H	2:G:114:GLN:HE22	1.44	0.64
1:T:300:ILE:HG23	1:T:308:TRP:HE3	1.62	0.64
2:J:6:GLN:H	2:J:114:GLN:HE22	1.45	0.64
2:H:6:GLN:H	2:H:114:GLN:HE22	1.46	0.64
2:Y:6:GLN:H	2:Y:114:GLN:HE22	1.44	0.63
1:P:238:ASP:OD1	1:P:239:ARG:N	2.31	0.63
1:B:10:PHE:CE2	1:B:83:HIS:HB3	2.33	0.63
1:T:27:PRO:HD3	3:g:95:SER:HB3	1.79	0.63
1:P:44:VAL:HG11	1:P:134:LEU:HD11	1.80	0.63
5:D:401:POV:H3A	1:E:223:PRO:HB3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASP:OD1	1:B:239:ARG:N	2.32	0.62
2:F:144:MET:HB2	2:F:191:THR:HG22	1.81	0.62
2:I:222:ARG:NH2	3:O:123:PRO:O	2.32	0.62
3:O:96:ASN:ND2	3:O:96:ASN:O	2.28	0.62
2:F:6:GLN:H	2:F:114:GLN:HE22	1.45	0.62
1:R:42:ILE:HG23	1:R:132:MET:HE1	1.81	0.62
3:L:107:THR:HG21	3:L:144:PRO:HB3	1.82	0.61
1:T:19:ARG:HH11	1:T:157:ASP:HA	1.65	0.61
2:I:30:THR:HA	2:I:53:PRO:HB2	1.82	0.61
1:P:180:SER:HA	1:T:271:SER:HB2	1.81	0.61
1:Q:42:ILE:HG23	1:Q:132:MET:HE1	1.81	0.61
1:Q:141:VAL:HG11	1:Q:208:GLN:HE21	1.66	0.61
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.82	0.61
1:S:267:LEU:HD12	1:S:268:PRO:HD2	1.83	0.61
1:E:42:ILE:HG23	1:E:132:MET:HE1	1.82	0.61
3:K:22:CYS:HB3	3:K:73:ALA:HB3	1.82	0.61
2:Y:24:ALA:HB1	2:Y:27:TYR:HE1	1.66	0.61
1:D:44:VAL:HG21	1:D:268:PRO:HG3	1.82	0.61
3:g:199:THR:HG22	3:g:204:THR:HG22	1.82	0.61
1:C:170:LEU:HD23	1:C:174:LEU:HD23	1.82	0.60
2:V:30:THR:HA	2:V:53:PRO:HB2	1.83	0.60
2:H:33:THR:HG21	2:H:50:LEU:HD12	1.84	0.60
2:I:98:ARG:NH2	2:I:110:ASP:OD2	2.27	0.60
1:A:44:VAL:HG11	1:A:134:LEU:HD11	1.83	0.60
1:D:213:PHE:CE2	1:D:217:LEU:HD12	2.37	0.60
1:D:220:LEU:HD22	1:D:263:ILE:HG13	1.83	0.60
2:F:98:ARG:NH2	2:F:110:ASP:OD2	2.29	0.60
3:K:188:TRP:CG	3:K:189:GLU:H	2.20	0.59
1:E:267:LEU:HD21	1:E:274:LYS:HE3	1.84	0.59
1:P:156:LYS:HA	3:f:95:SER:HB2	1.84	0.59
1:A:134:LEU:HD12	1:A:270:VAL:HG21	1.83	0.59
1:T:35:LEU:HB3	1:T:54:THR:HB	1.84	0.59
2:Y:24:ALA:HB1	2:Y:27:TYR:CE1	2.38	0.59
2:I:24:ALA:HB1	2:I:27:TYR:HE1	1.67	0.59
3:h:39:GLN:NE2	3:h:41:LYS:HE3	2.18	0.59
3:h:170:GLN:NE2	3:h:172:ASN:OD1	2.36	0.58
1:R:170:LEU:HD23	1:R:174:LEU:HD23	1.85	0.58
1:P:155:THR:OG1	2:W:107:ARG:NH2	2.37	0.58
1:S:218:LEU:HD23	1:S:222:ILE:HG13	1.83	0.58
3:N:94:TYR:O	3:N:96:ASN:N	2.36	0.58
1:S:42:ILE:HG23	1:S:132:MET:HE1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:LEU:HD13	2:H:219:ILE:HG13	1.84	0.58
2:Y:30:THR:HA	2:Y:53:PRO:HB2	1.86	0.58
1:P:249:GLY:HA3	1:P:291:LEU:HD13	1.85	0.58
1:S:134:LEU:HD12	1:S:270:VAL:HG21	1.86	0.58
1:A:42:ILE:HG23	1:A:132:MET:HE1	1.85	0.58
1:D:7:ALA:O	1:D:11:THR:HG23	2.04	0.58
1:C:98:ALA:HB3	1:D:103:ILE:HG13	1.85	0.57
2:H:98:ARG:NH2	2:H:110:ASP:OD2	2.33	0.57
1:T:9:LEU:O	1:T:12:SER:OG	2.21	0.57
3:K:39:GLN:NE2	3:K:41:LYS:HE3	2.18	0.57
1:R:239:ARG:NH1	1:R:301:ALA:HB1	2.19	0.57
3:g:153:VAL:HG12	3:g:158:VAL:HG22	1.85	0.57
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.69	0.57
3:L:135:LEU:HB2	3:L:181:LEU:HB3	1.86	0.57
1:A:7:ALA:O	1:A:11:THR:HG23	2.03	0.57
1:C:42:ILE:HG23	1:C:132:MET:HE1	1.86	0.57
1:S:154:THR:OG1	1:S:155:THR:N	2.34	0.57
2:Y:108:TYR:CB	3:g:51:GLY:HA3	2.35	0.57
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.85	0.57
1:C:238:ASP:OD1	1:C:239:ARG:N	2.37	0.57
2:G:30:THR:HA	2:G:53:PRO:HB2	1.85	0.57
1:P:107:ASN:OD1	1:P:123:ARG:NH1	2.38	0.57
1:P:227:LEU:HD13	5:P:403:POV:H22A	1.87	0.57
3:Z:41:LYS:HB2	3:Z:45:LEU:HB2	1.86	0.57
2:X:93:VAL:HG22	2:X:117:THR:HG22	1.86	0.57
3:N:135:LEU:HB2	3:N:181:LEU:HB3	1.87	0.57
2:W:128:PRO:HB3	2:W:154:TYR:HB3	1.86	0.56
2:X:30:THR:HA	2:X:53:PRO:HB2	1.86	0.56
3:i:85:GLU:HG3	3:i:107:THR:HA	1.86	0.56
2:F:27:TYR:CE2	2:F:98:ARG:HD2	2.41	0.56
2:H:24:ALA:HB1	2:H:27:TYR:HE1	1.68	0.56
3:M:41:LYS:HB2	3:M:45:LEU:HB2	1.87	0.56
1:C:154:THR:OG1	1:C:155:THR:N	2.38	0.56
3:N:152:LYS:HE3	3:N:155:GLY:HA2	1.86	0.56
1:Q:9:LEU:HD11	1:Q:66:TYR:HB3	1.86	0.56
1:A:239:ARG:HD3	1:A:312:SER:HB3	1.87	0.56
1:B:98:ALA:HB3	1:C:103:ILE:HG13	1.88	0.56
1:A:156:LYS:HA	3:L:95:SER:HB2	1.87	0.56
2:V:13:ARG:NH2	2:V:123:ALA:O	2.39	0.56
1:Q:258:ALA:HB1	5:Q:401:POV:H13B	1.87	0.56
1:T:220:LEU:HD22	1:T:263:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:30:THR:HA	2:U:53:PRO:HB2	1.89	0.55
2:F:24:ALA:HB1	2:F:27:TYR:HE1	1.69	0.55
1:P:36:LEU:HD21	1:P:39:ILE:HD11	1.87	0.55
2:J:93:VAL:HG22	2:J:117:THR:HG22	1.87	0.55
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.42	0.55
1:B:271:SER:HB2	1:C:180:SER:HA	1.89	0.55
1:T:302:ASN:OD1	1:T:303:ALA:N	2.40	0.55
2:X:6:GLN:H	2:X:114:GLN:HE22	1.53	0.55
3:f:37:TRP:CE2	3:f:75:LEU:HB2	2.41	0.55
1:A:126:LEU:HD13	1:A:128:LEU:HD21	1.87	0.55
1:A:219:GLN:NE2	5:A:402:POV:H12	2.21	0.55
2:U:60:TYR:HE1	2:U:70:LEU:HG	1.72	0.55
2:J:98:ARG:NH2	2:J:110:ASP:OD2	2.32	0.55
2:I:24:ALA:HB1	2:I:27:TYR:CE1	2.41	0.55
1:P:42:ILE:HG12	1:P:49:TYR:HB2	1.87	0.55
1:T:44:VAL:HG11	1:T:134:LEU:HD11	1.88	0.55
2:U:172:VAL:HA	2:U:190:VAL:HG12	1.87	0.55
3:g:37:TRP:CE2	3:g:75:LEU:HB2	2.41	0.55
3:h:152:LYS:HE3	3:h:155:GLY:HA2	1.89	0.55
1:Q:111:ARG:HD2	1:Q:119:LEU:HD23	1.89	0.55
1:R:137:TYR:HB3	1:R:274:LYS:HB3	1.88	0.55
1:B:107:ASN:OD1	1:B:123:ARG:NH1	2.39	0.55
1:E:184:THR:HG21	1:E:210:LYS:HD2	1.88	0.55
3:O:94:TYR:HB2	3:O:97:HIS:HB3	1.89	0.54
1:R:111:ARG:HD2	1:R:119:LEU:HD23	1.89	0.54
3:i:153:VAL:HG12	3:i:158:VAL:HG22	1.89	0.54
2:Y:39:GLN:HB3	2:Y:93:VAL:HG13	1.89	0.54
3:i:37:TRP:CE2	3:i:75:LEU:HB2	2.42	0.54
1:B:141:VAL:HG11	1:B:208:GLN:HE21	1.73	0.54
1:E:154:THR:OG1	1:E:155:THR:N	2.40	0.54
1:P:95:GLU:HG3	1:P:98:ALA:HB2	1.88	0.54
2:V:108:TYR:CB	3:Z:51:GLY:HA3	2.37	0.54
1:D:220:LEU:HD23	1:D:276:ILE:HD11	1.90	0.54
1:E:126:LEU:HD13	1:E:128:LEU:HD21	1.89	0.54
1:P:261:ALA:HA	5:Q:401:POV:H14B	1.90	0.54
2:G:172:VAL:HA	2:G:190:VAL:HG12	1.90	0.54
1:Q:154:THR:OG1	1:Q:155:THR:N	2.38	0.54
1:P:19:ARG:HH11	1:P:157:ASP:HA	1.73	0.54
1:R:34:MET:HE2	1:R:162:TRP:HH2	1.73	0.54
1:C:252:THR:HG22	1:C:287:ILE:HD13	1.88	0.54
1:E:252:THR:HG22	1:E:287:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:MET:HG2	5:D:401:POV:H1	1.88	0.54
1:A:103:ILE:HD11	1:E:91:PHE:HA	1.90	0.54
1:E:95:GLU:HG3	1:E:98:ALA:HB2	1.89	0.54
1:D:139:MET:HG2	8:D:403:LMT:H6D	1.90	0.53
1:S:249:GLY:HA3	1:S:291:LEU:HD13	1.90	0.53
1:D:95:GLU:HG3	1:D:98:ALA:HB2	1.89	0.53
3:K:170:GLN:HE21	3:K:176:MET:HB3	1.73	0.53
1:Q:302:ASN:OD1	1:Q:303:ALA:N	2.42	0.53
1:T:85:ILE:HD11	1:T:112:ILE:HD11	1.90	0.53
1:D:167:PRO:HB2	1:D:188:THR:HG21	1.90	0.53
3:L:152:LYS:HB2	3:L:195:SER:HB3	1.90	0.53
2:U:24:ALA:HB1	2:U:27:TYR:HE1	1.73	0.53
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.90	0.53
2:G:108:TYR:CB	3:K:51:GLY:HA3	2.38	0.53
3:O:135:LEU:HB2	3:O:181:LEU:HB3	1.90	0.53
1:T:154:THR:OG1	1:T:155:THR:N	2.38	0.53
1:A:95:GLU:HG3	1:A:98:ALA:HB2	1.90	0.53
1:E:107:ASN:OD1	1:E:123:ARG:NH1	2.41	0.53
3:K:119:THR:OG1	3:K:138:THR:OG1	2.26	0.53
1:Q:226:MET:HE2	5:Q:401:POV:H37	1.91	0.53
1:C:126:LEU:HD13	1:C:128:LEU:HD21	1.91	0.53
3:K:123:PRO:HD3	3:K:135:LEU:HG	1.91	0.53
2:Y:98:ARG:NH2	2:Y:110:ASP:OD2	2.40	0.53
1:D:267:LEU:HD12	1:D:268:PRO:HD2	1.90	0.53
1:B:134:LEU:HD12	1:B:270:VAL:HG21	1.91	0.53
5:D:401:POV:P	1:E:259:GLN:HE22	2.32	0.53
1:A:154:THR:OG1	1:A:155:THR:N	2.38	0.52
3:O:85:GLU:HG3	3:O:107:THR:HA	1.89	0.52
1:B:126:LEU:HD13	1:B:128:LEU:HD21	1.90	0.52
1:A:71:ASP:OD2	1:A:73:GLN:NE2	2.29	0.52
2:J:108:TYR:CB	3:M:51:GLY:HA3	2.39	0.52
2:F:108:TYR:HB2	3:N:51:GLY:HA2	1.91	0.52
2:V:132:PRO:HG3	2:V:217:LYS:HB3	1.92	0.52
1:A:46:ASN:ND2	1:B:41:LYS:HE2	2.25	0.52
2:H:30:THR:HA	2:H:53:PRO:HB2	1.91	0.52
1:S:126:LEU:HD13	1:S:128:LEU:HD21	1.92	0.52
3:N:131:ASN:HA	3:N:185:ALA:HB2	1.92	0.52
1:T:134:LEU:HD12	1:T:270:VAL:HG21	1.92	0.52
3:f:107:THR:HG21	3:f:144:PRO:HB3	1.90	0.52
1:A:220:LEU:HD22	1:A:263:ILE:HG13	1.92	0.51
1:A:267:LEU:HD11	1:A:274:LYS:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:LEU:HD23	1:C:256:MET:HE2	1.93	0.51
2:H:39:GLN:HB3	2:H:93:VAL:HG13	1.92	0.51
2:H:207:ALA:HB2	2:H:214:LYS:HD3	1.92	0.51
1:Q:252:THR:HG22	1:Q:287:ILE:HD13	1.92	0.51
3:Z:37:TRP:CE2	3:Z:75:LEU:HB2	2.46	0.51
3:f:96:ASN:HD22	3:f:96:ASN:C	2.13	0.51
2:V:176:PRO:HG2	3:Z:165:THR:HB	1.92	0.51
1:C:249:GLY:HA3	1:C:291:LEU:HD13	1.92	0.51
1:E:138:PRO:HD2	1:E:139:MET:SD	2.50	0.51
2:F:10:GLU:HG3	2:F:18:MET:HE3	1.91	0.51
2:G:147:LEU:HD13	2:G:219:ILE:HD13	1.93	0.51
2:I:6:GLN:N	2:I:114:GLN:HE22	2.08	0.51
1:R:239:ARG:HH11	1:R:301:ALA:HB1	1.76	0.51
1:S:220:LEU:HD22	1:S:263:ILE:HG13	1.92	0.51
1:T:263:ILE:HG21	1:T:276:ILE:HG12	1.93	0.51
2:U:39:GLN:HB3	2:U:93:VAL:HG13	1.92	0.51
2:F:24:ALA:HB1	2:F:27:TYR:CE1	2.45	0.51
1:P:213:PHE:CE2	1:P:217:LEU:HD12	2.45	0.51
1:Q:213:PHE:CE2	1:Q:217:LEU:HD12	2.45	0.51
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.45	0.51
1:P:105:LYS:HD2	1:P:105:LYS:N	2.26	0.51
1:Q:170:LEU:HD11	1:Q:186:THR:HG21	1.93	0.51
1:T:252:THR:HG22	1:T:287:ILE:HD13	1.93	0.51
2:J:30:THR:HA	2:J:53:PRO:HB2	1.93	0.51
1:A:89:ASP:HB2	1:B:105:LYS:HD3	1.93	0.51
1:A:227:LEU:HD23	1:A:256:MET:HE2	1.92	0.51
1:C:95:GLU:HG3	1:C:98:ALA:HB2	1.92	0.51
3:L:22:CYS:HB3	3:L:73:ALA:HB3	1.92	0.51
2:W:108:TYR:CB	3:f:51:GLY:HA3	2.40	0.51
1:P:239:ARG:NH1	1:P:301:ALA:HB1	2.26	0.51
1:S:95:GLU:HG3	1:S:98:ALA:HB2	1.92	0.51
1:S:154:THR:HG23	1:S:156:LYS:HG2	1.93	0.51
1:T:42:ILE:HG23	1:T:132:MET:HE1	1.93	0.51
2:U:24:ALA:HB1	2:U:27:TYR:CE1	2.45	0.51
1:B:7:ALA:O	1:B:11:THR:HG23	2.10	0.51
2:H:108:TYR:CB	3:L:51:GLY:HA3	2.41	0.51
1:R:85:ILE:HD11	1:R:112:ILE:HD11	1.92	0.51
2:W:161:VAL:HG22	2:W:206:VAL:HG22	1.92	0.51
1:D:183:LEU:HD21	1:D:186:THR:HG23	1.93	0.51
3:L:93:TRP:NE1	3:L:95:SER:HA	2.26	0.51
1:Q:19:ARG:HH11	1:Q:157:ASP:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:85:ILE:HD11	1:Q:112:ILE:HD11	1.93	0.51
1:T:154:THR:HG23	1:T:156:LYS:HG2	1.93	0.51
2:J:24:ALA:HB1	2:J:27:TYR:CE1	2.46	0.51
2:I:27:TYR:CE2	2:I:98:ARG:HD2	2.45	0.50
1:R:262:GLY:HA3	5:R:401:POV:H12	1.92	0.50
1:T:37:ARG:HH11	1:T:52:GLN:HE21	1.58	0.50
1:T:95:GLU:HG3	1:T:98:ALA:HB2	1.92	0.50
3:f:22:CYS:HB3	3:f:73:ALA:HB3	1.93	0.50
1:B:95:GLU:HG3	1:B:98:ALA:HB2	1.93	0.50
1:C:33:ASN:HB3	1:C:56:ARG:HB2	1.93	0.50
1:P:105:LYS:HE2	1:T:87:MET:HE3	1.92	0.50
1:S:38:THR:HG22	1:S:52:GLN:HB3	1.92	0.50
2:U:98:ARG:NH2	2:U:110:ASP:OD2	2.36	0.50
3:N:170:GLN:NE2	3:N:172:ASN:OD1	2.45	0.50
1:T:38:THR:HG22	1:T:52:GLN:HB3	1.92	0.50
2:I:132:PRO:HD3	2:I:217:LYS:HE2	1.93	0.50
2:Y:27:TYR:CE2	2:Y:98:ARG:HD2	2.46	0.50
1:T:126:LEU:HD13	1:T:128:LEU:HD21	1.92	0.50
2:U:133:LEU:HD23	2:U:150:LEU:HB2	1.92	0.50
1:C:154:THR:HG23	1:C:156:LYS:HG2	1.92	0.50
1:E:36:LEU:HD21	1:E:39:ILE:HD11	1.94	0.50
1:E:215:PHE:CE1	1:E:219:GLN:HG3	2.46	0.50
1:E:227:LEU:HD23	1:E:256:MET:HE2	1.92	0.50
1:R:95:GLU:HG3	1:R:98:ALA:HB2	1.94	0.50
1:D:42:ILE:HG13	1:D:132:MET:HE1	1.93	0.50
1:D:170:LEU:HD11	1:D:186:THR:HG21	1.94	0.50
1:P:10:PHE:HZ	1:P:85:ILE:HG22	1.77	0.50
1:R:137:TYR:O	1:R:275:ALA:HB3	2.12	0.50
1:S:19:ARG:HH11	1:S:157:ASP:HA	1.75	0.50
1:S:307:GLU:HG2	1:S:309:ASN:H	1.76	0.50
1:D:154:THR:HG22	1:D:155:THR:H	1.77	0.49
1:B:183:LEU:HD21	1:B:186:THR:HG23	1.93	0.49
1:R:226:MET:HE2	5:R:401:POV:H37A	1.94	0.49
1:S:194:VAL:O	2:X:55:ASN:ND2	2.43	0.49
2:V:162:THR:HG23	2:V:205:ASN:HB2	1.94	0.49
1:Q:126:LEU:HD13	1:Q:128:LEU:HD21	1.95	0.49
1:E:215:PHE:CZ	1:E:219:GLN:HG3	2.47	0.49
2:U:147:LEU:HD13	2:U:219:ILE:HD12	1.93	0.49
2:V:123:ALA:HB2	2:V:182:ASP:HB3	1.94	0.49
1:E:220:LEU:HD13	1:E:263:ILE:HG13	1.93	0.49
1:B:42:ILE:HG23	1:B:132:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:95:GLU:HG3	1:Q:98:ALA:HB2	1.93	0.49
1:Q:138:PRO:HD2	1:Q:139:MET:SD	2.52	0.49
1:B:137:TYR:HD2	1:B:276:ILE:HB	1.77	0.49
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.46	0.49
1:R:35:LEU:HB3	1:R:54:THR:HB	1.95	0.49
1:R:284:MET:HG2	5:R:402:POV:H1	1.95	0.49
2:Y:60:TYR:HE1	2:Y:70:LEU:HG	1.78	0.49
1:D:217:LEU:O	1:D:221:TYR:HB2	2.12	0.49
2:G:199:SER:OG	2:G:200:GLU:OE1	2.25	0.49
1:S:134:LEU:N	1:S:272:TYR:OH	2.42	0.49
1:E:220:LEU:HD11	1:E:280:ILE:HD11	1.94	0.49
1:P:271:SER:HB2	1:Q:180:SER:HA	1.95	0.49
1:Q:154:THR:HG23	1:Q:156:LYS:HG2	1.93	0.49
1:A:154:THR:HG23	1:A:156:LYS:HG2	1.95	0.49
2:I:197:TRP:CZ3	2:I:202:VAL:HG22	2.48	0.49
1:T:141:VAL:HG11	1:T:208:GLN:HE21	1.78	0.49
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.48	0.49
1:C:170:LEU:HD11	1:C:186:THR:HG21	1.94	0.48
1:P:98:ALA:HB3	1:Q:103:ILE:HG21	1.95	0.48
1:P:170:LEU:HD11	1:P:186:THR:HG21	1.95	0.48
1:P:241:ALA:HB2	1:T:302:ASN:ND2	2.24	0.48
1:Q:215:PHE:CE1	1:Q:219:GLN:HG3	2.48	0.48
2:J:27:TYR:CE2	2:J:98:ARG:HD2	2.47	0.48
1:D:126:LEU:HD13	1:D:128:LEU:HD21	1.95	0.48
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.78	0.48
1:P:226:MET:HE2	5:P:403:POV:H26	1.96	0.48
1:T:220:LEU:HB2	1:T:263:ILE:HD11	1.95	0.48
2:G:14:PRO:HG2	2:G:122:SER:HB3	1.95	0.48
1:S:111:ARG:HB2	1:S:119:LEU:HB3	1.94	0.48
2:Y:207:ALA:HB2	2:Y:214:LYS:HD3	1.95	0.48
2:I:176:PRO:HG2	3:O:165:THR:HB	1.94	0.48
1:S:264:ASN:HD21	5:T:401:POV:H14B	1.78	0.48
3:Z:107:THR:HG21	3:Z:144:PRO:HB3	1.94	0.48
3:i:213:ASP:OD1	3:i:213:ASP:N	2.46	0.48
1:C:1:SER:HA	1:C:4:LYS:HD2	1.94	0.48
2:H:157:GLU:HG3	2:H:184:TYR:CD2	2.49	0.48
1:S:264:ASN:ND2	5:T:401:POV:H14B	2.28	0.48
3:L:148:THR:HB	3:L:199:THR:HB	1.94	0.48
3:N:170:GLN:NE2	3:N:174:LYS:HB2	2.29	0.48
1:R:138:PRO:HD2	1:R:139:MET:SD	2.53	0.48
1:C:111:ARG:HD2	1:C:119:LEU:HD23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:VAL:O	1:C:231:SER:OG	2.29	0.48
2:U:6:GLN:N	2:U:114:GLN:HE22	2.12	0.48
3:f:120:LEU:HD13	3:f:209:LEU:HD22	1.95	0.48
3:h:170:GLN:NE2	3:h:174:LYS:HB2	2.28	0.48
1:B:134:LEU:N	1:B:272:TYR:OH	2.44	0.48
1:A:110:ILE:HG12	1:A:120:TYR:HD1	1.79	0.48
2:G:208:HIS:ND1	2:G:211:SER:OG	2.42	0.48
1:R:271:SER:HB2	1:S:180:SER:HA	1.96	0.48
2:J:152:LYS:HA	2:J:185:THR:HG23	1.96	0.48
1:C:288:PHE:HE1	1:D:230:VAL:HG11	1.78	0.47
3:L:85:GLU:HG3	3:L:107:THR:HA	1.96	0.47
1:T:311:ILE:O	1:T:315:VAL:HG23	2.14	0.47
1:C:271:SER:HB2	1:D:180:SER:HA	1.96	0.47
1:D:271:SER:HB2	1:E:180:SER:HA	1.95	0.47
1:S:220:LEU:C	1:S:223:PRO:HD2	2.38	0.47
2:W:168:LEU:HD13	2:W:190:VAL:HG21	1.96	0.47
1:B:300:ILE:O	1:B:308:TRP:HB3	2.13	0.47
2:J:24:ALA:HB1	2:J:27:TYR:HE1	1.77	0.47
1:A:170:LEU:HD22	1:A:174:LEU:HD23	1.96	0.47
1:D:285:THR:OG1	5:D:401:POV:O22	2.28	0.47
1:P:126:LEU:HD13	1:P:128:LEU:HD21	1.97	0.47
1:S:267:LEU:HG	1:S:268:PRO:O	2.15	0.47
2:G:157:GLU:HB2	2:G:158:PRO:HA	1.96	0.47
1:Q:259:GLN:O	1:Q:263:ILE:HG12	2.15	0.47
1:R:299:HIS:CE1	1:S:237:PHE:HA	2.49	0.47
1:B:220:LEU:O	1:B:224:SER:OG	2.21	0.47
1:C:230:VAL:O	1:C:233:VAL:HG22	2.14	0.47
1:E:228:VAL:O	1:E:231:SER:OG	2.32	0.47
2:H:6:GLN:N	2:H:114:GLN:HE22	2.12	0.47
1:Q:215:PHE:CZ	1:Q:219:GLN:HG3	2.49	0.47
1:Q:223:PRO:HB3	5:Q:401:POV:H3	1.97	0.47
1:S:85:ILE:HD11	1:S:112:ILE:HD11	1.97	0.47
1:S:137:TYR:HD2	1:S:276:ILE:HB	1.80	0.47
1:E:137:TYR:CE1	1:E:267:LEU:HD13	2.50	0.47
1:E:268:PRO:HA	1:E:269:PRO:HD3	1.77	0.47
2:G:44:ASN:ND2	3:K:102:GLY:HA2	2.30	0.47
2:G:161:VAL:HG22	2:G:206:VAL:HG22	1.96	0.47
2:X:155:PHE:HA	2:X:156:PRO:HA	1.76	0.47
1:R:220:LEU:HD22	1:R:263:ILE:HG13	1.96	0.47
1:R:230:VAL:O	1:R:233:VAL:HG22	2.14	0.47
1:T:170:LEU:HD11	1:T:186:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:259:GLN:NE2	5:T:401:POV:O13	2.48	0.47
3:g:39:GLN:NE2	3:g:41:LYS:HE3	2.29	0.47
3:M:120:LEU:HD13	3:M:209:LEU:HD22	1.97	0.47
1:E:184:THR:CG2	1:E:210:LYS:HD2	2.45	0.47
2:F:175:PHE:CZ	3:N:138:THR:HG23	2.50	0.47
2:H:133:LEU:HD13	3:L:121:PHE:CG	2.50	0.47
1:Q:230:VAL:O	1:Q:233:VAL:HG22	2.14	0.47
1:S:185:ASN:HD22	4:S:401:NAG:H61	1.80	0.47
2:G:6:GLN:N	2:G:114:GLN:HE22	2.10	0.46
1:R:215:PHE:CZ	1:R:219:GLN:HG3	2.50	0.46
2:U:163:TRP:HB3	2:U:168:LEU:HD12	1.98	0.46
1:A:228:VAL:O	1:A:231:SER:OG	2.29	0.46
2:G:128:PRO:HD3	2:G:208:HIS:HD1	1.80	0.46
2:U:157:GLU:HG3	2:U:184:TYR:CD2	2.50	0.46
1:B:215:PHE:O	1:B:219:GLN:N	2.46	0.46
1:E:154:THR:HG23	1:E:156:LYS:HG2	1.95	0.46
1:R:227:LEU:HD13	5:R:401:POV:H34A	1.96	0.46
1:T:230:VAL:O	1:T:233:VAL:HG22	2.15	0.46
5:Q:401:POV:H13B	5:Q:401:POV:H11	1.64	0.46
1:E:175:SER:HB2	1:E:182:GLN:OE1	2.16	0.46
2:H:27:TYR:CE2	2:H:98:ARG:HD2	2.50	0.46
2:J:197:TRP:CZ2	2:J:221:PRO:HG3	2.50	0.46
1:B:256:MET:HE2	1:B:283:CYS:HB2	1.97	0.46
2:G:208:HIS:NE2	2:G:210:ALA:HB3	2.31	0.46
1:Q:33:ASN:HB3	1:Q:56:ARG:HB2	1.98	0.46
1:R:297:VAL:HG13	1:R:312:SER:HB2	1.97	0.46
2:F:175:PHE:HZ	3:N:138:THR:HG23	1.81	0.46
3:K:122:PRO:HG3	3:K:209:LEU:HD11	1.98	0.46
2:Y:18:MET:HG3	2:Y:86:LEU:HD11	1.98	0.46
2:Y:208:HIS:CE1	2:Y:210:ALA:HB3	2.51	0.46
3:g:121:PHE:HA	3:g:122:PRO:HD3	1.81	0.46
1:A:170:LEU:HD11	1:A:186:THR:HG21	1.98	0.46
1:D:299:HIS:CE1	1:E:237:PHE:HA	2.51	0.46
3:K:151:TRP:O	3:K:157:PRO:HA	2.15	0.46
1:P:42:ILE:HG23	1:P:132:MET:HE1	1.98	0.46
2:U:18:MET:HG3	2:U:86:LEU:HD11	1.97	0.46
1:B:299:HIS:CE1	1:C:237:PHE:HA	2.51	0.46
2:I:155:PHE:HA	2:I:156:PRO:HA	1.75	0.46
2:V:6:GLN:HE22	2:V:96:CYS:H	1.64	0.46
2:Y:174:THR:HG23	2:Y:186:LEU:HD21	1.97	0.46
3:f:152:LYS:HA	3:f:157:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:85:GLU:HG3	3:h:107:THR:HA	1.96	0.46
1:C:35:LEU:HD12	1:C:169:GLN:O	2.16	0.46
1:T:137:TYR:HD2	1:T:276:ILE:HB	1.81	0.46
2:Y:169:SER:C	2:Y:171:GLY:H	2.24	0.46
1:A:35:LEU:HB3	1:A:54:THR:HB	1.98	0.45
1:B:305:THR:CG2	1:B:308:TRP:HD1	2.28	0.45
2:G:37:VAL:HG11	2:G:45:LEU:HD23	1.98	0.45
2:U:18:MET:HE1	2:U:20:ILE:HG12	1.98	0.45
3:h:121:PHE:HA	3:h:122:PRO:HD3	1.79	0.45
1:C:19:ARG:HG2	1:C:20:PRO:HD2	1.98	0.45
2:F:132:PRO:HD3	2:F:217:LYS:HE2	1.97	0.45
2:H:132:PRO:HG3	2:H:217:LYS:HE2	1.97	0.45
2:I:108:TYR:CB	3:O:51:GLY:HA3	2.44	0.45
1:R:111:ARG:HB2	1:R:119:LEU:HB3	1.99	0.45
1:R:186:THR:HG22	1:R:207:ILE:HG22	1.98	0.45
1:R:228:VAL:O	1:R:231:SER:OG	2.33	0.45
1:S:271:SER:HB2	1:T:180:SER:HA	1.98	0.45
3:Z:22:CYS:HB3	3:Z:73:ALA:HB3	1.99	0.45
1:D:227:LEU:HG	1:D:252:THR:HG23	1.99	0.45
2:I:6:GLN:H	2:I:114:GLN:NE2	2.12	0.45
3:K:141:ASP:H	3:K:170:GLN:HE22	1.64	0.45
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.99	0.45
1:S:170:LEU:HD22	1:S:174:LEU:HD23	1.99	0.45
2:V:6:GLN:N	2:V:114:GLN:HE22	2.11	0.45
2:H:127:PRO:HA	2:H:128:PRO:HD3	1.83	0.45
2:V:166:GLY:C	2:V:168:LEU:H	2.24	0.45
3:g:135:LEU:HB2	3:g:181:LEU:HB3	1.98	0.45
1:A:252:THR:HG22	1:A:287:ILE:HD13	1.98	0.45
1:B:98:ALA:CB	1:C:103:ILE:HG13	2.46	0.45
1:B:130:CYS:O	1:B:132:MET:HG3	2.17	0.45
1:E:183:LEU:HD12	1:E:183:LEU:O	2.17	0.45
2:F:6:GLN:N	2:F:114:GLN:HE22	2.14	0.45
2:H:50:LEU:HD21	2:H:59:SER:HB3	1.97	0.45
1:T:228:VAL:O	1:T:231:SER:OG	2.28	0.45
2:W:18:MET:HE1	2:W:20:ILE:HG12	1.98	0.45
3:Z:150:ASP:O	3:Z:197:GLN:N	2.46	0.45
1:C:137:TYR:HA	1:C:138:PRO:HA	1.74	0.45
3:N:85:GLU:HG3	3:N:107:THR:HA	1.99	0.45
3:O:96:ASN:HD22	3:O:96:ASN:C	2.19	0.45
1:S:138:PRO:HD2	1:S:139:MET:SD	2.57	0.45
1:T:239:ARG:HD2	1:T:301:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:139:ILE:HG12	3:g:198:VAL:HG21	1.99	0.45
2:J:6:GLN:N	2:J:114:GLN:HE22	2.12	0.45
1:B:138:PRO:HG3	1:B:216:TYR:CG	2.51	0.45
1:D:137:TYR:HA	1:D:138:PRO:HA	1.80	0.45
1:S:154:THR:HA	1:S:200:TYR:CD1	2.52	0.45
2:U:174:THR:HG23	2:U:186:LEU:HD21	1.98	0.45
2:V:6:GLN:NE2	2:V:96:CYS:H	2.15	0.45
2:V:141:THR:OG1	2:V:142:ASN:N	2.49	0.45
1:A:215:PHE:HA	1:E:273:ILE:HD11	1.99	0.45
1:C:239:ARG:HD2	1:C:301:ALA:HB1	1.98	0.45
1:C:254:LEU:HD11	1:D:254:LEU:HD23	1.99	0.45
1:D:20:PRO:HA	1:D:21:PRO:HD3	1.88	0.45
2:F:48:ILE:HA	2:F:64:PHE:HD2	1.81	0.45
1:R:215:PHE:CE1	1:R:219:GLN:HG3	2.52	0.45
3:i:37:TRP:CD2	3:i:75:LEU:HB2	2.52	0.45
1:A:230:VAL:O	1:A:233:VAL:HG22	2.17	0.45
1:C:138:PRO:HD2	1:C:139:MET:SD	2.57	0.45
1:E:259:GLN:O	1:E:263:ILE:HG12	2.17	0.45
1:B:137:TYR:HA	1:B:138:PRO:HA	1.69	0.45
1:B:230:VAL:O	1:B:233:VAL:HG22	2.16	0.45
2:G:176:PRO:HG2	3:K:165:THR:HB	1.98	0.45
1:C:313:LYS:HA	1:C:313:LYS:HD3	1.80	0.44
2:I:46:GLU:OE1	2:I:63:LYS:HE2	2.16	0.44
3:K:122:PRO:HB3	3:K:209:LEU:HD21	1.98	0.44
3:N:22:CYS:HB3	3:N:73:ALA:HB3	1.99	0.44
1:T:256:MET:HE2	1:T:283:CYS:HB2	1.99	0.44
2:F:30:THR:HA	2:F:53:PRO:HB2	1.99	0.44
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.52	0.44
2:X:131:TYR:HA	2:X:132:PRO:HD3	1.83	0.44
3:h:39:GLN:HB2	3:h:49:LEU:HD11	1.99	0.44
1:E:267:LEU:HD12	1:E:268:PRO:HD2	1.99	0.44
1:P:239:ARG:HH11	1:P:301:ALA:HB1	1.81	0.44
1:S:259:GLN:O	1:S:263:ILE:HG12	2.18	0.44
2:U:199:SER:OG	2:U:200:GLU:OE1	2.28	0.44
2:V:163:TRP:HB2	2:V:168:LEU:HD11	1.99	0.44
2:H:146:THR:HG22	2:H:191:THR:HG22	2.00	0.44
1:P:137:TYR:HA	1:P:138:PRO:HA	1.78	0.44
1:S:299:HIS:CE1	1:T:237:PHE:HA	2.52	0.44
1:A:107:ASN:OD1	1:A:123:ARG:NH1	2.50	0.44
3:K:109:LEU:HD21	3:K:144:PRO:HG3	2.00	0.44
1:Q:224:SER:HB2	1:Q:279:TRP:CZ3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:267:LEU:HG	1:R:268:PRO:O	2.17	0.44
3:h:37:TRP:CE2	3:h:75:LEU:HB2	2.53	0.44
1:A:33:ASN:HB3	1:A:56:ARG:HB2	1.99	0.44
2:I:127:PRO:HA	2:I:128:PRO:HD3	1.83	0.44
3:N:172:ASN:OD1	3:N:172:ASN:N	2.48	0.44
1:R:252:THR:HG22	1:R:287:ILE:HD13	2.00	0.44
1:R:305:THR:HG22	1:R:307:GLU:OE1	2.18	0.44
1:T:192:THR:O	2:Y:105:TYR:N	2.49	0.44
2:Y:6:GLN:N	2:Y:114:GLN:HE22	2.12	0.44
2:J:60:TYR:HE1	2:J:70:LEU:HG	1.83	0.44
1:C:224:SER:OG	1:C:283:CYS:SG	2.72	0.44
1:E:49:TYR:CE1	1:E:144:CYS:HB3	2.52	0.44
5:P:403:POV:H13B	5:P:403:POV:H11A	1.77	0.44
1:Q:311:ILE:O	1:Q:315:VAL:HG23	2.18	0.44
1:S:33:ASN:HB3	1:S:56:ARG:HB2	2.00	0.44
1:T:156:LYS:HA	3:g:95:SER:HB2	2.00	0.44
2:X:208:HIS:CE1	2:X:210:ALA:HB3	2.53	0.44
2:Y:110:ASP:OD1	3:g:58:PRO:HD2	2.18	0.44
2:J:208:HIS:CE1	2:J:210:ALA:HB3	2.53	0.44
1:A:310:ASP:O	1:A:314:ARG:HG3	2.18	0.44
1:C:194:VAL:HG13	2:G:52:ASN:HD22	1.82	0.44
1:D:175:SER:HB2	1:D:182:GLN:OE1	2.18	0.44
1:D:194:VAL:HG13	2:I:52:ASN:HD22	1.82	0.44
2:G:6:GLN:H	2:G:114:GLN:NE2	2.13	0.44
3:h:22:CYS:HB3	3:h:73:ALA:HB3	1.99	0.44
2:G:153:GLY:HA2	2:G:183:LEU:HD22	2.00	0.44
3:L:37:TRP:CZ3	3:L:90:CYS:HB3	2.53	0.44
1:P:68:VAL:N	1:P:71:ASP:OD2	2.49	0.44
1:Q:111:ARG:HB2	1:Q:119:LEU:HB3	1.99	0.44
1:R:96:LYS:HD2	1:R:129:SER:HB3	2.00	0.44
2:W:60:TYR:CE1	2:W:70:LEU:HG	2.53	0.44
2:W:157:GLU:HG3	2:W:184:TYR:CD2	2.53	0.44
2:Y:144:MET:HG2	2:Y:193:PRO:HA	2.00	0.44
3:g:41:LYS:HB2	3:g:45:LEU:HB2	2.00	0.44
3:M:113:LYS:NZ	3:M:201:GLU:OE2	2.37	0.44
1:A:299:HIS:CE1	1:B:237:PHE:HA	2.53	0.43
1:C:19:ARG:HH11	1:C:157:ASP:HA	1.82	0.43
3:O:37:TRP:CZ3	3:O:90:CYS:HB3	2.53	0.43
1:R:256:MET:HE2	1:R:283:CYS:HB2	2.00	0.43
1:R:311:ILE:O	1:R:315:VAL:HG23	2.18	0.43
1:S:309:ASN:OD1	1:S:311:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:177:ALA:HB2	2:J:186:LEU:HD23	2.00	0.43
3:M:152:LYS:HB2	3:M:195:SER:HB3	1.99	0.43
1:E:230:VAL:O	1:E:233:VAL:HG22	2.18	0.43
1:T:137:TYR:O	1:T:275:ALA:HB3	2.18	0.43
2:W:6:GLN:N	2:W:114:GLN:HE22	2.11	0.43
2:W:208:HIS:CE1	2:W:210:ALA:HB3	2.53	0.43
2:H:153:GLY:HA2	2:H:183:LEU:HB3	1.99	0.43
1:S:100:LYS:HE2	1:T:104:ASP:H	1.83	0.43
3:M:41:LYS:HE2	3:M:83:GLU:O	2.18	0.43
1:A:300:ILE:HG13	1:A:312:SER:OG	2.18	0.43
1:D:252:THR:HG22	1:D:287:ILE:HD13	2.00	0.43
1:P:230:VAL:O	1:P:233:VAL:HG22	2.18	0.43
1:R:220:LEU:HD23	1:R:276:ILE:HD11	2.01	0.43
1:S:224:SER:HB2	1:S:279:TRP:CZ3	2.53	0.43
2:F:48:ILE:HG12	2:F:64:PHE:CE2	2.54	0.43
2:F:108:TYR:HB3	3:N:52:GLY:H	1.84	0.43
3:N:199:THR:HA	3:N:204:THR:HA	2.01	0.43
1:P:259:GLN:HE22	5:P:403:POV:P	2.42	0.43
1:P:305:THR:HB	1:P:308:TRP:HD1	1.83	0.43
1:R:249:GLY:HA3	1:R:291:LEU:HD13	1.99	0.43
1:S:170:LEU:HD11	1:S:186:THR:HG21	2.01	0.43
1:S:183:LEU:HD11	1:S:207:ILE:HB	2.01	0.43
8:T:403:LMT:H5B	8:T:403:LMT:H6D	2.01	0.43
1:C:311:ILE:O	1:C:315:VAL:HG23	2.19	0.43
2:I:161:VAL:HG22	2:I:206:VAL:HG22	1.99	0.43
3:K:188:TRP:CG	3:K:189:GLU:N	2.87	0.43
3:L:41:LYS:HB2	3:L:45:LEU:HB2	1.99	0.43
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.83	0.43
2:H:164:ASN:HB3	2:H:167:SER:HB3	1.99	0.43
1:P:137:TYR:O	1:P:275:ALA:HB3	2.18	0.43
2:U:27:TYR:CE2	2:U:98:ARG:HD2	2.53	0.43
1:A:220:LEU:HD23	1:A:276:ILE:HD11	2.01	0.43
2:F:108:TYR:CB	3:N:51:GLY:HA2	2.49	0.43
1:Q:183:LEU:HD12	1:Q:183:LEU:O	2.19	0.43
1:Q:267:LEU:HA	1:Q:268:PRO:HD2	1.87	0.43
1:S:87:MET:HE3	1:T:105:LYS:NZ	2.33	0.43
1:S:222:ILE:HB	1:S:223:PRO:HD3	2.00	0.43
3:f:37:TRP:CZ3	3:f:90:CYS:HB3	2.54	0.43
3:f:150:ASP:O	3:f:197:GLN:N	2.45	0.43
3:h:56:ARG:HH21	3:h:60:VAL:HG12	1.83	0.43
2:J:20:ILE:HD13	2:J:81:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:85:GLU:HG3	3:K:107:THR:HA	1.99	0.43
1:P:138:PRO:HD2	1:P:139:MET:SD	2.59	0.43
1:R:137:TYR:HA	1:R:138:PRO:HA	1.79	0.43
1:S:49:TYR:CE1	1:S:144:CYS:HB3	2.54	0.43
3:i:115:SER:HA	3:i:116:PRO:HD3	1.88	0.43
1:B:111:ARG:HD2	1:B:119:LEU:HD23	2.00	0.43
1:B:267:LEU:HD12	1:B:268:PRO:HD2	2.00	0.43
2:F:133:LEU:HD13	3:N:121:PHE:CG	2.53	0.43
3:L:139:ILE:HD12	3:L:198:VAL:HG21	2.00	0.43
1:R:20:PRO:HA	1:R:21:PRO:HD3	1.86	0.43
2:U:135:PRO:HB2	2:U:140:GLN:HE22	1.84	0.43
2:X:18:MET:HG3	2:X:86:LEU:HD11	2.00	0.43
1:B:20:PRO:HA	1:B:21:PRO:HD3	1.86	0.42
1:B:87:MET:HE3	1:C:105:LYS:NZ	2.34	0.42
1:B:215:PHE:CZ	1:B:219:GLN:HG2	2.54	0.42
1:D:138:PRO:HD2	1:D:139:MET:SD	2.59	0.42
1:D:267:LEU:HA	1:D:268:PRO:HD2	1.92	0.42
2:G:144:MET:HB2	2:G:191:THR:HG22	2.01	0.42
3:O:45:LEU:HD13	3:O:45:LEU:HA	1.87	0.42
1:Q:134:LEU:HD12	1:Q:270:VAL:HG21	2.00	0.42
1:R:300:ILE:HB	1:R:308:TRP:HE3	1.84	0.42
2:U:208:HIS:CE1	2:U:210:ALA:HB3	2.54	0.42
1:A:136:TYR:O	1:A:140:ASP:HB3	2.19	0.42
1:A:138:PRO:HD2	1:A:139:MET:SD	2.59	0.42
1:B:10:PHE:HE2	1:B:83:HIS:HB3	1.80	0.42
1:B:267:LEU:HA	1:B:268:PRO:HD2	1.90	0.42
2:F:127:PRO:HA	2:F:128:PRO:HD3	1.85	0.42
1:P:27:PRO:HD3	3:f:95:SER:HB3	2.01	0.42
1:R:33:ASN:HB3	1:R:56:ARG:HB2	2.00	0.42
3:h:56:ARG:NH2	3:h:61:PRO:O	2.52	0.42
3:M:122:PRO:HG3	3:M:209:LEU:HD11	2.00	0.42
1:C:299:HIS:CE1	1:D:237:PHE:HA	2.54	0.42
3:K:129:GLU:CD	3:K:130:THR:HG23	2.45	0.42
1:R:19:ARG:HH11	1:R:157:ASP:HA	1.84	0.42
1:B:170:LEU:HD11	1:B:186:THR:HG21	2.01	0.42
1:D:313:LYS:HA	1:D:313:LYS:HD3	1.88	0.42
2:F:18:MET:HE2	2:F:18:MET:HB2	1.94	0.42
1:P:311:ILE:O	1:P:315:VAL:HG23	2.19	0.42
1:B:227:LEU:HG	1:B:252:THR:HG23	2.01	0.42
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.55	0.42
1:P:20:PRO:HA	1:P:21:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:189:THR:OG1	1:R:190:TYR:N	2.52	0.42
5:R:402:POV:H211	5:R:402:POV:H28A	1.73	0.42
1:C:130:CYS:O	1:C:132:MET:HG3	2.20	0.42
3:f:181:LEU:HG	3:f:183:LEU:HD13	2.01	0.42
1:B:220:LEU:HD23	1:B:276:ILE:HD11	2.01	0.42
1:C:217:LEU:HA	1:C:221:TYR:HB2	2.01	0.42
1:C:267:LEU:HD12	1:C:268:PRO:HD2	2.02	0.42
2:I:18:MET:HE2	2:I:18:MET:HB2	1.93	0.42
3:K:141:ASP:H	3:K:170:GLN:NE2	2.18	0.42
3:N:118:VAL:O	3:N:207:LYS:HE3	2.20	0.42
1:S:300:ILE:HD11	1:S:312:SER:HA	2.02	0.42
1:T:224:SER:HB2	1:T:279:TRP:CZ3	2.55	0.42
2:X:33:THR:HA	2:X:53:PRO:HD3	2.00	0.42
1:A:76:PHE:CD2	1:A:111:ARG:HD3	2.55	0.42
1:B:273:ILE:HD11	1:C:215:PHE:HA	2.02	0.42
1:C:8:HIS:O	1:C:11:THR:HG22	2.19	0.42
1:D:76:PHE:CD2	1:D:111:ARG:HD3	2.55	0.42
1:D:168:LEU:HD23	1:D:186:THR:HB	2.01	0.42
1:D:227:LEU:HD12	1:D:227:LEU:HA	1.88	0.42
2:I:133:LEU:HD13	3:O:121:PHE:CG	2.55	0.42
1:P:252:THR:HG22	1:P:287:ILE:HD13	2.01	0.42
1:S:114:ASN:OD1	1:S:114:ASN:N	2.53	0.42
1:T:138:PRO:HD2	1:T:139:MET:SD	2.59	0.42
1:T:261:ALA:O	1:T:264:ASN:HB2	2.20	0.42
3:g:151:TRP:CE3	3:g:181:LEU:HD22	2.55	0.42
1:D:215:PHE:CE1	1:D:219:GLN:HG3	2.55	0.42
1:E:267:LEU:HA	1:E:268:PRO:HD2	1.81	0.42
2:H:18:MET:HE1	2:H:20:ILE:HG12	2.01	0.42
2:J:18:MET:HG3	2:J:86:LEU:HD11	2.01	0.42
1:C:221:TYR:HA	1:C:279:TRP:CZ3	2.55	0.42
1:D:139:MET:HE2	1:D:139:MET:HB2	1.95	0.42
2:F:48:ILE:HA	2:F:64:PHE:CD2	2.55	0.42
2:F:178:VAL:HG12	2:F:180:GLN:H	1.85	0.42
2:I:61:ASN:HD21	3:O:97:HIS:HE1	1.66	0.42
3:K:129:GLU:O	3:K:130:THR:OG1	2.34	0.42
1:P:111:ARG:HD2	1:P:119:LEU:HD23	2.01	0.42
1:S:75:ASP:O	1:S:114:ASN:N	2.53	0.42
1:S:194:VAL:HG13	2:X:52:ASN:HD22	1.85	0.42
2:V:155:PHE:HA	2:V:156:PRO:HA	1.76	0.42
2:X:170:SER:OG	2:X:171:GLY:N	2.52	0.42
3:f:94:TYR:O	3:f:95:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:39:GLN:HB2	3:g:49:LEU:HD11	2.02	0.42
1:B:102:THR:HA	1:B:106:PRO:HA	2.02	0.41
1:C:114:ASN:OD1	1:C:114:ASN:N	2.53	0.41
1:C:134:LEU:HD12	1:C:270:VAL:HG21	2.01	0.41
1:C:137:TYR:O	1:C:275:ALA:HB3	2.20	0.41
2:F:144:MET:HG2	2:F:193:PRO:HA	2.02	0.41
3:L:94:TYR:O	3:L:95:SER:OG	2.29	0.41
2:W:18:MET:HG3	2:W:86:LEU:HD11	2.01	0.41
3:f:37:TRP:CD2	3:f:75:LEU:HB2	2.55	0.41
3:i:135:LEU:HB2	3:i:181:LEU:HB3	2.02	0.41
2:J:53:PRO:O	2:J:74:LYS:HE2	2.20	0.41
1:B:189:THR:OG1	1:B:190:TYR:N	2.53	0.41
1:D:138:PRO:HB2	1:D:211:ARG:HD2	2.02	0.41
2:F:144:MET:HB3	2:F:192:VAL:C	2.45	0.41
3:N:152:LYS:HD3	3:N:197:GLN:OE1	2.20	0.41
1:Q:130:CYS:HA	1:Q:131:PRO:HD2	1.95	0.41
1:R:130:CYS:O	1:R:132:MET:HG3	2.19	0.41
2:V:157:GLU:HG3	2:V:184:TYR:CD2	2.56	0.41
3:f:166:GLN:HA	3:f:167:PRO:HD3	1.96	0.41
1:C:111:ARG:HB2	1:C:119:LEU:HB3	2.00	0.41
1:E:19:ARG:HG2	1:E:20:PRO:HD2	2.02	0.41
2:F:155:PHE:HA	2:F:156:PRO:HA	1.76	0.41
1:P:139:MET:HE2	1:P:139:MET:HB2	1.96	0.41
1:Q:256:MET:HE2	1:Q:283:CYS:HB2	2.02	0.41
1:T:307:GLU:O	1:T:311:ILE:HG12	2.19	0.41
2:U:100:GLY:HA3	2:U:108:TYR:CZ	2.55	0.41
3:f:85:GLU:HG3	3:f:107:THR:HA	2.03	0.41
2:H:208:HIS:NE2	2:H:210:ALA:HB3	2.34	0.41
3:K:94:TYR:O	3:K:96:ASN:N	2.53	0.41
3:i:36:ASN:ND2	3:i:52:GLY:H	2.19	0.41
1:C:273:ILE:HG12	1:D:215:PHE:HD1	1.85	0.41
1:P:279:TRP:HB2	1:P:334:TYR:CE1	2.56	0.41
1:Q:76:PHE:CD2	1:Q:111:ARG:HD3	2.56	0.41
1:S:154:THR:HA	1:S:200:TYR:HD1	1.85	0.41
2:Y:44:ASN:ND2	3:g:102:GLY:HA2	2.36	0.41
3:Z:181:LEU:HG	3:Z:183:LEU:HD13	2.01	0.41
3:f:152:LYS:HG2	3:f:157:PRO:HB3	2.01	0.41
1:A:237:PHE:HA	1:E:299:HIS:CE1	2.55	0.41
2:G:18:MET:HG3	2:G:86:LEU:HD11	2.01	0.41
1:P:288:PHE:CG	5:Q:401:POV:H34	2.56	0.41
2:U:197:TRP:HA	2:U:198:PRO:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:147:VAL:HG12	3:g:200:HIS:HB2	2.03	0.41
1:A:137:TYR:CE2	1:A:138:PRO:HB3	2.56	0.41
1:B:19:ARG:HG2	1:B:20:PRO:HD2	2.02	0.41
1:R:262:GLY:HA2	5:R:401:POV:H14B	2.03	0.41
3:Z:166:GLN:HA	3:Z:167:PRO:HD2	1.91	0.41
3:g:1:GLN:O	3:g:1:GLN:HG2	2.21	0.41
1:A:271:SER:HB2	1:B:180:SER:HA	2.03	0.41
3:K:121:PHE:HA	3:K:122:PRO:HD3	1.80	0.41
3:L:187:ALA:O	3:L:191:HIS:ND1	2.51	0.41
1:P:257:THR:OG1	1:P:284:MET:HE1	2.20	0.41
3:Z:115:SER:HA	3:Z:116:PRO:HD3	1.92	0.41
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.86	0.41
1:B:20:PRO:HD3	1:B:86:TRP:CD2	2.56	0.41
1:E:20:PRO:HA	1:E:21:PRO:HD3	1.85	0.41
1:E:35:LEU:HB3	1:E:54:THR:HB	2.03	0.41
1:E:130:CYS:O	1:E:132:MET:HG3	2.20	0.41
1:E:170:LEU:HD22	1:E:174:LEU:HD23	2.01	0.41
1:E:227:LEU:HA	1:E:227:LEU:HD12	1.89	0.41
1:E:279:TRP:HB2	1:E:334:TYR:CZ	2.56	0.41
2:H:6:GLN:H	2:H:114:GLN:NE2	2.17	0.41
3:L:128:LEU:HD21	3:L:188:TRP:CZ3	2.55	0.41
1:P:130:CYS:O	1:P:132:MET:HG3	2.21	0.41
1:R:49:TYR:CE1	1:R:144:CYS:HB3	2.56	0.41
1:T:130:CYS:O	1:T:132:MET:HG3	2.21	0.41
2:W:121:SER:OG	2:W:182:ASP:OD1	2.39	0.41
2:Y:13:ARG:HD2	2:Y:122:SER:HA	2.03	0.41
2:Y:27:TYR:HD2	2:Y:32:TYR:CD1	2.39	0.41
2:Y:153:GLY:HA2	2:Y:183:LEU:HB3	2.03	0.41
3:Z:188:TRP:HA	3:Z:194:TYR:OH	2.20	0.41
2:J:177:ALA:HA	2:J:186:LEU:HB3	2.02	0.41
3:M:40:GLU:O	3:M:86:ALA:HB1	2.20	0.41
1:T:220:LEU:HD23	1:T:276:ILE:HD11	2.02	0.41
2:Y:131:TYR:HA	2:Y:132:PRO:HD3	1.87	0.41
3:i:151:TRP:HD1	3:i:162:MET:HE3	1.86	0.41
2:J:218:LYS:HG2	2:J:219:ILE:H	1.86	0.41
1:A:35:LEU:HD12	1:A:169:GLN:O	2.21	0.40
1:A:137:TYR:HA	1:A:138:PRO:HA	1.79	0.40
1:B:43:ASP:OD1	1:B:45:VAL:N	2.51	0.40
1:Q:96:LYS:HD2	1:Q:129:SER:HB3	2.03	0.40
1:S:256:MET:HE2	1:S:283:CYS:HB2	2.03	0.40
1:E:110:ILE:HG12	1:E:120:TYR:HD1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:THR:HA	2:I:53:PRO:HD3	2.03	0.40
1:Q:107:ASN:OD1	1:Q:123:ARG:NH1	2.54	0.40
1:C:49:TYR:CE1	1:C:144:CYS:HB3	2.56	0.40
2:H:155:PHE:HA	2:H:156:PRO:HA	1.80	0.40
3:L:188:TRP:HA	3:L:194:TYR:OH	2.21	0.40
3:N:53:ILE:CG2	3:N:54:ASN:N	2.84	0.40
1:P:19:ARG:HA	1:P:20:PRO:HD3	1.97	0.40
1:P:220:LEU:O	1:P:224:SER:OG	2.23	0.40
1:S:5:ILE:O	1:S:8:HIS:HB3	2.20	0.40
1:S:302:ASN:ND2	1:T:241:ALA:HA	2.36	0.40
1:T:35:LEU:HD12	1:T:169:GLN:O	2.22	0.40
1:T:183:LEU:HD12	1:T:183:LEU:O	2.22	0.40
2:V:179:LEU:HD12	2:V:184:TYR:HE1	1.87	0.40
2:W:147:LEU:HD22	2:W:219:ILE:HG21	2.03	0.40
2:X:6:GLN:N	2:X:114:GLN:HE22	2.20	0.40
1:A:19:ARG:HG2	1:A:20:PRO:HD2	2.04	0.40
1:C:220:LEU:HD23	1:C:276:ILE:HD11	2.02	0.40
1:E:134:LEU:N	1:E:272:TYR:OH	2.41	0.40
2:H:18:MET:HG3	2:H:86:LEU:HD11	2.04	0.40
1:S:19:ARG:HG2	1:S:20:PRO:HD2	2.04	0.40
1:T:300:ILE:HG23	1:T:308:TRP:CE3	2.49	0.40
2:X:126:THR:HA	2:X:127:PRO:HD3	1.96	0.40
1:A:267:LEU:HD22	1:A:276:ILE:HG21	2.04	0.40
1:B:309:ASN:O	1:B:312:SER:OG	2.32	0.40
2:F:152:LYS:HA	2:F:185:THR:HG23	2.04	0.40
2:G:208:HIS:HD1	2:G:211:SER:HG	1.62	0.40
2:H:134:ALA:HA	2:H:135:PRO:HD3	1.97	0.40
2:I:48:ILE:HA	2:I:64:PHE:CD2	2.57	0.40
3:K:148:THR:HB	3:K:199:THR:HB	2.03	0.40
1:S:19:ARG:NH1	1:S:157:ASP:HA	2.37	0.40
1:S:137:TYR:OH	1:S:267:LEU:HB2	2.21	0.40
2:X:108:TYR:CB	3:i:51:GLY:HA3	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	340/347 (98%)	327 (96%)	13 (4%)	0	100	100
1	B	339/347 (98%)	325 (96%)	14 (4%)	0	100	100
1	C	338/347 (97%)	324 (96%)	14 (4%)	0	100	100
1	D	338/347 (97%)	328 (97%)	10 (3%)	0	100	100
1	E	338/347 (97%)	325 (96%)	13 (4%)	0	100	100
1	P	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	Q	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	R	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	S	338/347 (97%)	325 (96%)	12 (4%)	1 (0%)	36	68
1	T	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
2	F	219/224 (98%)	206 (94%)	13 (6%)	0	100	100
2	G	220/224 (98%)	203 (92%)	17 (8%)	0	100	100
2	H	221/224 (99%)	206 (93%)	15 (7%)	0	100	100
2	I	220/224 (98%)	206 (94%)	14 (6%)	0	100	100
2	J	220/224 (98%)	203 (92%)	16 (7%)	1 (0%)	24	59
2	U	219/224 (98%)	205 (94%)	14 (6%)	0	100	100
2	V	222/224 (99%)	203 (91%)	19 (9%)	0	100	100
2	W	222/224 (99%)	209 (94%)	13 (6%)	0	100	100
2	X	222/224 (99%)	206 (93%)	16 (7%)	0	100	100
2	Y	219/224 (98%)	202 (92%)	17 (8%)	0	100	100
3	K	208/215 (97%)	193 (93%)	14 (7%)	1 (0%)	24	59
3	L	209/215 (97%)	198 (95%)	11 (5%)	0	100	100
3	M	208/215 (97%)	193 (93%)	15 (7%)	0	100	100
3	N	209/215 (97%)	194 (93%)	14 (7%)	1 (0%)	24	59
3	O	209/215 (97%)	194 (93%)	15 (7%)	0	100	100
3	Z	213/215 (99%)	193 (91%)	19 (9%)	1 (0%)	24	59
3	f	213/215 (99%)	195 (92%)	16 (8%)	2 (1%)	14	47
3	g	209/215 (97%)	196 (94%)	11 (5%)	2 (1%)	12	45
3	h	209/215 (97%)	194 (93%)	15 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	i	212/215 (99%)	199 (94%)	12 (6%)	1 (0%)	24 59
All	All	7686/7860 (98%)	7256 (94%)	420 (6%)	10 (0%)	48 79

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	95	SER
3	N	95	SER
3	i	95	SER
3	f	95	SER
1	S	309	ASN
3	f	96	ASN
2	J	221	PRO
3	g	96	ASN
3	g	52	GLY
3	Z	52	GLY

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	311/316 (98%)	307 (99%)	4 (1%)	61 78
1	B	310/316 (98%)	306 (99%)	4 (1%)	61 78
1	C	309/316 (98%)	305 (99%)	4 (1%)	61 78
1	D	309/316 (98%)	304 (98%)	5 (2%)	55 75
1	E	309/316 (98%)	306 (99%)	3 (1%)	68 80
1	P	309/316 (98%)	304 (98%)	5 (2%)	55 75
1	Q	309/316 (98%)	307 (99%)	2 (1%)	78 84
1	R	309/316 (98%)	307 (99%)	2 (1%)	78 84
1	S	309/316 (98%)	305 (99%)	4 (1%)	61 78
1	T	309/316 (98%)	306 (99%)	3 (1%)	68 80
2	F	190/193 (98%)	188 (99%)	2 (1%)	65 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	191/193 (99%)	190 (100%)	1 (0%)	81	85
2	H	192/193 (100%)	190 (99%)	2 (1%)	68	80
2	I	191/193 (99%)	190 (100%)	1 (0%)	81	85
2	J	191/193 (99%)	187 (98%)	4 (2%)	47	71
2	U	190/193 (98%)	187 (98%)	3 (2%)	55	75
2	V	193/193 (100%)	191 (99%)	2 (1%)	68	80
2	W	193/193 (100%)	193 (100%)	0	100	100
2	X	193/193 (100%)	191 (99%)	2 (1%)	68	80
2	Y	190/193 (98%)	188 (99%)	2 (1%)	65	79
3	K	178/182 (98%)	177 (99%)	1 (1%)	78	84
3	L	179/182 (98%)	175 (98%)	4 (2%)	45	71
3	M	178/182 (98%)	174 (98%)	4 (2%)	45	71
3	N	179/182 (98%)	178 (99%)	1 (1%)	78	84
3	O	179/182 (98%)	175 (98%)	4 (2%)	45	71
3	Z	182/182 (100%)	180 (99%)	2 (1%)	65	79
3	f	182/182 (100%)	180 (99%)	2 (1%)	65	79
3	g	179/182 (98%)	175 (98%)	4 (2%)	45	71
3	h	179/182 (98%)	175 (98%)	4 (2%)	45	71
3	i	181/182 (100%)	175 (97%)	6 (3%)	33	65
All	All	6803/6910 (98%)	6716 (99%)	87 (1%)	61	78

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	95	GLU
1	A	227	LEU
1	A	267	LEU
1	B	95	GLU
1	B	172	VAL
1	B	194	VAL
1	B	227	LEU
1	C	95	GLU
1	C	172	VAL
1	C	194	VAL

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Mol	Chain	Res	Type
1	C	227	LEU
1	D	95	GLU
1	D	154	THR
1	D	172	VAL
1	D	194	VAL
1	D	227	LEU
1	E	95	GLU
1	E	194	VAL
1	E	227	LEU
2	F	27	TYR
2	F	145	VAL
2	G	220	VAL
2	H	27	TYR
2	H	133	LEU
2	I	27	TYR
3	K	149	VAL
3	L	75	LEU
3	L	139	ILE
3	L	149	VAL
3	L	158	VAL
3	N	53	ILE
3	O	45	LEU
3	O	75	LEU
3	O	97	HIS
3	O	139	ILE
1	P	95	GLU
1	P	105	LYS
1	P	172	VAL
1	P	194	VAL
1	P	227	LEU
1	Q	95	GLU
1	Q	264	ASN
1	R	95	GLU
1	R	172	VAL
1	S	95	GLU
1	S	172	VAL
1	S	194	VAL
1	S	227	LEU
1	T	95	GLU
1	T	172	VAL
1	T	227	LEU
2	U	27	TYR

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Mol	Chain	Res	Type
2	U	133	LEU
2	U	196	THR
2	V	149	CYS
2	V	220	VAL
2	X	45	LEU
2	X	172	VAL
2	Y	27	TYR
2	Y	45	LEU
3	Z	56	ARG
3	Z	75	LEU
3	f	45	LEU
3	f	75	LEU
3	g	75	LEU
3	g	130	THR
3	g	149	VAL
3	g	158	VAL
3	h	75	LEU
3	h	118	VAL
3	h	149	VAL
3	h	205	VAL
3	i	75	LEU
3	i	97	HIS
3	i	118	VAL
3	i	139	ILE
3	i	149	VAL
3	i	214	CYS
2	J	27	TYR
2	J	120	VAL
2	J	178	VAL
2	J	215	VAL
3	M	75	LEU
3	M	118	VAL
3	M	130	THR
3	M	149	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	46	ASN
1	A	219	GLN
1	A	298	ASN
1	A	302	ASN

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Mol	Chain	Res	Type
1	B	169	GLN
1	C	46	ASN
1	C	83	HIS
1	C	196	ASN
1	C	264	ASN
1	D	298	ASN
1	E	83	HIS
1	E	259	GLN
1	E	298	ASN
2	H	140	GLN
2	I	55	ASN
3	K	39	GLN
3	K	170	GLN
3	K	172	ASN
3	L	200	HIS
3	N	39	GLN
3	N	55	ASN
3	N	170	GLN
3	O	39	GLN
3	O	97	HIS
3	O	111	GLN
3	O	172	ASN
1	P	73	GLN
1	P	83	HIS
1	P	259	GLN
1	P	298	ASN
1	Q	73	GLN
1	Q	83	HIS
1	Q	208	GLN
1	Q	219	GLN
1	Q	266	GLN
1	Q	299	HIS
1	R	52	GLN
1	R	83	HIS
1	R	196	ASN
1	R	219	GLN
1	S	83	HIS
1	S	219	GLN
1	S	264	ASN
1	S	266	GLN
1	T	46	ASN
1	T	208	GLN

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Mol	Chain	Res	Type
1	T	259	GLN
1	T	266	GLN
2	V	6	GLN
2	V	55	ASN
2	Y	44	ASN
2	Y	173	HIS
3	Z	97	HIS
3	g	39	GLN
3	h	39	GLN
3	i	170	GLN
2	J	173	HIS
2	J	180	GLN
3	M	170	GLN
3	M	172	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 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	POV	A	402	-	22,22,51	1.11	1 (4%)	27,29,59	1.19	2 (7%)
4	NAG	A	401	1	14,14,15	0.29	0	17,19,21	1.02	1 (5%)
4	NAG	B	402	1	14,14,15	0.26	0	17,19,21	0.80	0
4	NAG	Q	402	1	14,14,15	0.27	0	17,19,21	0.63	0
8	LMT	D	403	-	24,24,36	1.08	2 (8%)	35,35,47	1.15	2 (5%)
7	GOL	B	401	-	5,5,5	0.37	0	5,5,5	0.29	0
8	LMT	B	403	-	24,24,36	1.02	2 (8%)	35,35,47	1.43	5 (14%)
5	POV	R	401	-	33,33,51	1.18	2 (6%)	39,41,59	1.14	3 (7%)
5	POV	Q	401	-	45,45,51	1.03	2 (4%)	51,53,59	1.05	3 (5%)
4	NAG	D	402	1	14,14,15	0.35	0	17,19,21	1.32	1 (5%)
4	NAG	C	401	1	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
4	NAG	T	402	1	14,14,15	0.37	0	17,19,21	0.77	1 (5%)
8	LMT	T	403	-	24,24,36	1.04	2 (8%)	35,35,47	1.25	5 (14%)
5	POV	D	401	-	25,25,51	1.36	2 (8%)	31,33,59	1.32	4 (12%)
4	NAG	P	401	1	14,14,15	0.34	0	17,19,21	0.71	0
8	LMT	C	402	-	24,24,36	1.10	2 (8%)	35,35,47	1.12	4 (11%)
4	NAG	E	401	1	14,14,15	0.27	0	17,19,21	0.59	0
5	POV	R	402	-	34,34,51	1.15	2 (5%)	37,39,59	1.33	5 (13%)
8	LMT	P	402	-	24,24,36	1.04	2 (8%)	35,35,47	1.18	2 (5%)
4	NAG	S	401	1	14,14,15	0.35	0	17,19,21	1.32	1 (5%)
5	POV	P	403	-	41,41,51	1.07	2 (4%)	47,49,59	1.12	4 (8%)
5	POV	T	401	-	42,42,51	1.04	2 (4%)	48,50,59	1.14	4 (8%)
8	LMT	E	402	-	24,24,36	1.04	2 (8%)	35,35,47	1.15	3 (8%)
8	LMT	S	402	-	24,24,36	1.05	2 (8%)	35,35,47	1.23	2 (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
5	POV	A	402	-	-	4/25/25/55	-
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	402	1	-	0/6/23/26	0/1/1/1
4	NAG	Q	402	1	-	0/6/23/26	0/1/1/1
8	LMT	D	403	-	-	4/8/48/61	0/2/2/2
7	GOL	B	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LMT	B	403	-	-	4/8/48/61	0/2/2/2
5	POV	R	401	-	-	17/37/37/55	-
5	POV	Q	401	-	-	14/49/49/55	-
4	NAG	D	402	1	-	3/6/23/26	0/1/1/1
4	NAG	C	401	1	-	5/6/23/26	0/1/1/1
4	NAG	T	402	1	-	3/6/23/26	0/1/1/1
8	LMT	T	403	-	-	2/8/48/61	0/2/2/2
5	POV	D	401	-	-	10/29/29/55	-
4	NAG	P	401	1	-	4/6/23/26	0/1/1/1
8	LMT	C	402	-	-	6/8/48/61	0/2/2/2
4	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	POV	R	402	-	-	12/36/36/55	-
8	LMT	P	402	-	-	1/8/48/61	0/2/2/2
4	NAG	S	401	1	-	0/6/23/26	0/1/1/1
5	POV	P	403	-	-	12/45/45/55	-
5	POV	T	401	-	-	16/46/46/55	-
8	LMT	E	402	-	-	3/8/48/61	0/2/2/2
8	LMT	S	402	-	-	1/8/48/61	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	POV	O31-C31	4.48	1.46	1.33
5	P	403	POV	O31-C31	4.35	1.46	1.33
5	Q	401	POV	O31-C31	4.33	1.46	1.33
5	R	401	POV	O31-C31	4.26	1.45	1.33
5	T	401	POV	O31-C31	4.22	1.45	1.33
5	R	402	POV	O31-C31	4.20	1.45	1.33
5	R	402	POV	O21-C21	4.15	1.46	1.34
5	A	402	POV	O21-C21	4.12	1.45	1.34
5	Q	401	POV	O21-C21	4.07	1.45	1.34
5	T	401	POV	O21-C21	4.07	1.45	1.34
5	P	403	POV	O21-C21	4.06	1.45	1.34
5	R	401	POV	O21-C21	4.03	1.45	1.34
5	D	401	POV	O21-C21	3.95	1.45	1.34
8	C	402	LMT	O5B-C1B	2.98	1.49	1.41
8	D	403	LMT	O5B-C1B	2.94	1.49	1.41
8	B	403	LMT	O5B-C1B	2.85	1.49	1.41
8	P	402	LMT	O5B-C1B	2.82	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	402	LMT	O5B-C1B	2.69	1.48	1.41
8	T	403	LMT	O5B-C1B	2.63	1.48	1.41
8	E	402	LMT	O5B-C1B	2.56	1.48	1.41
8	S	402	LMT	O5'-C1'	2.36	1.48	1.42
8	T	403	LMT	O5'-C1'	2.34	1.48	1.42
8	C	402	LMT	O5'-C1'	2.34	1.48	1.42
8	P	402	LMT	O5'-C1'	2.25	1.48	1.42
8	D	403	LMT	O5'-C1'	2.20	1.48	1.42
8	E	402	LMT	O5'-C1'	2.15	1.48	1.42
8	B	403	LMT	O5'-C1'	2.05	1.47	1.42

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	401	NAG	C1-O5-C5	4.58	118.32	112.19
4	D	402	NAG	C1-O5-C5	-4.40	106.29	112.19
5	R	402	POV	O21-C21-C22	4.30	120.79	111.48
5	T	401	POV	O21-C21-C22	4.18	120.53	111.48
5	A	402	POV	O21-C21-C22	4.07	120.28	111.48
5	D	401	POV	O21-C21-C22	4.04	120.23	111.48
5	P	403	POV	O21-C21-C22	3.83	119.76	111.48
8	E	402	LMT	O5'-C5'-C4'	3.68	117.32	109.72
8	S	402	LMT	C1B-O1B-C4'	-3.60	109.45	117.98
8	P	402	LMT	C1B-O1B-C4'	-3.57	109.52	117.98
4	A	401	NAG	C1-O5-C5	-3.57	107.41	112.19
5	D	401	POV	C2-O21-C21	-3.37	109.72	117.80
5	R	401	POV	C2-O21-C21	-3.34	109.79	117.80
5	R	401	POV	O21-C21-C22	3.27	118.55	111.48
5	Q	401	POV	O21-C21-C22	3.26	118.53	111.48
8	T	403	LMT	C1B-O1B-C4'	-3.07	110.71	117.98
5	Q	401	POV	O31-C31-C32	3.05	121.15	111.83
5	P	403	POV	C2-O21-C21	-2.94	110.75	117.80
5	T	401	POV	C2-O21-C21	-2.85	110.99	117.80
8	D	403	LMT	C1B-O1B-C4'	-2.80	111.35	117.98
5	R	401	POV	O31-C31-C32	2.79	120.35	111.83
8	B	403	LMT	C2'-C3'-C4'	2.77	115.97	109.68
5	R	402	POV	O31-C31-C32	2.76	120.25	111.83
8	B	403	LMT	O5B-C5B-C4B	2.75	114.65	109.70
5	D	401	POV	O31-C31-C32	2.75	120.21	111.83
8	B	403	LMT	C1'-C2'-C3'	2.74	115.93	110.36
5	P	403	POV	O31-C31-C32	2.64	119.89	111.83
5	R	402	POV	C2-O21-C21	-2.58	111.62	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	POV	C2-O21-C21	-2.53	111.75	117.80
8	P	402	LMT	C2'-C3'-C4'	2.51	115.37	109.68
5	T	401	POV	O31-C31-C32	2.50	119.45	111.83
8	T	403	LMT	O5'-C5'-C4'	2.42	114.72	109.72
8	C	402	LMT	C1B-O1B-C4'	-2.38	112.33	117.98
8	T	403	LMT	O5B-C5B-C4B	2.33	113.90	109.70
5	Q	401	POV	C2-O21-C21	-2.32	112.24	117.80
8	S	402	LMT	C4B-C3B-C2B	2.32	114.90	110.83
5	T	401	POV	C11-C12-N	-2.28	108.50	115.82
5	R	402	POV	O13-P-O14	2.28	119.72	110.83
8	T	403	LMT	C2'-C3'-C4'	2.28	114.84	109.68
5	P	403	POV	C11-C12-N	-2.27	108.53	115.82
8	E	402	LMT	C1B-O1B-C4'	-2.26	112.62	117.98
4	C	401	NAG	C1-O5-C5	2.24	115.19	112.19
4	T	402	NAG	C1-O5-C5	2.13	115.04	112.19
8	C	402	LMT	C1B-C2B-C3B	2.13	114.49	110.01
8	B	403	LMT	C3B-C4B-C5B	2.13	114.09	110.23
5	R	402	POV	O21-C21-O22	-2.10	118.79	123.70
8	B	403	LMT	O3'-C3'-C2'	-2.10	105.42	110.38
8	C	402	LMT	C4B-C3B-C2B	2.07	114.46	110.83
8	E	402	LMT	C3'-C4'-C5'	2.06	115.50	110.93
8	C	402	LMT	O5B-C5B-C4B	2.06	113.41	109.70
8	T	403	LMT	O5'-C1'-C2'	2.03	113.86	110.30
8	D	403	LMT	C1'-C2'-C3'	2.02	114.48	110.36
5	D	401	POV	O21-C21-O22	-2.00	119.02	123.70

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	NAG	C8-C7-N2-C2
4	C	401	NAG	O7-C7-N2-C2
4	D	402	NAG	C8-C7-N2-C2
4	D	402	NAG	O7-C7-N2-C2
4	T	402	NAG	C8-C7-N2-C2
4	T	402	NAG	O7-C7-N2-C2
5	A	402	POV	C11-O12-P-O14
5	A	402	POV	O12-C11-C12-N
5	A	402	POV	C22-C21-O21-C2
5	D	401	POV	C11-O12-P-O14
5	D	401	POV	O12-C11-C12-N
5	P	403	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
5	P	403	POV	C11-O12-P-O14
5	P	403	POV	O12-C11-C12-N
5	R	401	POV	C1-O11-P-O12
5	R	401	POV	C1-O11-P-O14
5	R	401	POV	O22-C21-O21-C2
5	R	402	POV	C1-O11-P-O12
5	T	401	POV	C1-O11-P-O12
5	T	401	POV	C1-O11-P-O13
5	T	401	POV	C11-O12-P-O11
5	T	401	POV	C11-O12-P-O13
5	T	401	POV	O12-C11-C12-N
7	B	401	GOL	O1-C1-C2-C3
8	B	403	LMT	O5B-C1B-O1B-C4'
5	A	402	POV	O22-C21-O21-C2
5	R	401	POV	C22-C21-O21-C2
4	A	401	NAG	O7-C7-N2-C2
8	C	402	LMT	C4B-C5B-C6B-O6B
5	R	402	POV	C22-C21-O21-C2
8	C	402	LMT	O5B-C5B-C6B-O6B
8	D	403	LMT	O5'-C5'-C6'-O6'
4	P	401	NAG	C4-C5-C6-O6
4	A	401	NAG	C8-C7-N2-C2
8	D	403	LMT	C4B-C5B-C6B-O6B
5	R	402	POV	O22-C21-O21-C2
4	P	401	NAG	O5-C5-C6-O6
5	Q	401	POV	C22-C21-O21-C2
4	P	401	NAG	C8-C7-N2-C2
8	D	403	LMT	O5B-C5B-C6B-O6B
5	R	401	POV	C32-C31-O31-C3
5	Q	401	POV	O22-C21-O21-C2
4	P	401	NAG	O7-C7-N2-C2
8	E	402	LMT	C4'-C5'-C6'-O6'
4	C	401	NAG	O5-C5-C6-O6
5	R	401	POV	C22-C23-C24-C25
5	T	401	POV	C34-C35-C36-C37
8	C	402	LMT	C2B-C1B-O1B-C4'
5	R	401	POV	O32-C31-O31-C3
5	T	401	POV	C22-C21-O21-C2
5	Q	401	POV	C22-C23-C24-C25
5	R	401	POV	C21-C22-C23-C24
5	P	403	POV	C22-C21-O21-C2
8	T	403	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
5	P	403	POV	O22-C21-O21-C2
5	R	402	POV	O11-C1-C2-O21
5	Q	401	POV	C211-C212-C213-C214
4	D	402	NAG	O5-C5-C6-O6
8	E	402	LMT	O5B-C5B-C6B-O6B
8	C	402	LMT	O5B-C1B-O1B-C4'
5	Q	401	POV	O11-C1-C2-C3
8	B	403	LMT	C3'-C4'-O1B-C1B
8	S	402	LMT	O5'-C5'-C6'-O6'
5	T	401	POV	C24-C25-C26-C27
8	D	403	LMT	C4'-C5'-C6'-O6'
5	T	401	POV	O22-C21-O21-C2
5	D	401	POV	C1-C2-C3-O31
5	R	402	POV	C26-C27-C28-C29
4	T	402	NAG	O5-C5-C6-O6
5	R	402	POV	C1-O11-P-O14
8	B	403	LMT	C5'-C4'-O1B-C1B
4	E	401	NAG	C8-C7-N2-C2
5	T	401	POV	C32-C31-O31-C3
7	B	401	GOL	O1-C1-C2-O2
5	R	402	POV	O11-C1-C2-C3
5	P	403	POV	C311-C310-C39-C38
5	Q	401	POV	C215-C216-C217-C218
5	R	402	POV	C1-C2-C3-O31
5	Q	401	POV	O11-C1-C2-O21
5	Q	401	POV	O21-C21-C22-C23
5	R	402	POV	C32-C31-O31-C3
8	B	403	LMT	C4B-C5B-C6B-O6B
5	T	401	POV	O32-C31-O31-C3
5	D	401	POV	O11-C1-C2-O21
5	T	401	POV	C1-C2-C3-O31
5	D	401	POV	O21-C2-C3-O31
5	T	401	POV	C311-C310-C39-C38
4	C	401	NAG	C4-C5-C6-O6
8	C	402	LMT	C4'-C5'-C6'-O6'
5	R	401	POV	O12-C11-C12-N
5	P	403	POV	C39-C310-C311-C312
4	E	401	NAG	O7-C7-N2-C2
5	D	401	POV	O11-C1-C2-C3
5	R	401	POV	O11-C1-C2-C3
5	Q	401	POV	C23-C24-C25-C26
5	T	401	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
5	R	402	POV	O32-C31-O31-C3
5	R	401	POV	C2-C1-O11-P
5	R	401	POV	O11-C1-C2-O21
5	R	401	POV	O21-C2-C3-O31
5	R	402	POV	O21-C2-C3-O31
4	C	401	NAG	C3-C2-N2-C7
5	P	403	POV	C1-O11-P-O12
5	R	401	POV	C1-O11-P-O13
5	R	401	POV	C11-O12-P-O14
5	P	403	POV	C32-C31-O31-C3
5	Q	401	POV	C24-C25-C26-C27
5	P	403	POV	O32-C31-O31-C3
8	P	402	LMT	O5B-C5B-C6B-O6B
5	P	403	POV	C31-C32-C33-C34
5	Q	401	POV	C26-C27-C28-C29
5	P	403	POV	C33-C34-C35-C36
5	D	401	POV	O22-C21-O21-C2
5	R	402	POV	C23-C24-C25-C26
5	Q	401	POV	C27-C28-C29-C210
8	T	403	LMT	O5B-C5B-C6B-O6B
5	D	401	POV	O32-C31-O31-C3
5	Q	401	POV	O22-C21-C22-C23
5	T	401	POV	O21-C2-C3-O31
5	D	401	POV	C22-C21-O21-C2
5	R	401	POV	C1-C2-C3-O31
8	E	402	LMT	O5'-C5'-C6'-O6'
8	C	402	LMT	O5'-C5'-C6'-O6'
5	D	401	POV	C32-C31-O31-C3
5	R	401	POV	C35-C36-C37-C38
5	T	401	POV	C313-C314-C315-C316
5	Q	401	POV	C31-C32-C33-C34

There are no ring outliers.

11 monomers are involved in 29 short contacts:

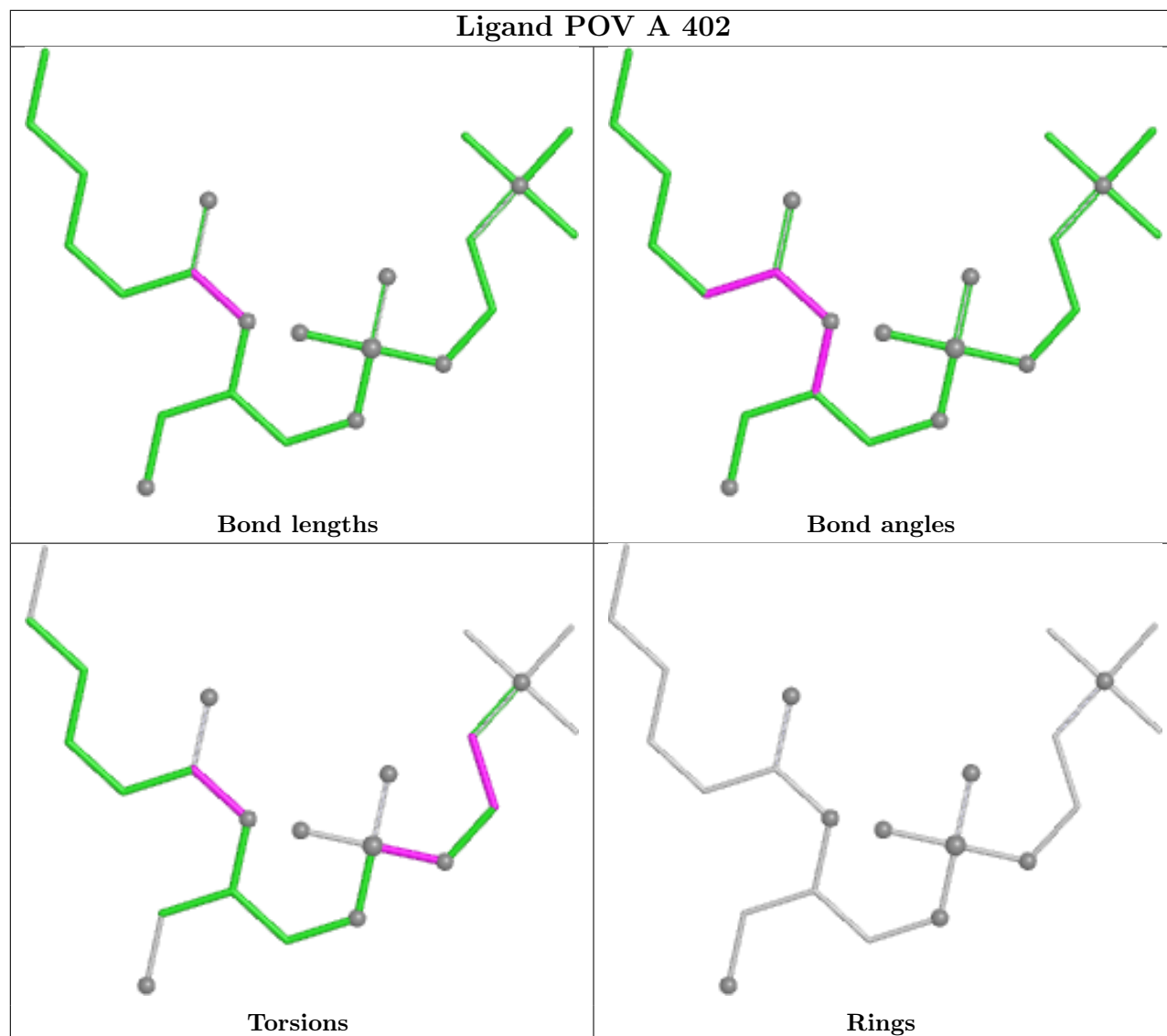
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	POV	1	0
8	D	403	LMT	1	0
5	R	401	POV	4	0
5	Q	401	POV	6	0
8	T	403	LMT	1	0
5	D	401	POV	5	0

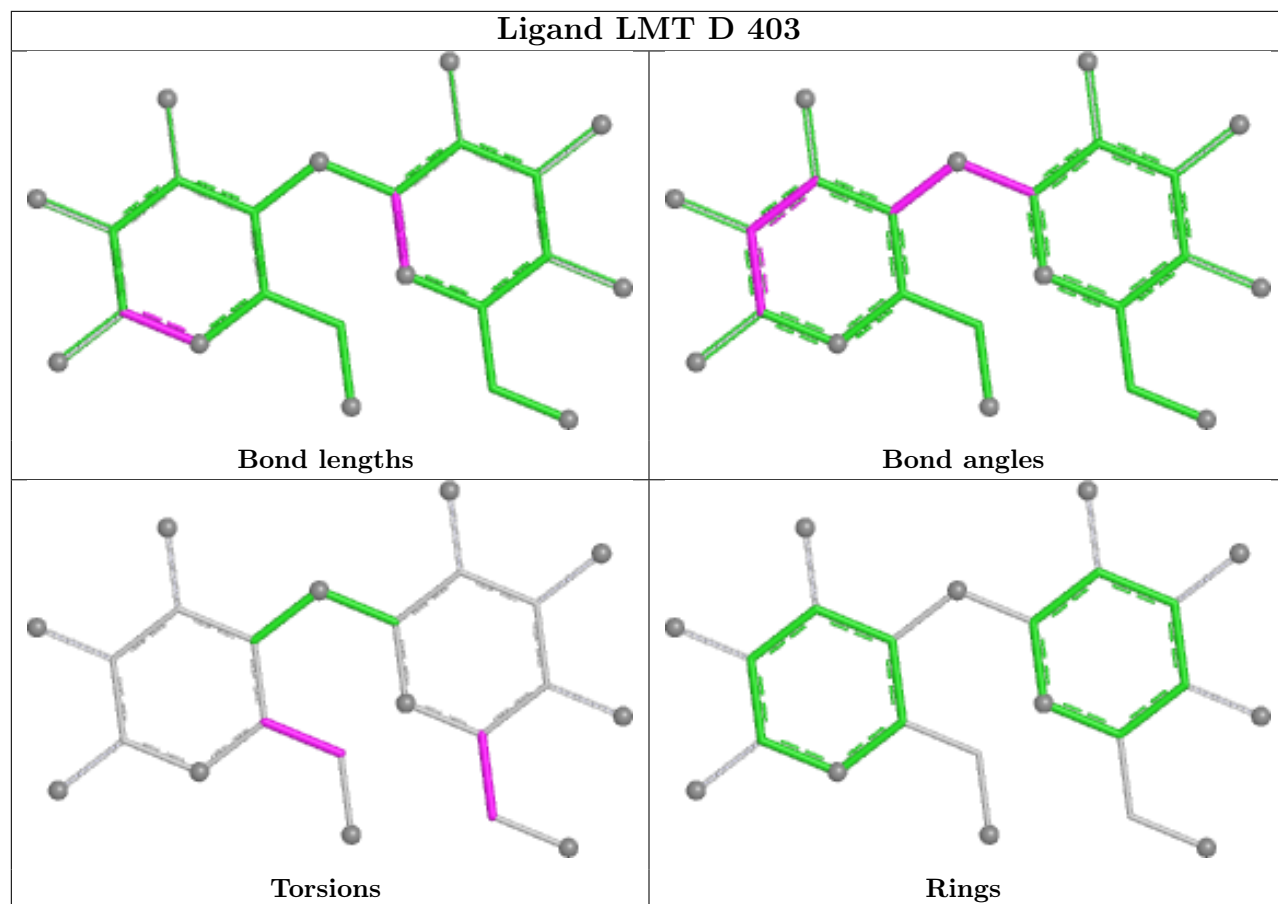
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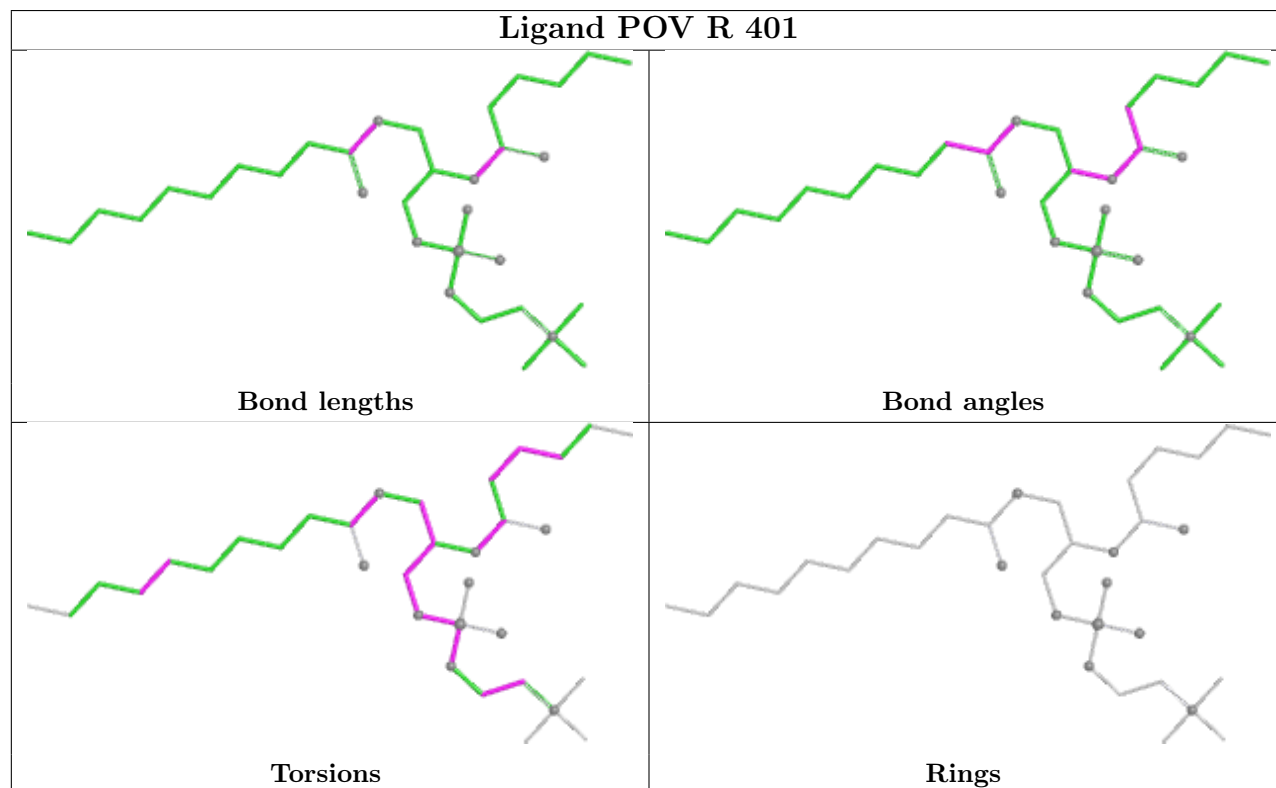
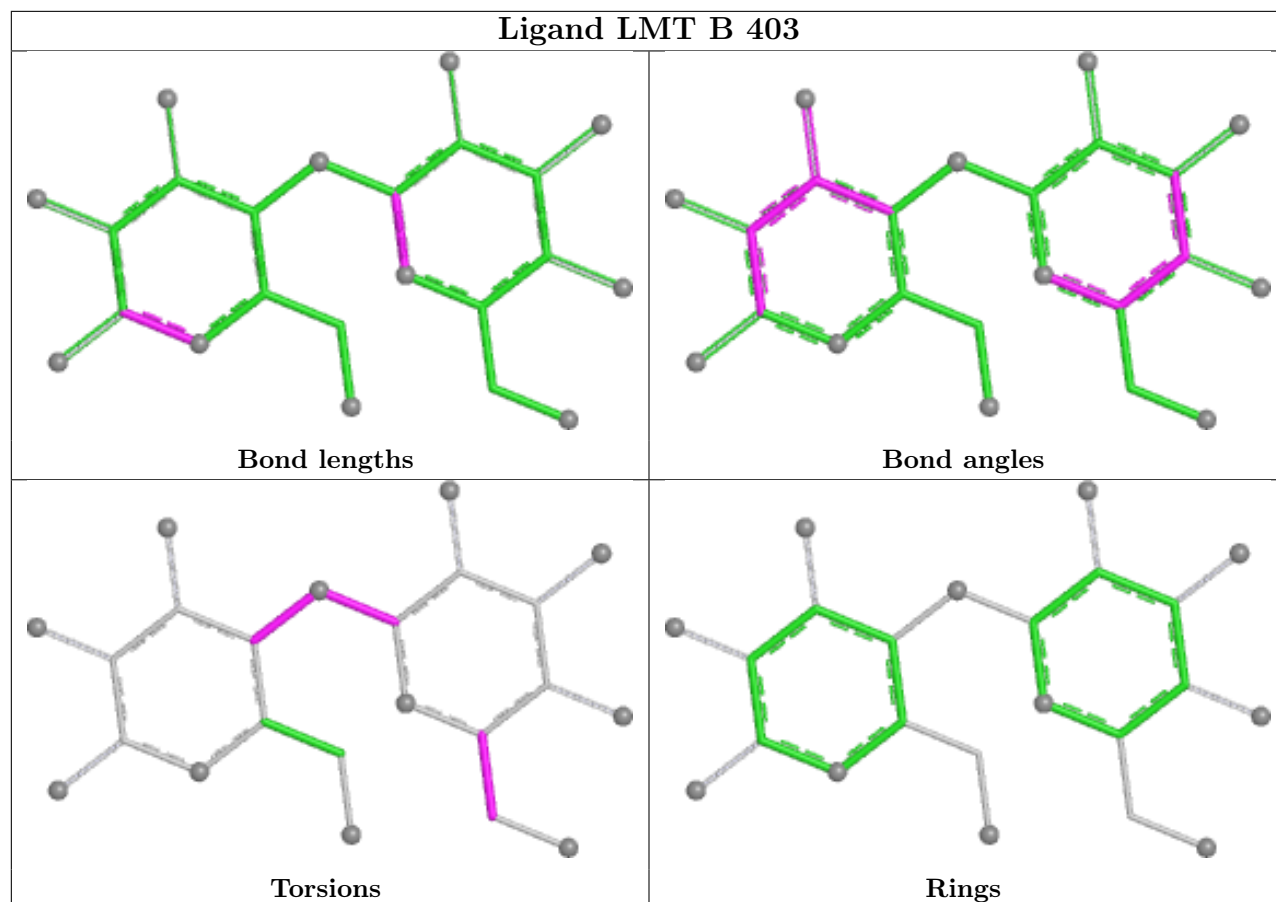
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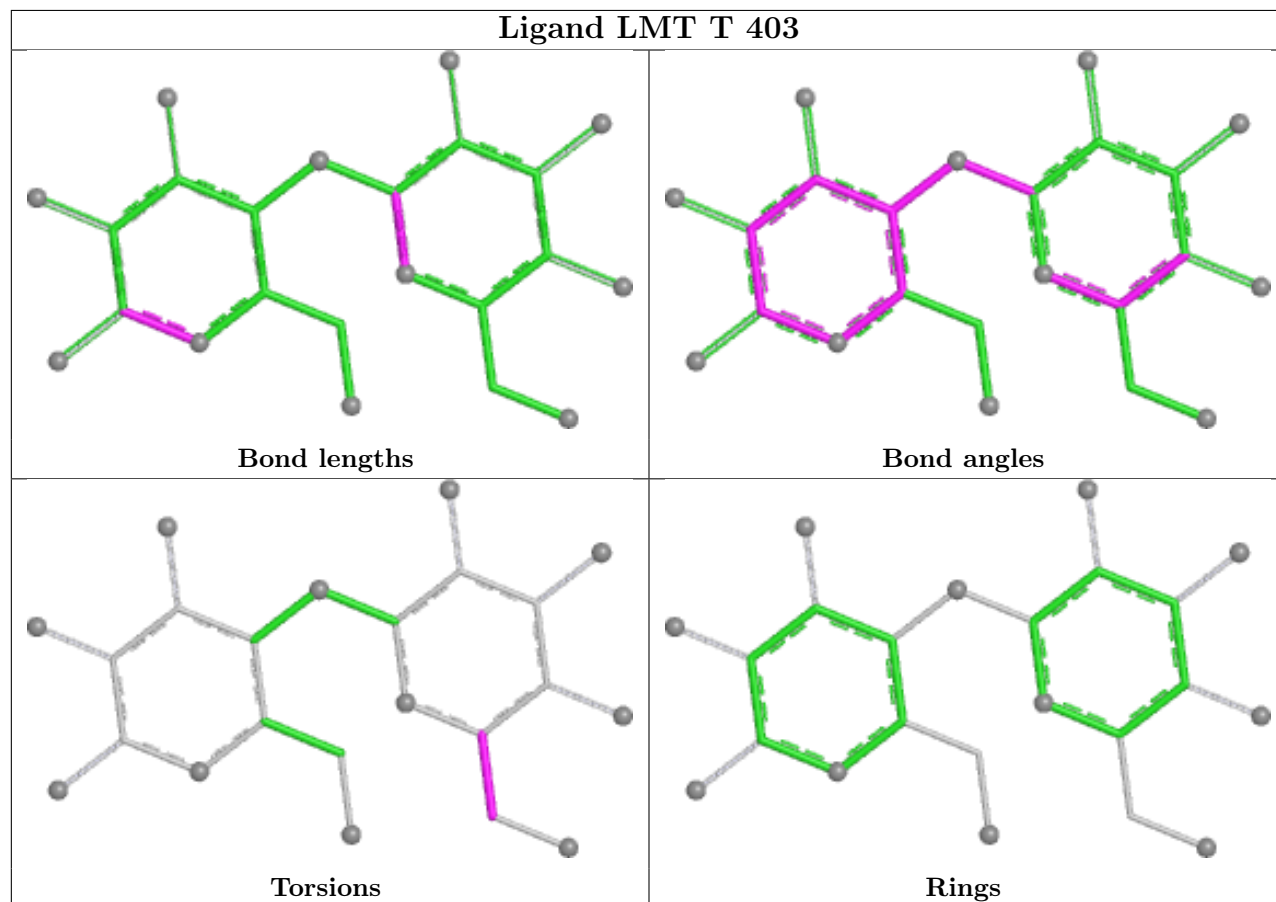
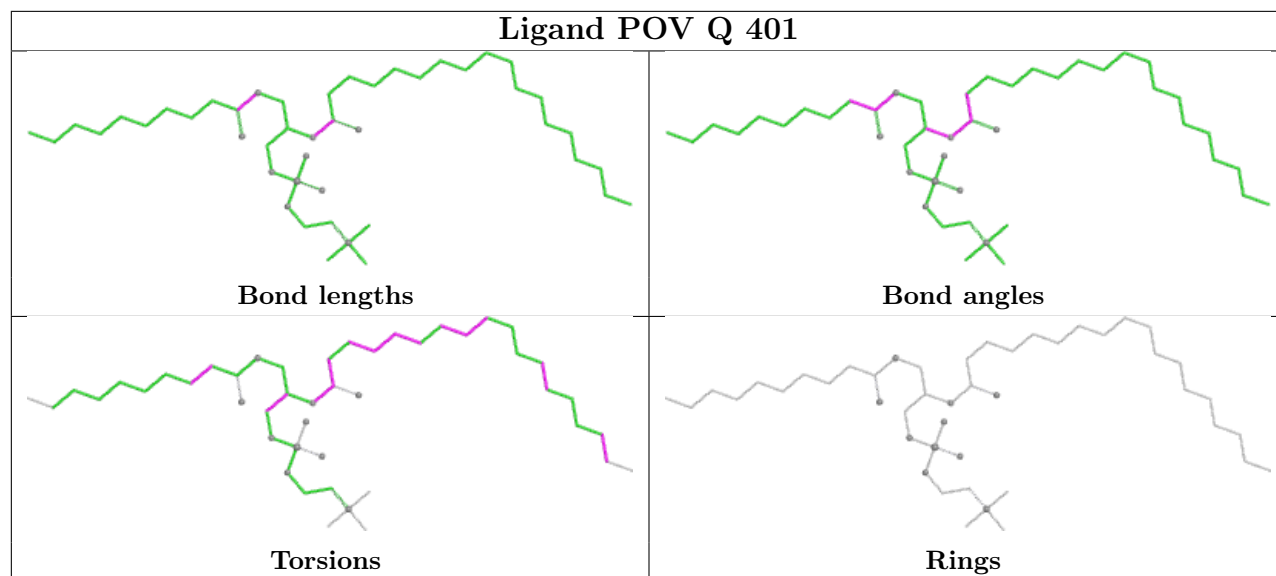
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	402	POV	2	0
4	S	401	NAG	1	0
5	P	403	POV	4	0
5	T	401	POV	3	0
8	S	402	LMT	1	0

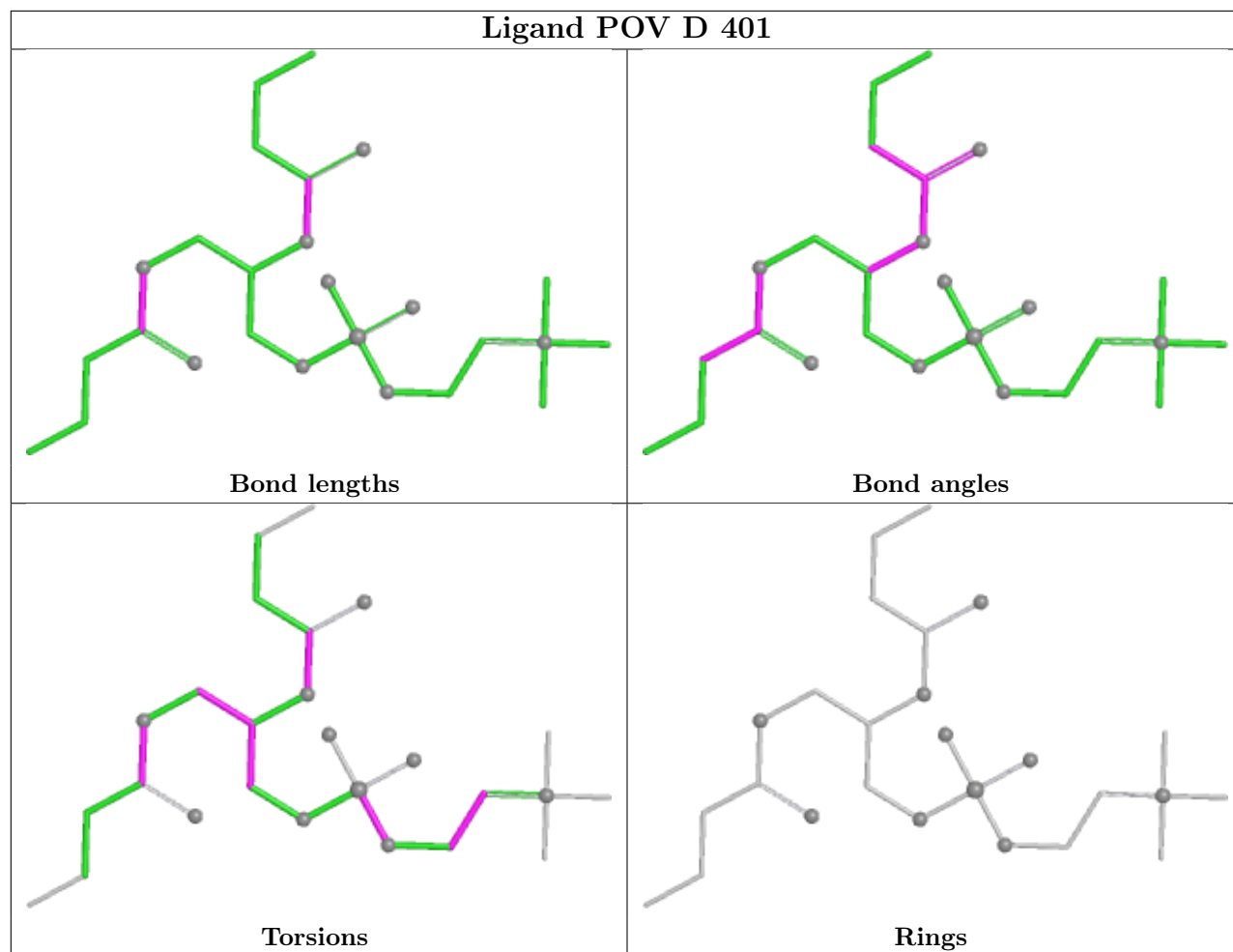
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

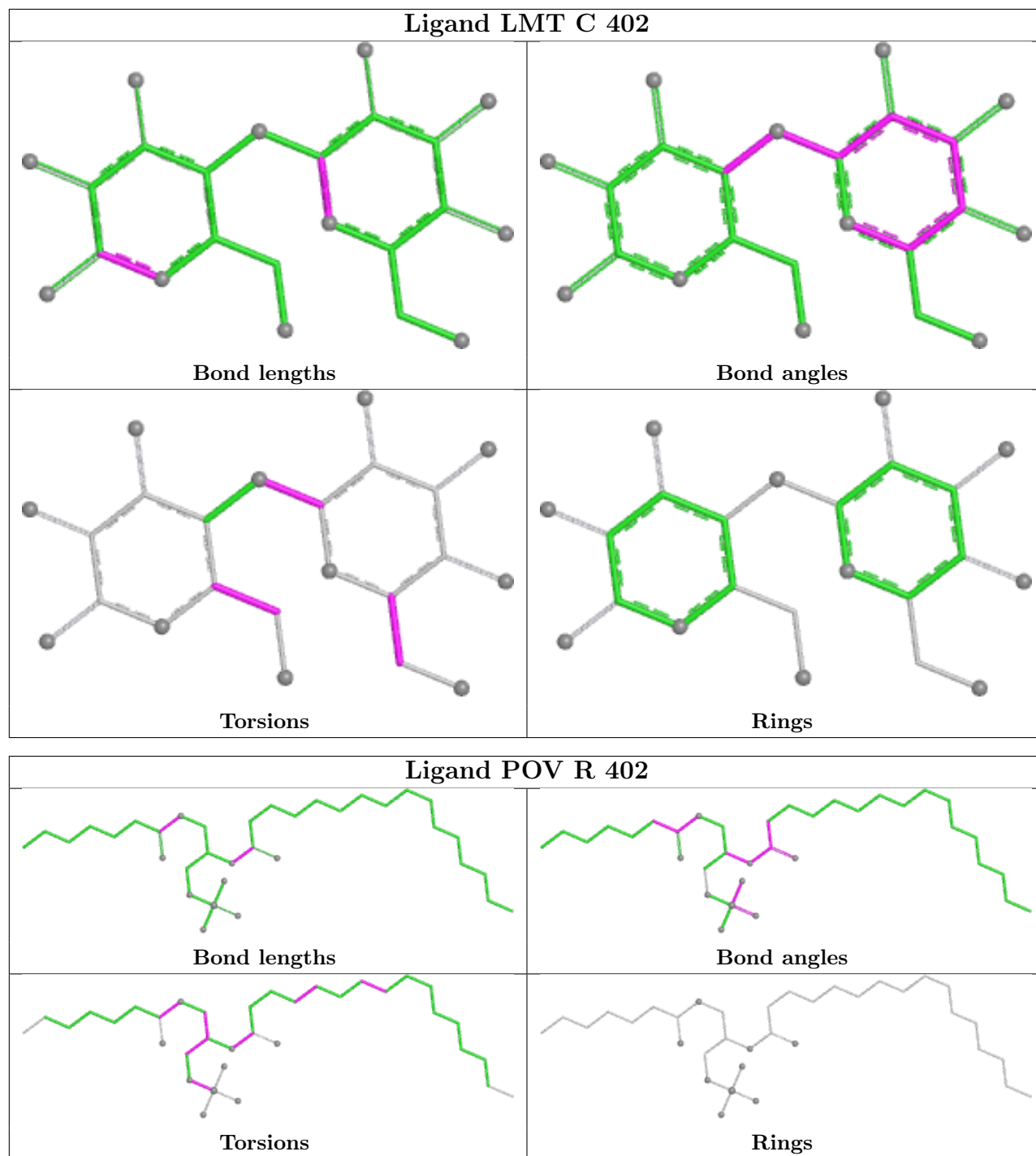


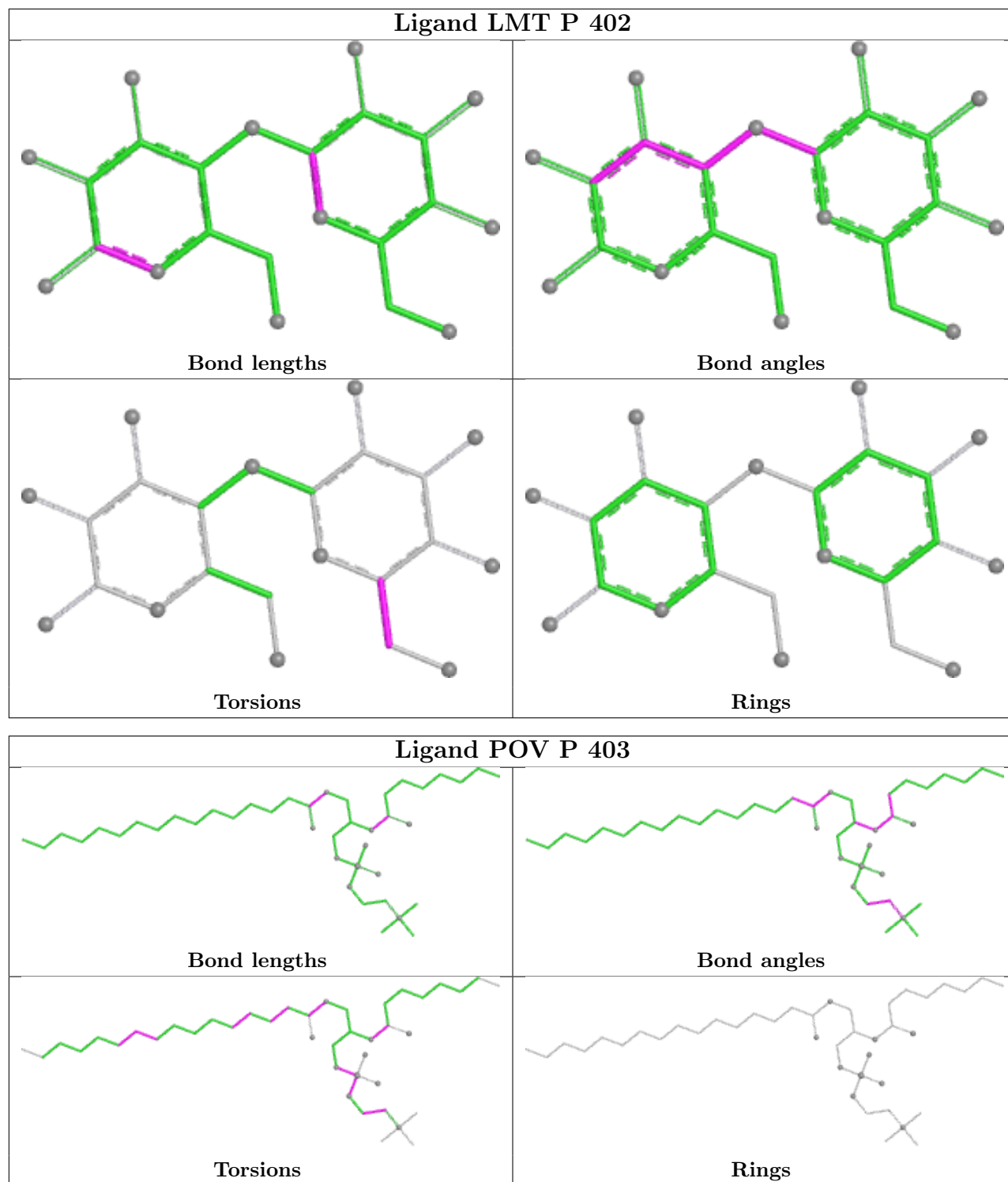


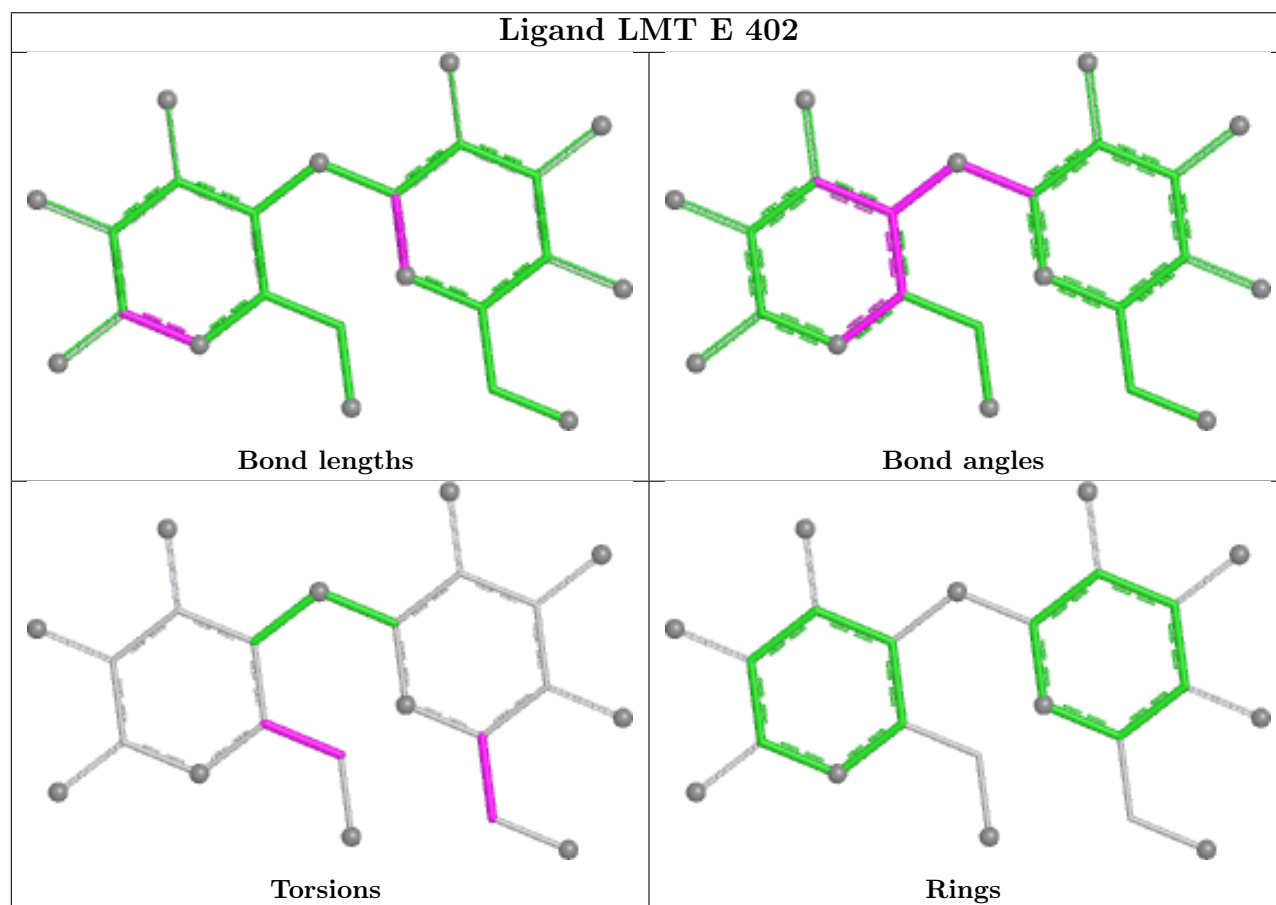
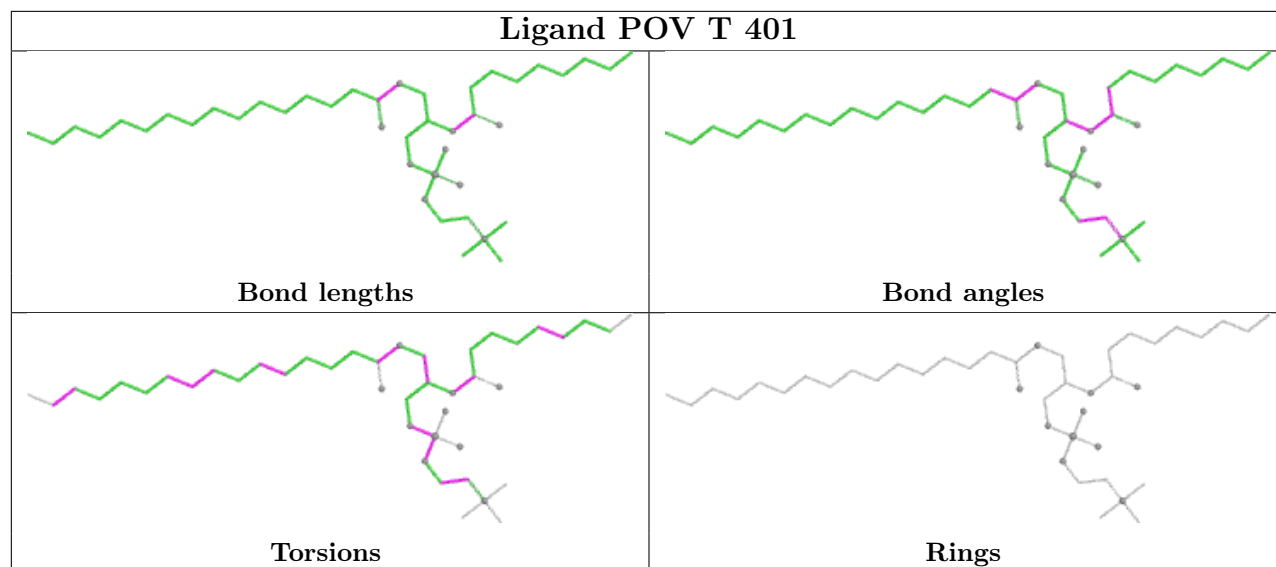


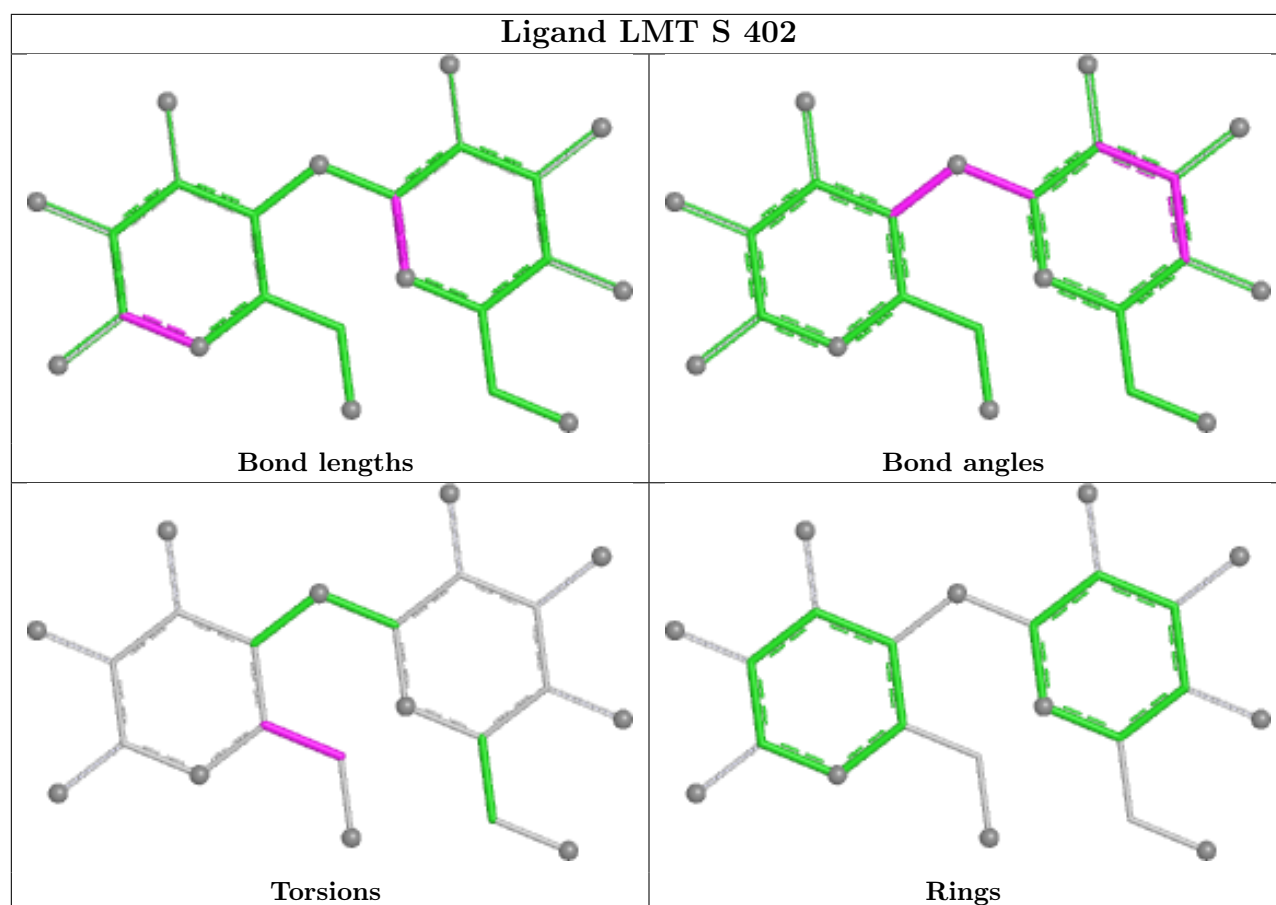












5.7 Other polymers [i](#)

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(Å²)	Q<0.9
1	A	342/347 (98%)	0.46	32 (9%)	14	9	56, 102, 165, 226	0
1	B	341/347 (98%)	0.37	15 (4%)	39	24	58, 109, 175, 270	0
1	C	340/347 (97%)	0.42	21 (6%)	26	17	58, 106, 185, 251	0
1	D	340/347 (97%)	0.40	17 (5%)	34	22	54, 106, 170, 263	0
1	E	340/347 (97%)	0.35	16 (4%)	36	23	57, 105, 170, 230	0
1	P	340/347 (97%)	0.40	19 (5%)	30	19	51, 93, 156, 239	0
1	Q	340/347 (97%)	0.39	14 (4%)	41	25	58, 99, 167, 242	0
1	R	340/347 (97%)	0.32	10 (2%)	53	35	58, 97, 158, 274	0
1	S	340/347 (97%)	0.32	13 (3%)	44	27	53, 89, 144, 247	0
1	T	340/347 (97%)	0.31	20 (5%)	28	18	49, 88, 151, 210	0
2	F	221/224 (98%)	0.35	12 (5%)	31	20	68, 113, 202, 265	0
2	G	222/224 (99%)	0.65	14 (6%)	26	17	75, 142, 230, 309	0
2	H	223/224 (99%)	0.35	12 (5%)	31	20	52, 100, 158, 275	0
2	I	222/224 (99%)	0.27	6 (2%)	56	36	63, 105, 192, 239	0
2	J	222/224 (99%)	0.67	26 (11%)	9	6	64, 146, 281, 313	0
2	U	221/224 (98%)	0.49	8 (3%)	46	28	75, 131, 220, 317	0
2	V	224/224 (100%)	0.27	7 (3%)	51	32	70, 117, 169, 269	0
2	W	224/224 (100%)	0.24	10 (4%)	38	24	68, 102, 155, 257	0
2	X	224/224 (100%)	0.37	12 (5%)	31	20	57, 98, 169, 249	0
2	Y	221/224 (98%)	0.37	6 (2%)	56	36	64, 127, 195, 277	0
3	K	210/215 (97%)	0.49	14 (6%)	24	15	59, 114, 222, 295	0
3	L	211/215 (98%)	0.25	12 (5%)	29	19	49, 91, 170, 224	0
3	M	210/215 (97%)	0.34	9 (4%)	40	24	69, 130, 248, 270	0
3	N	211/215 (98%)	0.28	6 (2%)	55	35	66, 116, 158, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	O	211/215 (98%)	0.23	6 (2%) 55 35	65, 108, 143, 157	0
3	Z	215/215 (100%)	0.29	8 (3%) 45 28	71, 120, 160, 199	0
3	f	215/215 (100%)	0.31	12 (5%) 30 19	69, 104, 153, 231	0
3	g	211/215 (98%)	0.30	10 (4%) 36 23	71, 127, 173, 218	0
3	h	211/215 (98%)	0.34	5 (2%) 59 40	75, 137, 177, 249	0
3	i	214/215 (99%)	0.08	3 (1%) 73 54	60, 99, 135, 165	0
All	All	7746/7860 (98%)	0.36	375 (4%) 35 22	49, 107, 191, 317	0

All (375) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	ALA	5.8
2	X	224	CYS	5.5
2	H	139	ALA	5.3
3	K	123	PRO	5.2
1	D	267	LEU	5.1
1	B	260	SER	5.1
1	P	240	THR	4.8
1	T	304	GLY	4.7
3	K	122	PRO	4.6
2	X	220	VAL	4.4
3	L	131	ASN	4.4
1	A	13	GLY	4.3
2	J	55	ASN	4.3
2	G	134	ALA	4.2
2	U	137	SER	4.2
2	X	142	ASN	4.1
2	X	138	ALA	4.1
1	A	104	ASP	4.0
1	E	261	ALA	4.0
1	Q	103	ILE	3.9
2	H	44	ASN	3.9
3	L	96	ASN	3.9
3	f	156	THR	3.9
2	J	146	THR	3.9
2	F	149	CYS	3.8
2	W	110	ASP	3.8
1	T	263	ILE	3.8
3	f	154	ASP	3.8
1	D	266	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	S	104	ASP	3.7
1	C	24	ASN	3.7
1	R	180	SER	3.7
3	M	210	SER	3.7
1	P	104	ASP	3.6
1	C	23	ASP	3.6
1	C	157	ASP	3.6
1	A	308	TRP	3.6
2	G	149	CYS	3.6
2	Y	55	ASN	3.6
2	H	195	SER	3.6
1	S	242	ILE	3.5
2	J	44	ASN	3.5
2	X	139	ALA	3.5
1	E	242	ILE	3.5
2	Y	221	PRO	3.5
2	Y	170	SER	3.5
3	K	105	LYS	3.4
2	G	150	LEU	3.4
1	E	243	PRO	3.4
1	Q	304	GLY	3.4
2	V	44	ASN	3.4
1	C	213	PHE	3.4
1	P	316	ASP	3.4
1	R	104	ASP	3.4
2	U	136	GLY	3.4
2	H	191	THR	3.4
2	Y	147	LEU	3.3
2	I	55	ASN	3.3
1	D	260	SER	3.3
2	V	122	SER	3.3
1	R	249	GLY	3.3
3	K	194	TYR	3.3
1	A	240	THR	3.3
1	E	260	SER	3.3
2	V	121	SER	3.3
3	K	125	SER	3.2
1	Q	263	ILE	3.2
3	L	53	ILE	3.2
2	J	134	ALA	3.2
3	g	53	ILE	3.2
1	A	305	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	Y	191	THR	3.2
3	K	162	MET	3.1
1	A	266	GLN	3.1
2	W	122	SER	3.1
3	K	126	GLU	3.1
1	A	216	TYR	3.1
1	P	37	ARG	3.1
1	B	104	ASP	3.1
2	J	46	GLU	3.1
1	E	37	ARG	3.1
2	G	135	PRO	3.1
2	X	135	PRO	3.1
3	O	54	ASN	3.1
1	B	341	HIS	3.1
2	G	133	LEU	3.1
1	T	37	ARG	3.1
3	M	95	SER	3.1
1	T	303	ALA	3.0
1	T	249	GLY	3.0
3	f	155	GLY	3.0
1	A	242	ILE	3.0
2	U	181	SER	3.0
1	B	157	ASP	3.0
1	T	135	GLN	3.0
2	F	181	SER	3.0
1	Q	340	HIS	3.0
2	W	222	ARG	3.0
1	A	249	GLY	3.0
2	F	148	GLY	3.0
1	P	260	SER	2.9
1	A	218	LEU	2.9
3	i	96	ASN	2.9
1	E	241	ALA	2.9
3	O	185	ALA	2.9
1	E	249	GLY	2.9
2	U	149	CYS	2.9
2	J	151	VAL	2.9
2	I	144	MET	2.9
3	g	96	ASN	2.9
2	F	192	VAL	2.9
3	f	190	ARG	2.9
2	J	144	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	J	188	SER	2.9
3	g	81	GLN	2.9
2	X	223	ASP	2.9
2	I	89	GLU	2.9
1	A	141	VAL	2.9
3	f	126	GLU	2.8
1	E	239	ARG	2.8
1	C	141	VAL	2.8
1	E	263	ILE	2.8
3	N	52	GLY	2.8
3	L	43	ASP	2.8
3	K	210	SER	2.8
1	R	2	ASP	2.8
1	S	263	ILE	2.8
3	Z	94	TYR	2.8
1	T	301	ALA	2.8
2	V	139	ALA	2.8
1	A	164	GLU	2.8
1	E	304	GLY	2.7
2	J	166	GLY	2.7
3	g	95	SER	2.7
3	Z	158	VAL	2.7
1	A	234	SER	2.7
2	W	136	GLY	2.7
2	J	165	SER	2.7
1	C	308	TRP	2.7
3	L	132	LYS	2.7
2	X	55	ASN	2.7
2	G	1	GLU	2.7
3	Z	95	SER	2.7
1	C	263	ILE	2.7
1	P	103	ILE	2.7
1	T	199	ILE	2.7
1	R	308	TRP	2.7
1	A	271	SER	2.7
1	C	271	SER	2.7
1	A	89	ASP	2.7
1	A	341	HIS	2.7
1	A	143	GLN	2.6
1	D	132	MET	2.6
3	N	48	GLY	2.6
2	Y	137	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	136	VAL	2.6
2	H	102	TYR	2.6
3	O	95	SER	2.6
1	E	104	ASP	2.6
1	A	214	SER	2.6
1	T	260	SER	2.6
2	F	44	ASN	2.6
2	V	55	ASN	2.6
2	J	150	LEU	2.6
1	D	239	ARG	2.6
1	D	265	SER	2.6
1	R	12	SER	2.6
1	Q	182	GLN	2.6
1	Q	249	GLY	2.6
2	G	55	ASN	2.6
2	J	220	VAL	2.6
3	f	204	THR	2.6
2	J	189	SER	2.5
3	N	51	GLY	2.5
1	E	75	ASP	2.5
2	H	55	ASN	2.5
2	W	55	ASN	2.5
3	K	159	THR	2.5
2	J	149	CYS	2.5
1	S	271	SER	2.5
2	H	133	LEU	2.5
3	Z	43	ASP	2.5
1	T	11	THR	2.5
3	M	98	TRP	2.5
1	C	237	PHE	2.5
1	E	216	TYR	2.5
1	S	6	LEU	2.5
1	C	175	SER	2.5
3	f	210	SER	2.5
3	N	98	TRP	2.5
1	A	231	SER	2.5
1	A	263	ILE	2.5
1	Q	251	THR	2.5
2	H	141	THR	2.5
1	T	243	PRO	2.5
1	P	169	GLN	2.5
1	Q	143	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	O	96	ASN	2.4
1	Q	11	THR	2.4
2	F	147	LEU	2.4
3	Z	157	PRO	2.4
3	f	153	VAL	2.4
1	A	290	ALA	2.4
3	i	53	ILE	2.4
2	H	146	THR	2.4
3	f	96	ASN	2.4
2	X	110	ASP	2.4
1	C	246	VAL	2.4
1	A	303	ALA	2.4
3	f	169	LYS	2.4
1	Q	237	PHE	2.4
3	f	189	GLU	2.4
1	T	234	SER	2.4
3	h	95	SER	2.4
1	P	296	LEU	2.4
1	Q	308	TRP	2.4
2	J	196	THR	2.4
3	M	188	TRP	2.4
1	P	243	PRO	2.4
2	J	164	ASN	2.4
1	S	238	ASP	2.4
1	A	304	GLY	2.4
1	C	249	GLY	2.4
1	P	249	GLY	2.4
2	X	222	ARG	2.4
2	J	157	GLU	2.4
2	G	143	SER	2.4
1	A	243	PRO	2.4
3	M	130	THR	2.4
1	D	104	ASP	2.4
2	J	110	ASP	2.4
3	M	121	PHE	2.4
1	B	193	SER	2.4
2	H	59	SER	2.4
1	D	216	TYR	2.3
1	R	37	ARG	2.3
1	T	242	ILE	2.3
1	T	298	ASN	2.3
1	B	213	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	S	10	PHE	2.3
3	K	16	GLU	2.3
2	J	137	SER	2.3
1	B	105	LYS	2.3
2	V	174	THR	2.3
2	F	138	ALA	2.3
2	W	44	ASN	2.3
3	g	211	ARG	2.3
3	M	122	PRO	2.3
1	D	305	THR	2.3
1	Q	271	SER	2.3
3	h	185	ALA	2.3
2	W	96	CYS	2.3
2	G	168	LEU	2.3
3	K	121	PHE	2.3
1	B	246	VAL	2.3
2	U	123	ALA	2.3
1	C	260	SER	2.3
3	L	130	THR	2.3
3	i	128	LEU	2.3
3	M	194	TYR	2.3
1	C	327	PHE	2.3
1	Q	298	ASN	2.3
1	T	104	ASP	2.3
1	C	212	GLU	2.3
2	W	107	ARG	2.3
3	L	186	ARG	2.3
3	L	201	GLU	2.3
1	B	263	ILE	2.3
2	W	106	GLY	2.3
2	J	177	ALA	2.3
2	G	88	SER	2.3
2	G	202	VAL	2.3
2	U	110	ASP	2.3
1	P	263	ILE	2.2
1	D	249	GLY	2.2
1	D	261	ALA	2.2
1	T	244	ALA	2.2
2	X	144	MET	2.2
1	C	234	SER	2.2
1	E	182	GLN	2.2
3	L	173	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	W	224	CYS	2.2
1	B	175	SER	2.2
1	S	312	SER	2.2
1	Q	246	VAL	2.2
1	P	135	GLN	2.2
2	J	140	GLN	2.2
1	A	103	ILE	2.2
1	A	212	GLU	2.2
2	J	193	PRO	2.2
3	g	52	GLY	2.2
3	L	190	ARG	2.2
3	h	204	THR	2.2
1	T	266	GLN	2.2
3	K	160	GLN	2.2
1	D	264	ASN	2.2
2	I	42	GLY	2.2
1	C	316	ASP	2.2
1	E	105	LYS	2.2
2	J	213	THR	2.2
2	G	130	VAL	2.2
2	F	62	GLN	2.2
1	B	303	ALA	2.2
1	D	37	ARG	2.2
1	S	37	ARG	2.2
1	S	277	ASP	2.2
3	N	90	CYS	2.2
3	h	130	THR	2.1
1	C	182	GLN	2.1
1	P	241	ALA	2.1
2	F	55	ASN	2.1
2	U	221	PRO	2.1
2	J	174	THR	2.1
1	B	296	LEU	2.1
1	A	241	ALA	2.1
1	R	212	GLU	2.1
1	S	260	SER	2.1
1	S	268	PRO	2.1
3	Z	52	GLY	2.1
1	T	277	ASP	2.1
3	f	188	TRP	2.1
1	B	218	LEU	2.1
1	P	183	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	160	THR	2.1
2	X	219	ILE	2.1
3	L	176	MET	2.1
1	D	131	PRO	2.1
1	B	180	SER	2.1
1	R	234	SER	2.1
2	I	28	SER	2.1
3	g	210	SER	2.1
1	A	277	ASP	2.1
1	C	242	ILE	2.1
1	D	340	HIS	2.1
1	R	263	ILE	2.1
1	C	137	TYR	2.1
1	C	216	TYR	2.1
1	S	99	TYR	2.1
1	D	259	GLN	2.1
2	I	143	SER	2.1
2	J	199	SER	2.1
1	A	226	MET	2.1
1	P	139	MET	2.1
1	P	137	TYR	2.1
1	T	144	CYS	2.1
3	K	130	THR	2.1
3	O	119	THR	2.1
3	Z	205	VAL	2.0
1	A	177	SER	2.0
2	F	59	SER	2.0
1	B	89	ASP	2.0
1	P	11	THR	2.0
1	T	89	ASP	2.0
1	A	173	GLY	2.0
1	A	181	PHE	2.0
2	G	132	PRO	2.0
2	U	147	LEU	2.0
2	V	107	ARG	2.0
3	Z	128	LEU	2.0
1	D	125	SER	2.0
2	F	121	SER	2.0
3	L	13	SER	2.0
3	g	188	TRP	2.0
1	E	240	THR	2.0
1	P	136	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	201	THR	2.0
3	K	30	THR	2.0
3	h	156	THR	2.0
2	H	110	ASP	2.0
1	P	10	PHE	2.0
2	J	135	PRO	2.0
3	N	146	VAL	2.0
3	O	146	VAL	2.0
3	g	83	GLU	2.0
3	g	45	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	401	14/15	0.45	0.17	191,210,218,223	0
8	LMT	S	402	23/35	0.45	0.17	169,214,224,235	0
8	LMT	E	402	23/35	0.46	0.16	218,239,254,257	0
4	NAG	S	401	14/15	0.48	0.17	153,184,189,195	0
8	LMT	T	403	23/35	0.50	0.17	156,202,217,222	0
4	NAG	T	402	14/15	0.54	0.14	153,200,210,211	0
4	NAG	P	401	14/15	0.56	0.11	133,182,192,201	0
4	NAG	B	402	14/15	0.56	0.14	139,168,176,177	0
4	NAG	Q	402	14/15	0.58	0.13	146,184,202,207	0
4	NAG	E	401	14/15	0.58	0.15	157,190,206,212	0
7	GOL	B	401	6/6	0.59	0.22	115,145,151,167	0
8	LMT	P	402	23/35	0.61	0.16	221,221,221,221	0
4	NAG	D	402	14/15	0.63	0.16	153,197,214,221	0

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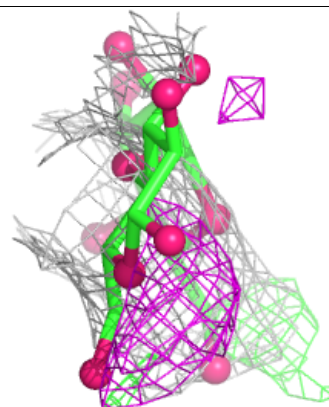
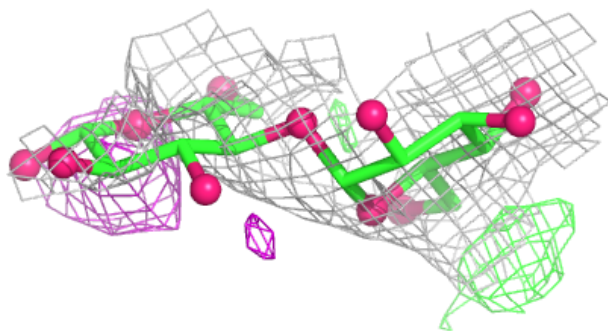
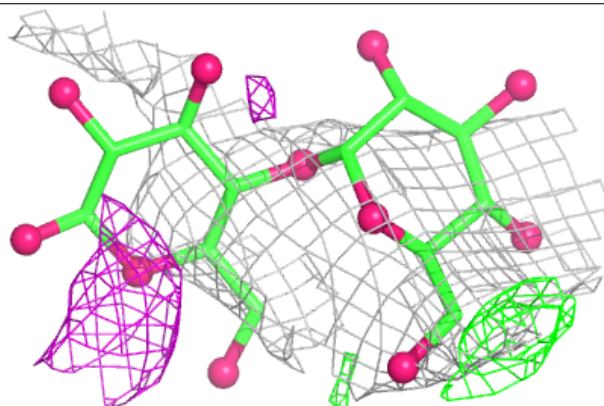
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	LMT	C	402	23/35	0.64	0.15	179,179,179,179	0
4	NAG	A	401	14/15	0.69	0.14	137,181,192,196	0
8	LMT	B	403	23/35	0.70	0.14	176,217,235,242	0
8	LMT	D	403	23/35	0.71	0.14	196,218,239,247	0
5	POV	A	402	23/52	0.78	0.30	137,177,208,241	0
5	POV	R	401	34/52	0.81	0.29	99,146,200,535	0
5	POV	D	401	26/52	0.86	0.32	125,176,201,334	0
5	POV	T	401	43/52	0.88	0.24	77,129,177,205	0
5	POV	Q	401	46/52	0.88	0.25	108,149,198,237	0
5	POV	P	403	42/52	0.88	0.25	82,125,179,206	0
5	POV	R	402	35/52	0.90	0.23	96,123,186,208	0
6	CL	A	403	1/1	0.94	0.07	119,119,119,119	0
6	CL	P	404	1/1	0.95	0.21	90,90,90,90	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.

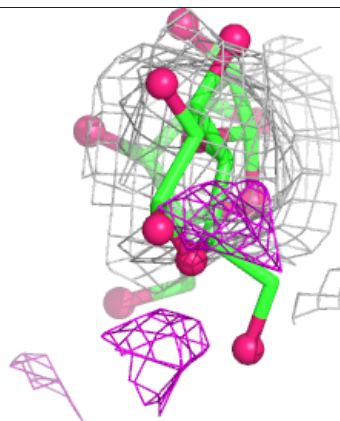
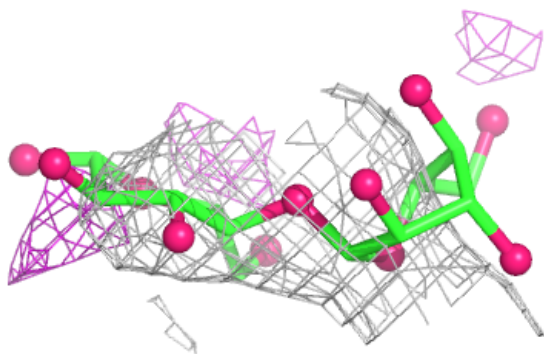
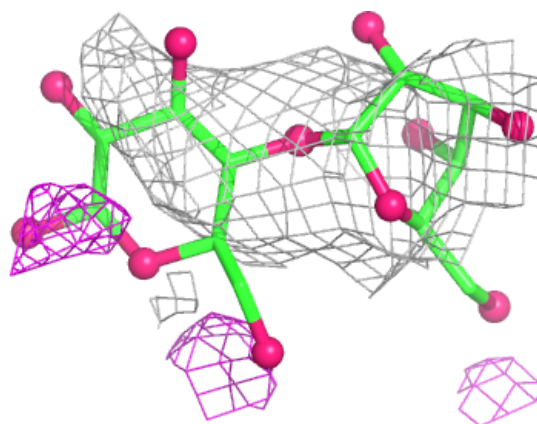
Electron density around LMT S 402:

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



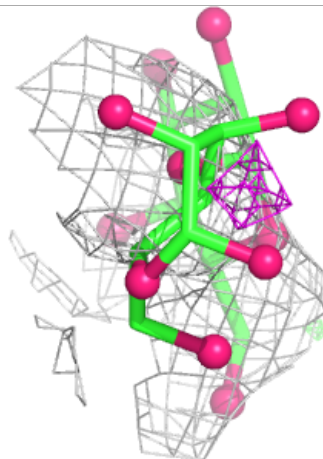
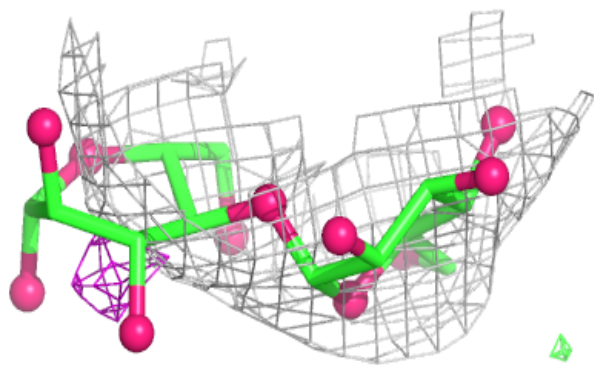
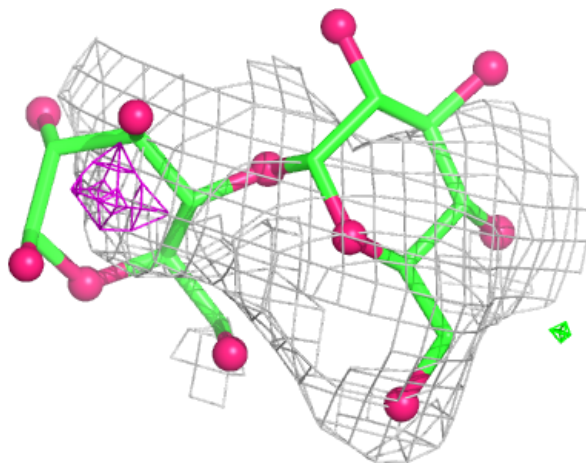
Electron density around LMT E 402:

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



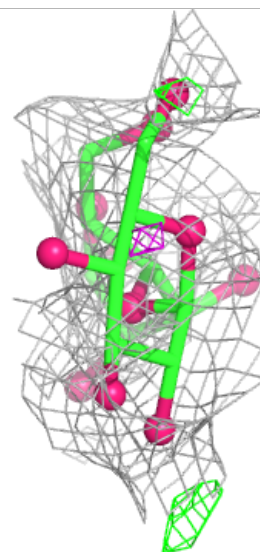
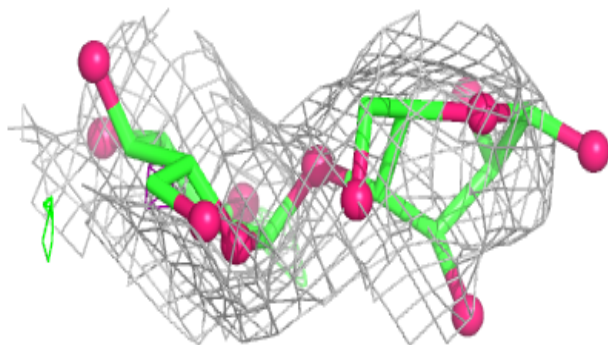
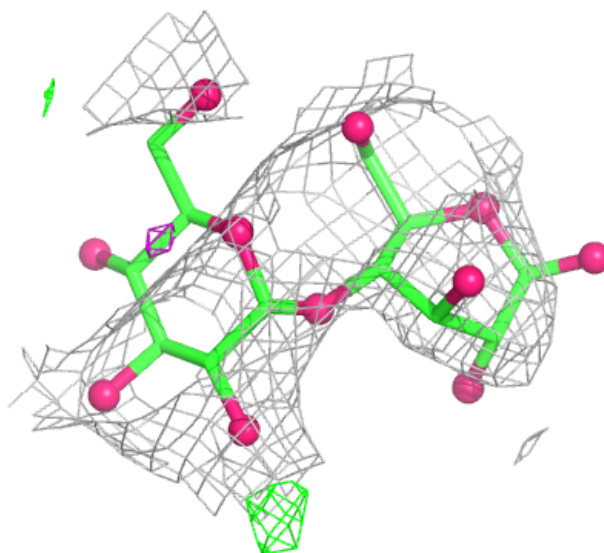
Electron density around LMT T 403:

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



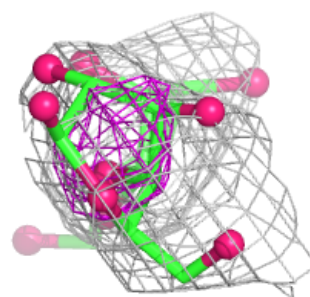
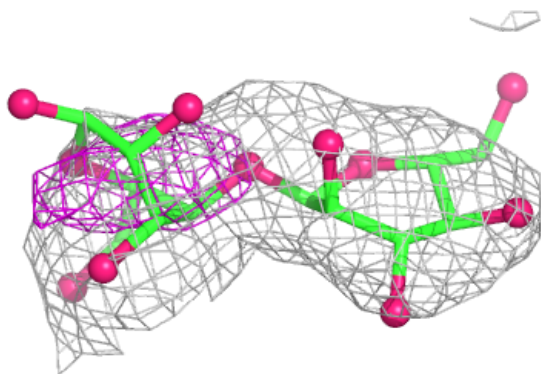
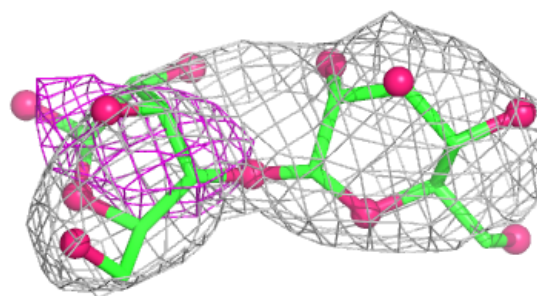
Electron density around LMT P 402:

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

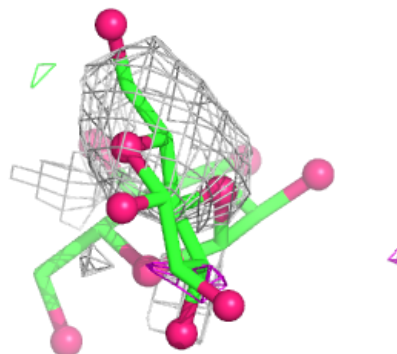
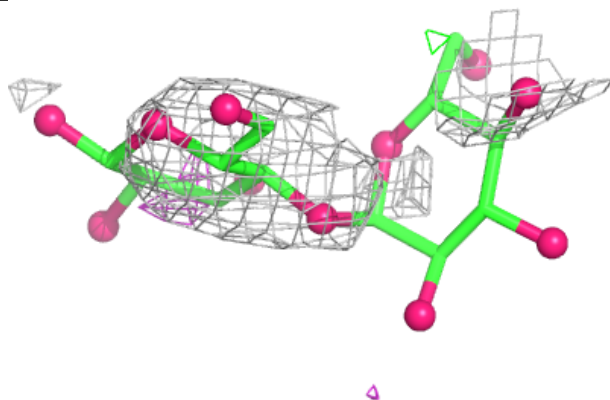
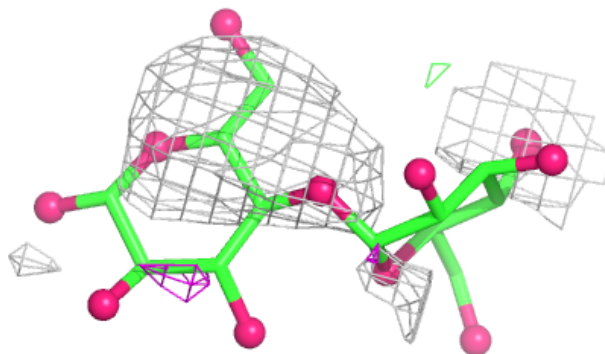


Electron density around LMT C 402:

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

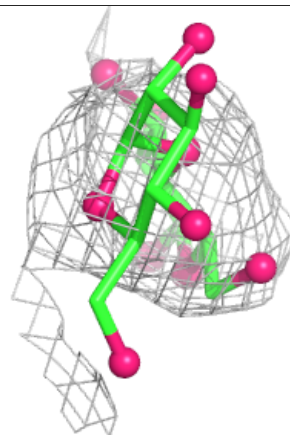
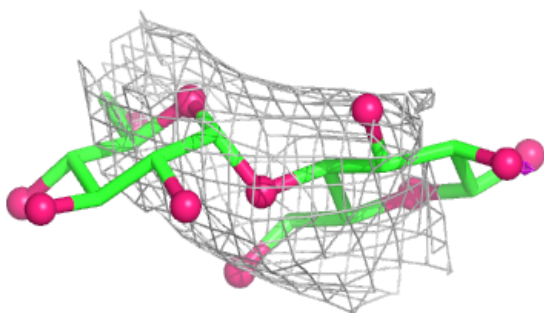
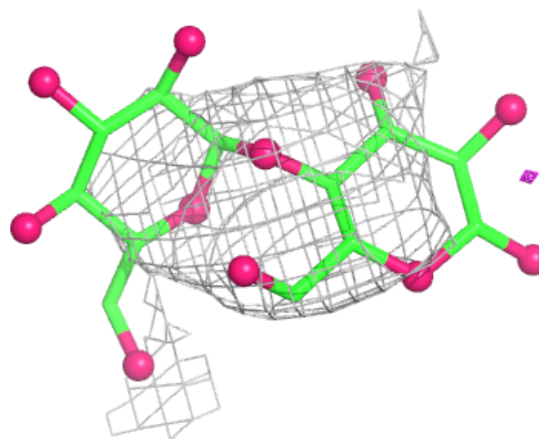
**Electron density around LMT B 403:**

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

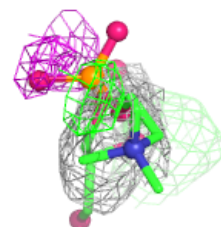
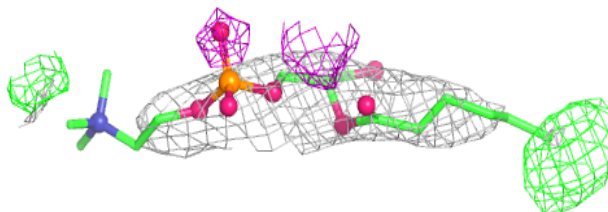
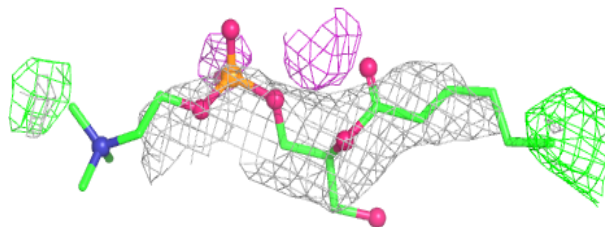


Electron density around LMT D 403:

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

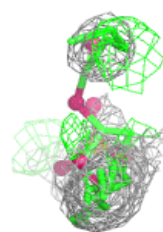
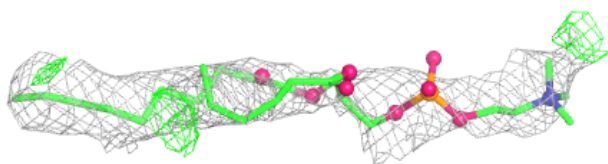
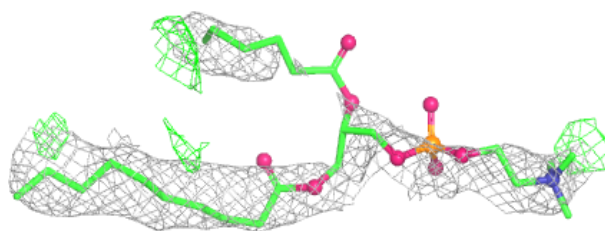
**Electron density around POV A 402:**

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

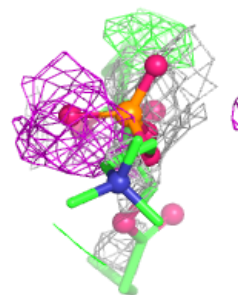
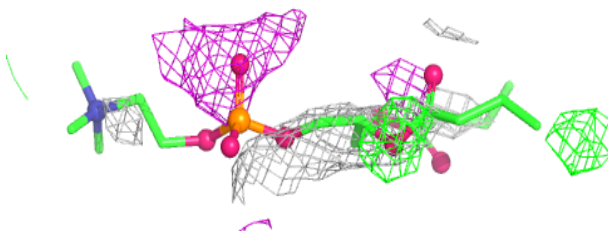
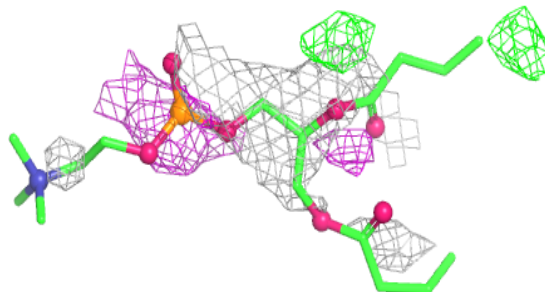


Electron density around POV R 401:

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

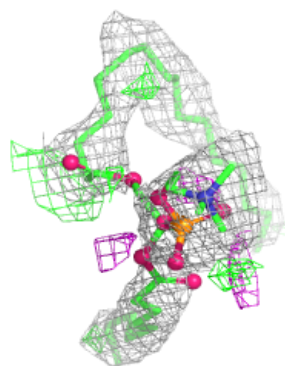
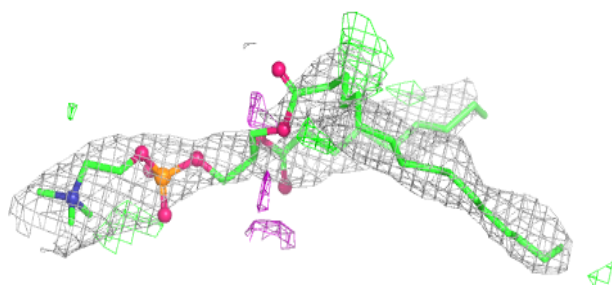
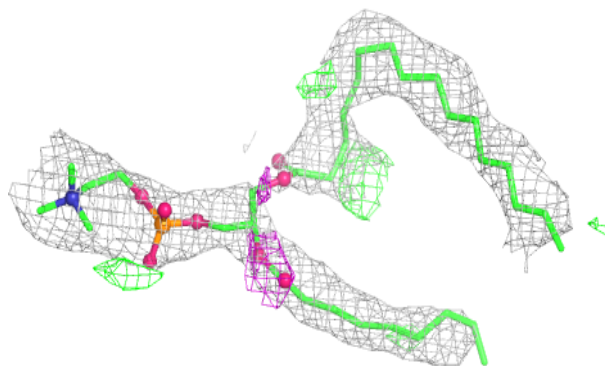
**Electron density around POV D 401:**

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

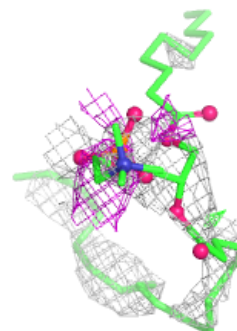
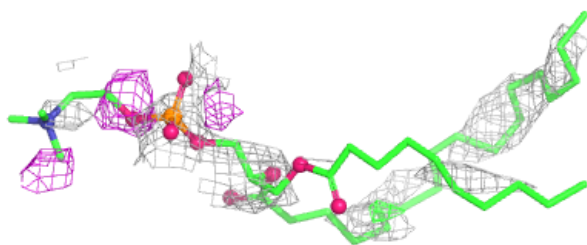
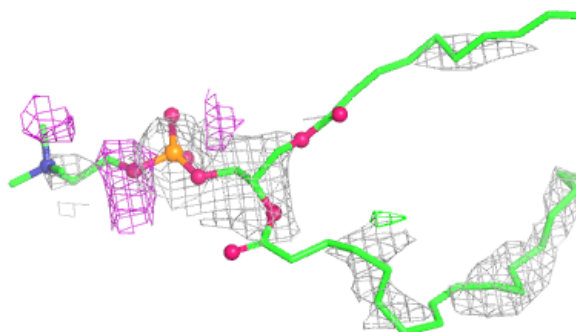


Electron density around POV T 401:

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

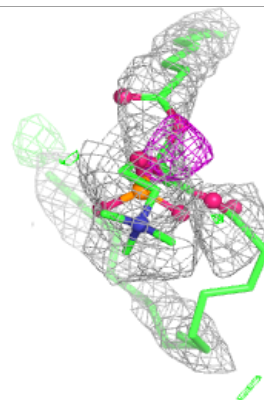
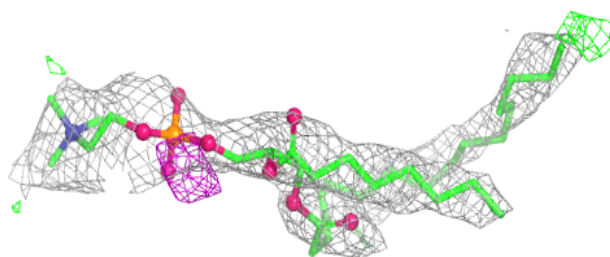
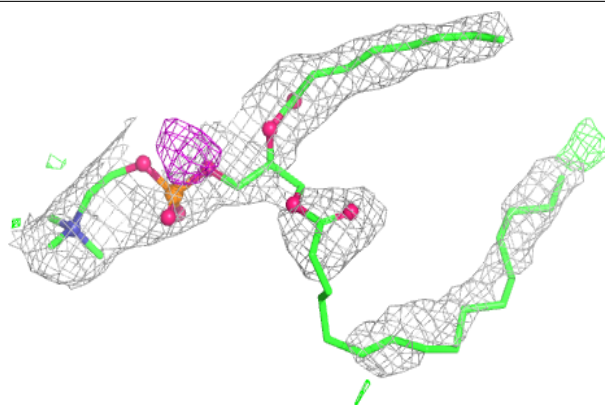
**Electron density around POV Q 401:**

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



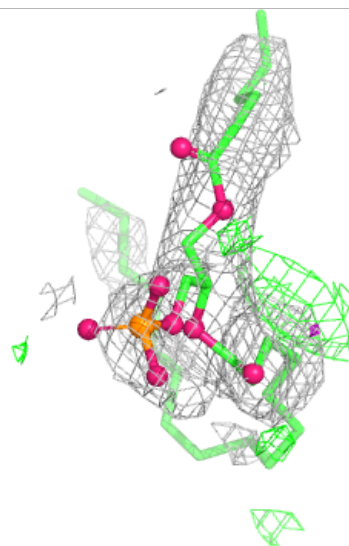
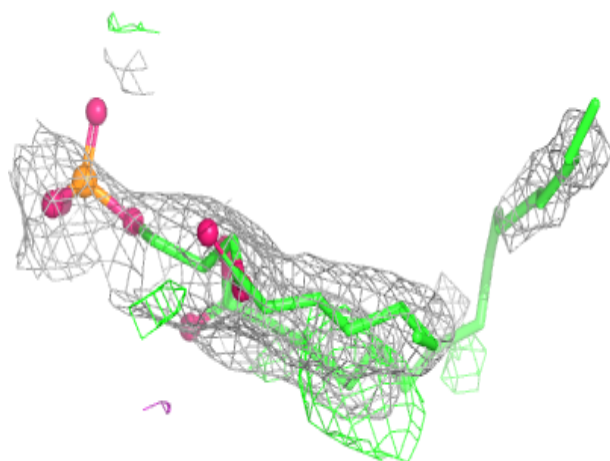
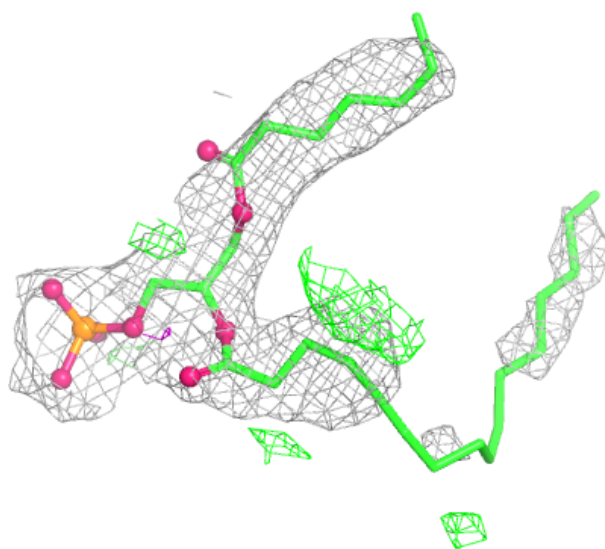
Electron density around POV P 403:

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



Electron density around POV 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.