



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:33 AM BST

PDB ID : 3RHW
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab and ivermectin
Authors : Hibbs, R.E.; Gouaux, E.
Deposited on : 2011-04-12
Resolution : 3.26 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

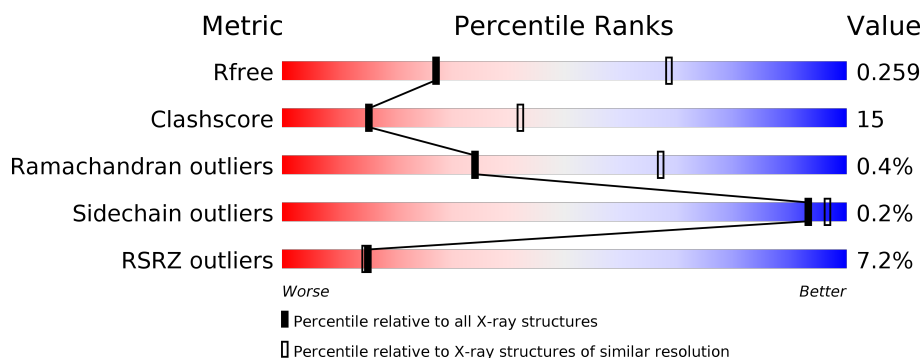
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div></div> </div> <div></div> </div>
1	B	347	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div></div> </div> <div></div> </div>
1	C	347	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div></div> </div> <div></div> </div>
1	D	347	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div></div> </div> <div></div> </div>
1	E	347	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>34%</div> <div></div> </div> <div></div> </div>
2	F	221	<div> <div>14%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>14%</div> </div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
2	G	221	
2	H	221	
2	I	221	
2	J	221	
3	K	210	
3	L	210	
3	M	210	
3	N	210	
3	O	210	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	400	-	-	-	X
6	NAG	E	400	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29197 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	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			
1	B	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			
1	C	339	Total	C	N	O	S	0	0	0
			2706	1762	438	491	15			
1	D	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	linker	UNP O17793
A	304	GLY	-	linker	UNP O17793
A	305	THR	-	linker	UNP O17793
A	340	HIS	-	expression tag	UNP O17793
A	341	HIS	-	expression tag	UNP O17793
A	342	HIS	-	expression tag	UNP O17793
A	343	HIS	-	expression tag	UNP O17793
A	344	HIS	-	expression tag	UNP O17793
A	345	HIS	-	expression tag	UNP O17793
A	346	HIS	-	expression tag	UNP O17793
A	347	HIS	-	expression tag	UNP O17793
B	303	ALA	-	linker	UNP O17793
B	304	GLY	-	linker	UNP O17793
B	305	THR	-	linker	UNP O17793
B	340	HIS	-	expression tag	UNP O17793
B	341	HIS	-	expression tag	UNP O17793
B	342	HIS	-	expression tag	UNP O17793
B	343	HIS	-	expression tag	UNP O17793

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	HIS	-	expression tag	UNP O17793
B	345	HIS	-	expression tag	UNP O17793
B	346	HIS	-	expression tag	UNP O17793
B	347	HIS	-	expression tag	UNP O17793
C	303	ALA	-	linker	UNP O17793
C	304	GLY	-	linker	UNP O17793
C	305	THR	-	linker	UNP O17793
C	340	HIS	-	expression tag	UNP O17793
C	341	HIS	-	expression tag	UNP O17793
C	342	HIS	-	expression tag	UNP O17793
C	343	HIS	-	expression tag	UNP O17793
C	344	HIS	-	expression tag	UNP O17793
C	345	HIS	-	expression tag	UNP O17793
C	346	HIS	-	expression tag	UNP O17793
C	347	HIS	-	expression tag	UNP O17793
D	303	ALA	-	linker	UNP O17793
D	304	GLY	-	linker	UNP O17793
D	305	THR	-	linker	UNP O17793
D	340	HIS	-	expression tag	UNP O17793
D	341	HIS	-	expression tag	UNP O17793
D	342	HIS	-	expression tag	UNP O17793
D	343	HIS	-	expression tag	UNP O17793
D	344	HIS	-	expression tag	UNP O17793
D	345	HIS	-	expression tag	UNP O17793
D	346	HIS	-	expression tag	UNP O17793
D	347	HIS	-	expression tag	UNP O17793
E	303	ALA	-	linker	UNP O17793
E	304	GLY	-	linker	UNP O17793
E	305	THR	-	linker	UNP O17793
E	340	HIS	-	expression tag	UNP O17793
E	341	HIS	-	expression tag	UNP O17793
E	342	HIS	-	expression tag	UNP O17793
E	343	HIS	-	expression tag	UNP O17793
E	344	HIS	-	expression tag	UNP O17793
E	345	HIS	-	expression tag	UNP O17793
E	346	HIS	-	expression tag	UNP O17793
E	347	HIS	-	expression tag	UNP O17793

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	191	Total	C	N	O	S	0	0	0
			1478	942	240	289	7			

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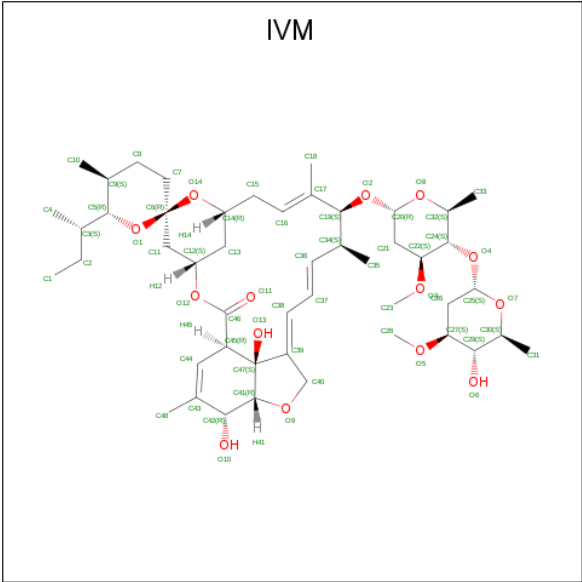
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	200	Total	C	N	O	S	0	0	0
			1529	973	248	301	7			
2	H	221	Total	C	N	O	S	0	0	0
			1683	1067	273	335	8			
2	I	199	Total	C	N	O	S	0	0	0
			1525	969	247	301	8			
2	J	215	Total	C	N	O	S	0	0	0
			1639	1043	265	324	7			

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

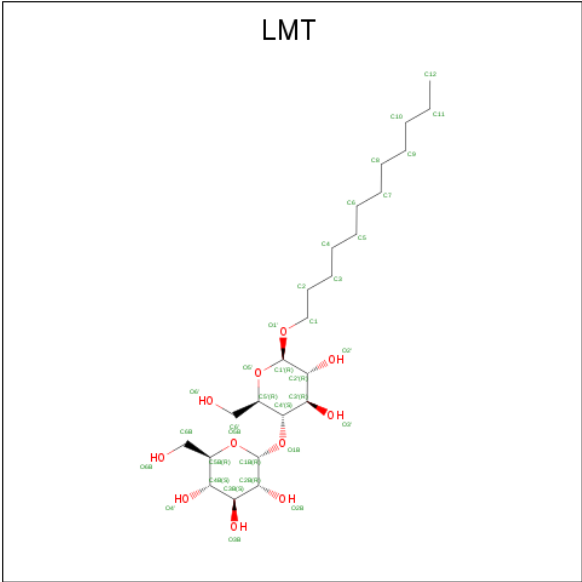
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	199	Total	C	N	O	S	0	0	0
			1496	941	246	303	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1584	996	263	319	6			
3	N	158	Total	C	N	O	S	0	0	0
			1165	736	192	233	4			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	243	294	6			

- Molecule 4 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacy clooctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄).



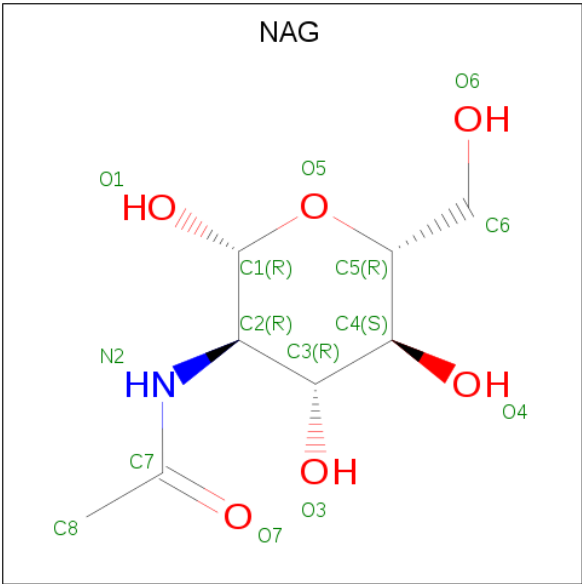
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			62	48	14		
4	B	1	Total	C	O	0	0
			62	48	14		
4	B	1	Total	C	O	0	0
			62	48	14		
4	D	1	Total	C	O	0	0
			62	48	14		
4	D	1	Total	C	O	0	0
			62	48	14		

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



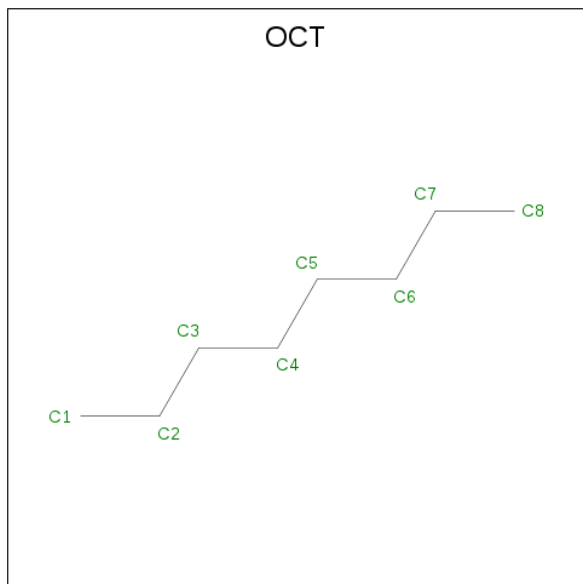
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			26	15	11		
5	A	1	Total	C	O	0	0
			27	16	11		
5	B	1	Total	C	O	0	0
			26	15	11		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



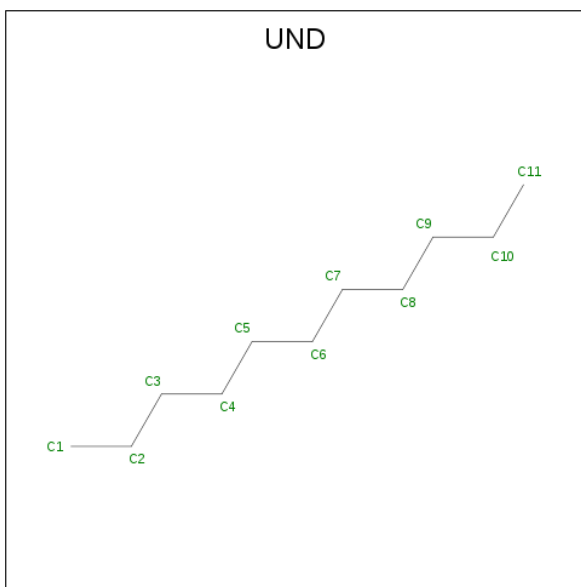
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C 8 8	0	0
7	D	1	Total C 8 8	0	0
7	E	1	Total C 8 8	0	0

- Molecule 8 is UNDECANE (three-letter code: UND) (formula: C₁₁H₂₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 11 11	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

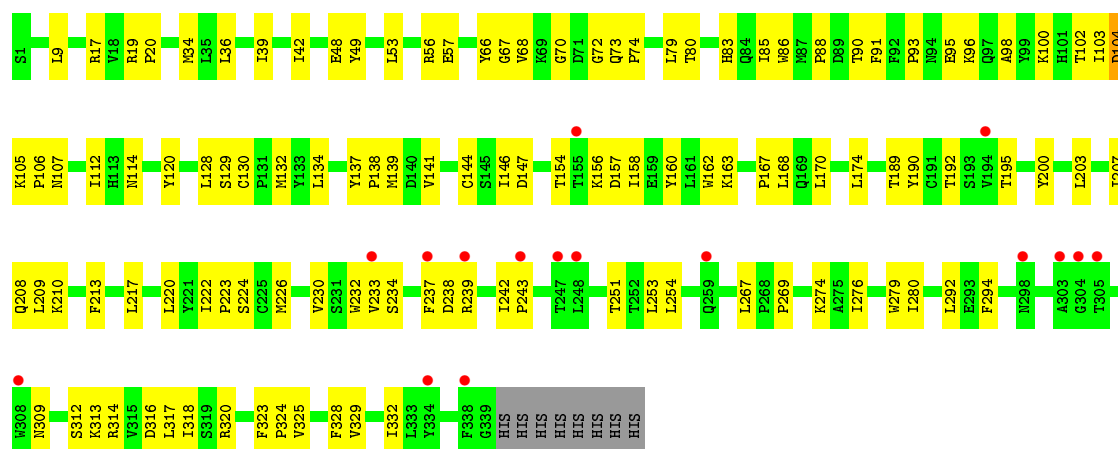
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cl 1 1	0	0

3 Residue-property plots

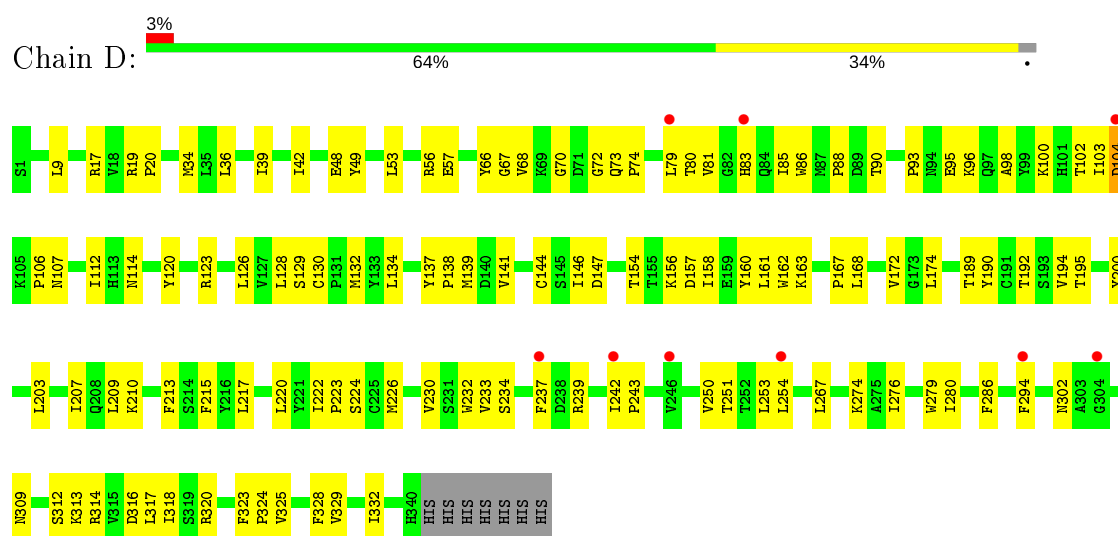
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

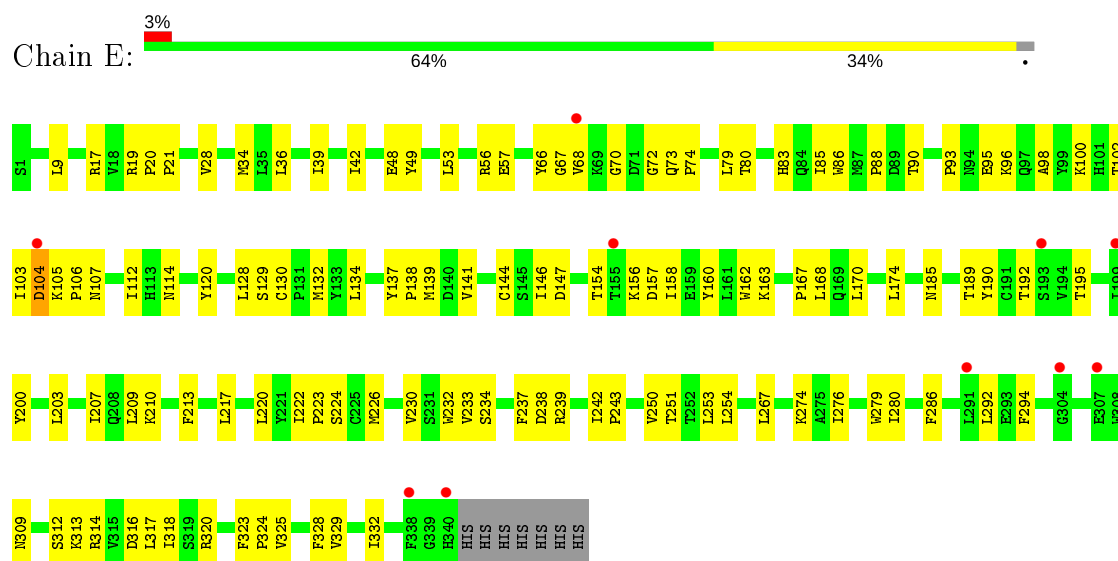




- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

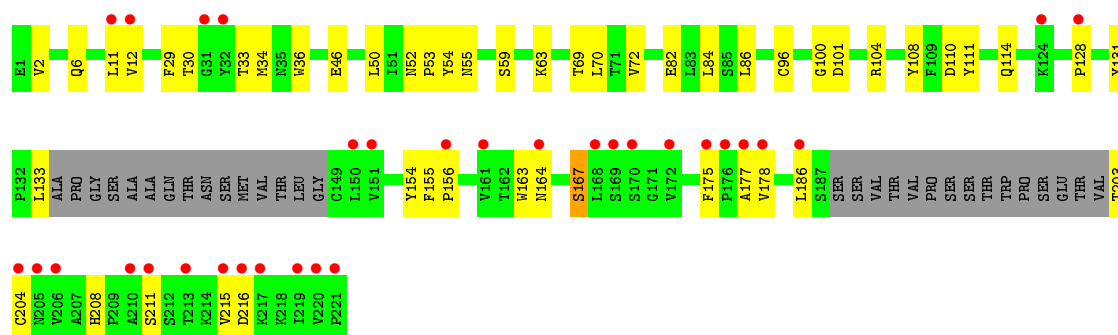


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



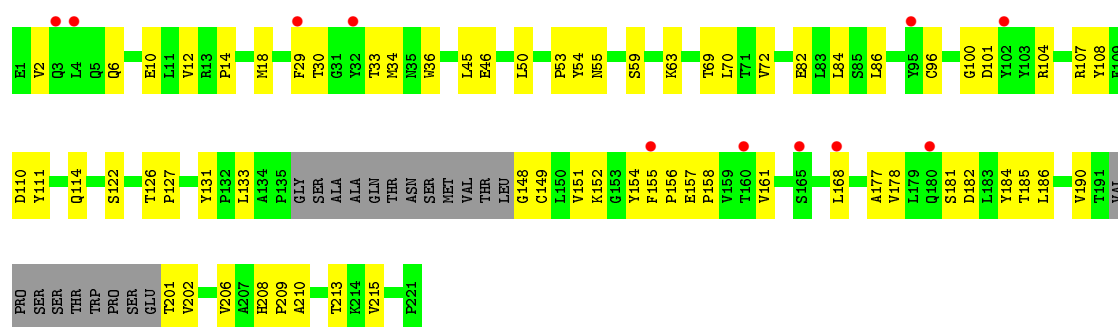
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F: 




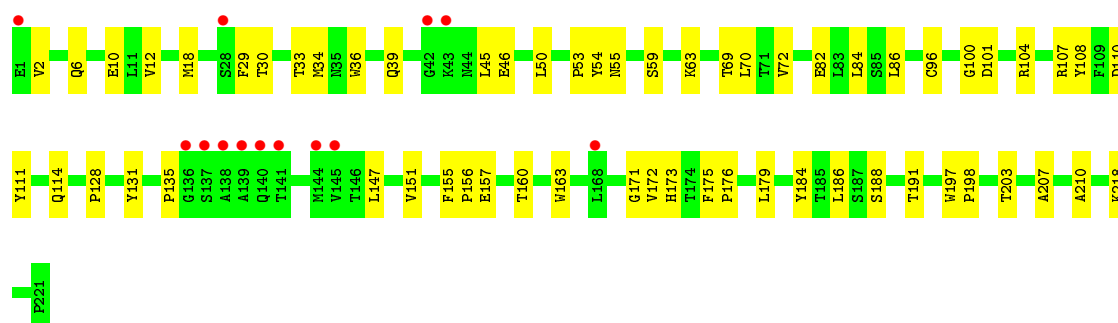
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain G: 



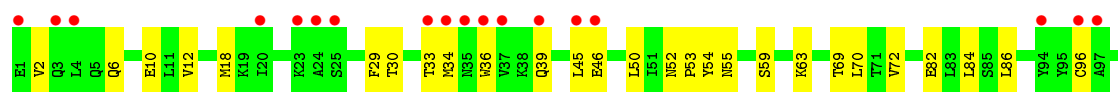
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

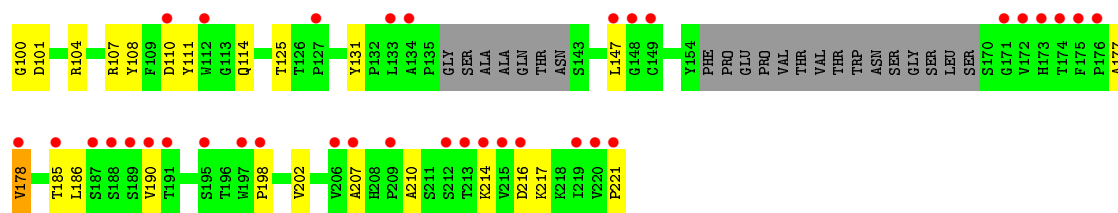
Chain H: 



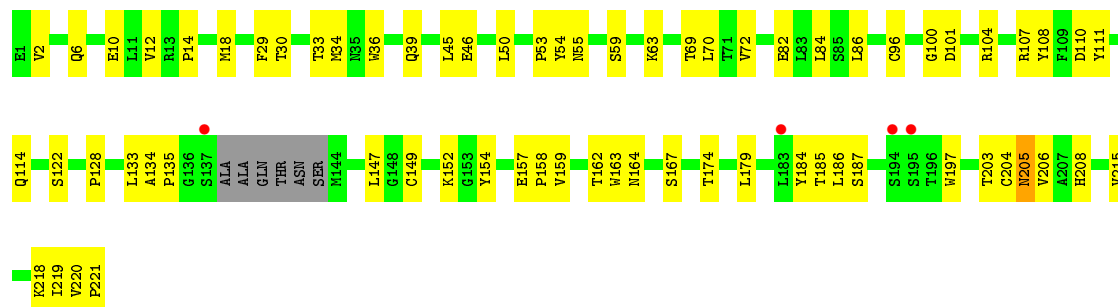
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain I: 

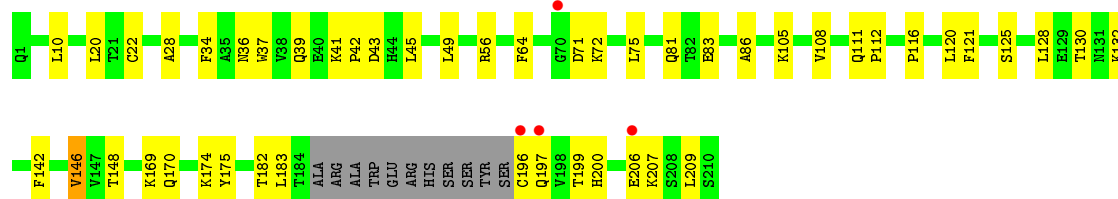




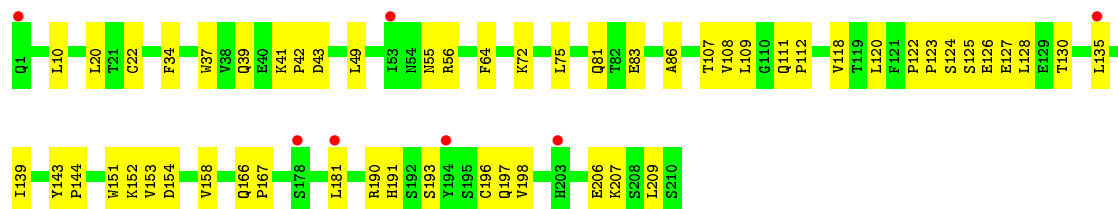
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



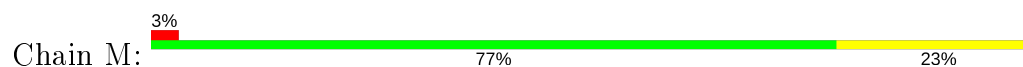
- Molecule 3: Mouse monoclonal Fab fragment, light chain

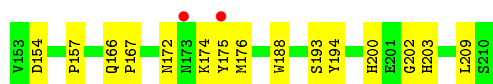


- Molecule 3: Mouse monoclonal Fab fragment, light chain

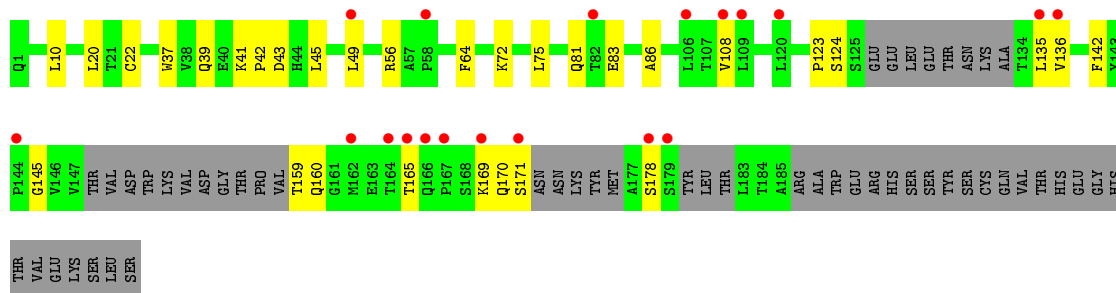


- Molecule 3: Mouse monoclonal Fab fragment, light chain

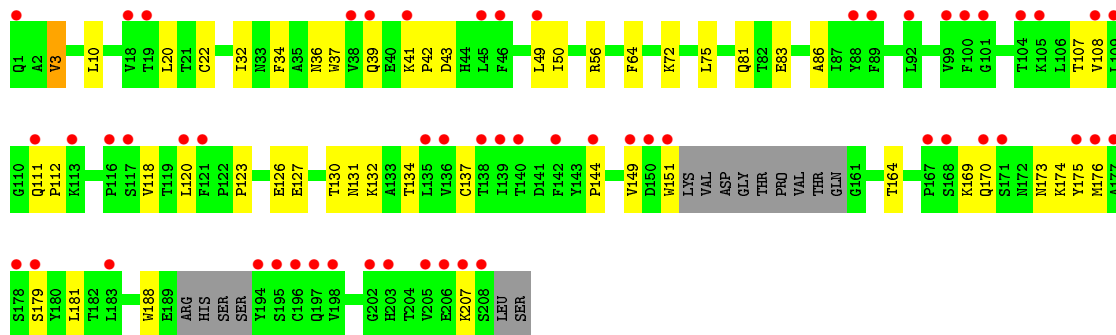




- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.85Å 154.85Å 574.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.50 – 3.26 109.50 – 3.26	Depositor EDS
% Data completeness (in resolution range)	93.7 (109.50-3.26) 99.7 (109.50-3.26)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.239 , 0.270 0.229 , 0.259	Depositor DCC
R_{free} test set	5474 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	86.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	29197	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, IVM, LMT, UND, OCT

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	0.26	0/2789	0.42	0/3809
1	B	0.26	0/2789	0.42	0/3809
1	C	0.25	0/2778	0.42	0/3794
1	D	0.25	0/2789	0.42	0/3809
1	E	0.26	0/2789	0.42	0/3809
2	F	0.23	0/1517	0.41	0/2062
2	G	0.24	0/1569	0.44	0/2138
2	H	0.25	0/1729	0.43	0/2360
2	I	0.24	0/1564	0.42	0/2128
2	J	0.24	0/1684	0.43	0/2299
3	K	0.24	0/1529	0.43	0/2089
3	L	0.25	0/1629	0.45	0/2226
3	M	0.24	0/1622	0.43	0/2219
3	N	0.24	0/1188	0.44	0/1621
3	O	0.32	1/1504 (0.1%)	0.47	1/2056 (0.0%)
All	All	0.25	1/29469 (0.0%)	0.43	1/40228 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3	VAL	CB-CG2	8.11	1.69	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	3	VAL	CG1-CB-CG2	7.33	122.63	110.90

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	2716	0	2709	109	0
1	B	2716	0	2708	109	0
1	C	2706	0	2701	109	0
1	D	2716	0	2709	109	0
1	E	2716	0	2708	105	0
2	F	1478	0	1432	39	0
2	G	1529	0	1478	49	0
2	H	1683	0	1632	46	0
2	I	1525	0	1485	42	0
2	J	1639	0	1588	48	0
3	K	1496	0	1458	34	0
3	L	1591	0	1542	38	0
3	M	1584	0	1531	33	0
3	N	1165	0	1142	22	0
3	O	1470	0	1412	41	0
4	A	62	0	74	1	0
4	B	124	0	148	3	0
4	D	124	0	148	5	0
5	A	53	0	52	12	0
5	B	26	0	25	4	0
6	B	14	0	13	1	0
6	C	14	0	13	1	0
6	E	14	0	13	1	0
7	B	8	0	18	2	0
7	D	8	0	18	2	0
7	E	8	0	18	2	0
8	B	11	0	24	0	0
9	C	1	0	0	0	0
All	All	29197	0	28799	861	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 15.

All (861) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG22	1:A:160:TYR:OH	1.62	1.00
1:D:90:THR:HG22	1:D:160:TYR:OH	1.63	0.99
2:F:208:HIS:HD2	2:F:211:SER:H	1.10	0.98
1:B:90:THR:HG22	1:B:160:TYR:OH	1.63	0.98
1:E:90:THR:HG22	1:E:160:TYR:OH	1.65	0.96
1:C:90:THR:HG22	1:C:160:TYR:OH	1.63	0.96
1:E:195:THR:HA	2:J:55:ASN:ND2	1.84	0.92
1:C:208:GLN:HB2	6:C:400:NAG:H82	1.53	0.90
3:L:107:THR:HG21	3:L:144:PRO:HB3	1.53	0.90
1:E:195:THR:HA	2:J:55:ASN:HD21	1.38	0.89
2:F:208:HIS:CD2	2:F:211:SER:H	1.93	0.87
3:L:206:GLU:O	3:L:207:LYS:HD2	1.76	0.86
1:D:195:THR:HA	2:I:55:ASN:ND2	1.91	0.85
1:B:195:THR:HA	2:F:55:ASN:ND2	1.92	0.84
1:A:195:THR:HA	2:H:55:ASN:ND2	1.93	0.84
1:B:195:THR:HA	2:F:55:ASN:HD21	1.44	0.82
1:A:303:ALA:HB2	5:A:349:LMT:H6D	1.61	0.81
3:M:105:LYS:HD2	3:M:146:VAL:HG22	1.62	0.80
1:D:195:THR:HA	2:I:55:ASN:HD21	1.47	0.80
1:A:195:THR:HA	2:H:55:ASN:HD21	1.45	0.79
1:A:299:HIS:CD2	5:A:349:LMT:H11	2.18	0.78
1:A:303:ALA:CB	5:A:349:LMT:H6D	2.14	0.77
3:O:149:VAL:HB	3:O:164:THR:HG21	1.65	0.77
3:L:139:ILE:HD12	3:L:198:VAL:HG21	1.68	0.76
3:L:122:PRO:HB3	3:L:209:LEU:HD11	1.67	0.74
2:J:164:ASN:CB	2:J:167:SER:HB3	2.18	0.73
1:B:36:LEU:HD23	1:B:39:ILE:HD11	1.71	0.73
1:D:36:LEU:HD23	1:D:39:ILE:HD11	1.71	0.73
1:D:79:LEU:HD22	1:D:85:ILE:HD12	1.71	0.73
2:H:179:LEU:HD13	2:H:184:TYR:CE1	2.23	0.72
2:J:164:ASN:HB2	2:J:167:SER:HB3	1.72	0.72
3:O:118:VAL:O	3:O:207:LYS:HE3	1.89	0.72
1:E:79:LEU:HD22	1:E:85:ILE:HD12	1.72	0.72
1:C:79:LEU:HD22	1:C:85:ILE:HD12	1.72	0.72
1:A:36:LEU:HD23	1:A:39:ILE:HD11	1.70	0.71
1:E:36:LEU:HD23	1:E:39:ILE:HD11	1.72	0.71
3:K:170:GLN:HG2	3:K:174:LYS:O	1.90	0.71
1:C:195:THR:HA	2:G:55:ASN:ND2	2.05	0.70
3:L:125:SER:HA	3:L:128:LEU:HD12	1.74	0.70
1:C:17:ARG:HB3	1:D:80:THR:HB	1.73	0.70
1:C:36:LEU:HD23	1:C:39:ILE:HD11	1.72	0.70
4:D:349:IVM:H11A	1:E:226:MET:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD22	1:B:85:ILE:HD12	1.75	0.69
4:B:349:IVM:H11A	1:C:226:MET:HG3	1.74	0.69
1:A:79:LEU:HD22	1:A:85:ILE:HD12	1.74	0.69
2:I:147:LEU:HD12	2:I:202:VAL:HG11	1.73	0.69
1:C:195:THR:HA	2:G:55:ASN:HD21	1.57	0.68
1:B:250:VAL:CG1	1:C:251:THR:HG21	2.22	0.68
3:O:111:GLN:HG2	3:O:112:PRO:HD2	1.74	0.68
3:L:120:LEU:HD12	3:L:196:CYS:HB3	1.73	0.68
3:O:169:LYS:HA	3:O:175:TYR:HA	1.75	0.68
3:M:22:CYS:O	3:M:72:LYS:HB2	1.94	0.67
1:B:253:LEU:HD11	1:C:226:MET:CE	2.24	0.67
1:C:90:THR:HG22	1:C:160:TYR:CZ	2.29	0.67
1:A:90:THR:HG22	1:A:160:TYR:CZ	2.30	0.67
1:C:224:SER:HB2	1:C:279:TRP:CH2	2.30	0.67
1:D:224:SER:HB2	1:D:279:TRP:CH2	2.30	0.67
3:K:22:CYS:O	3:K:72:LYS:HB2	1.95	0.67
1:E:85:ILE:HD11	1:E:112:ILE:HD11	1.77	0.67
2:H:50:LEU:HD21	2:H:59:SER:HB3	1.77	0.67
2:J:128:PRO:HB3	2:J:154:TYR:HB3	1.76	0.67
1:D:85:ILE:HD11	1:D:112:ILE:HD11	1.77	0.66
3:L:22:CYS:O	3:L:72:LYS:HB2	1.96	0.66
3:O:22:CYS:O	3:O:72:LYS:HB2	1.95	0.66
1:B:90:THR:HG22	1:B:160:TYR:CZ	2.31	0.66
1:B:224:SER:HB2	1:B:279:TRP:CH2	2.31	0.66
2:J:50:LEU:HD21	2:J:59:SER:HB3	1.78	0.66
1:B:85:ILE:HD11	1:B:112:ILE:HD11	1.78	0.65
1:D:90:THR:HG22	1:D:160:TYR:CZ	2.31	0.65
1:E:224:SER:HB2	1:E:279:TRP:CH2	2.31	0.65
1:E:96:LYS:HD2	1:E:129:SER:HB3	1.79	0.65
1:B:96:LYS:HD2	1:B:129:SER:HB3	1.78	0.65
1:A:224:SER:HB2	1:A:279:TRP:CH2	2.32	0.65
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.78	0.65
2:F:50:LEU:HD21	2:F:59:SER:HB3	1.79	0.64
3:K:111:GLN:HG3	3:K:112:PRO:HD2	1.79	0.64
3:N:22:CYS:O	3:N:72:LYS:HB2	1.96	0.64
2:I:50:LEU:HD21	2:I:59:SER:HB3	1.79	0.64
1:A:253:LEU:HD11	1:B:226:MET:CE	2.27	0.64
1:A:66:TYR:CE2	1:A:114:ASN:HA	2.32	0.64
1:C:96:LYS:HD2	1:C:129:SER:HB3	1.79	0.64
2:H:2:VAL:HG21	2:H:111:TYR:CD2	2.32	0.64
2:J:2:VAL:HG21	2:J:111:TYR:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:THR:HG22	1:E:160:TYR:CZ	2.32	0.64
2:I:2:VAL:HG21	2:I:111:TYR:CD2	2.33	0.64
2:G:50:LEU:HD21	2:G:59:SER:HB3	1.79	0.64
1:A:96:LYS:HD2	1:A:129:SER:HB3	1.79	0.64
1:B:302:ASN:HD22	1:C:238:ASP:HB3	1.63	0.64
2:G:2:VAL:HG21	2:G:111:TYR:CD2	2.33	0.63
1:D:189:THR:HG22	1:D:190:TYR:H	1.62	0.63
2:H:50:LEU:CD2	2:H:59:SER:HB3	2.29	0.63
3:M:41:LYS:HE2	3:M:83:GLU:O	1.99	0.63
2:H:157:GLU:HG3	2:H:184:TYR:CE2	2.32	0.63
1:A:299:HIS:CD2	5:A:349:LMT:C1	2.82	0.63
1:C:66:TYR:CE2	1:C:114:ASN:HA	2.33	0.63
1:E:66:TYR:CE2	1:E:114:ASN:HA	2.34	0.63
1:B:66:TYR:CE2	1:B:114:ASN:HA	2.34	0.63
1:B:189:THR:HG22	1:B:190:TYR:H	1.63	0.63
1:B:254:LEU:HD12	1:C:251:THR:HG23	1.81	0.62
1:A:189:THR:HG22	1:A:190:TYR:H	1.64	0.62
2:F:2:VAL:HG21	2:F:111:TYR:CD2	2.33	0.62
3:L:41:LYS:HE2	3:L:83:GLU:O	2.00	0.62
1:A:85:ILE:HD11	1:A:112:ILE:HD11	1.81	0.62
1:C:189:THR:HG22	1:C:190:TYR:H	1.63	0.62
1:D:96:LYS:HD2	1:D:129:SER:HB3	1.81	0.62
1:B:302:ASN:ND2	1:C:238:ASP:HB3	2.15	0.62
1:D:226:MET:HG3	4:D:348:IVM:H11A	1.82	0.62
3:O:41:LYS:HE2	3:O:83:GLU:O	1.99	0.62
3:O:170:GLN:OE1	3:O:176:MET:HB3	2.00	0.62
1:B:17:ARG:HB3	1:C:80:THR:HB	1.81	0.62
1:D:242:ILE:HG22	1:D:243:PRO:HD3	1.82	0.62
2:G:50:LEU:CD2	2:G:59:SER:HB3	2.30	0.62
2:J:203:THR:HA	2:J:218:LYS:HA	1.82	0.62
3:N:41:LYS:HE2	3:N:83:GLU:O	1.99	0.62
1:D:66:TYR:CE2	1:D:114:ASN:HA	2.34	0.61
3:K:125:SER:HA	3:K:128:LEU:HD12	1.82	0.61
1:D:239:ARG:CZ	1:D:313:LYS:HG2	2.31	0.61
1:B:39:ILE:HD13	1:B:207:ILE:CD1	2.30	0.61
2:J:14:PRO:HD2	2:J:122:SER:HB3	1.83	0.61
2:H:156:PRO:HD2	2:H:210:ALA:CB	2.29	0.61
1:A:239:ARG:CZ	1:A:313:LYS:HG2	2.30	0.61
1:E:57:GLU:OE2	1:E:90:THR:HG21	2.01	0.61
2:J:50:LEU:CD2	2:J:59:SER:HB3	2.30	0.61
3:M:10:LEU:HD12	3:M:20:LEU:HD23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:CZ	1:C:313:LYS:HG2	2.31	0.61
1:E:189:THR:HG22	1:E:190:TYR:H	1.65	0.60
1:E:39:ILE:HD13	1:E:207:ILE:CD1	2.30	0.60
5:A:349:LMT:H1B	5:A:349:LMT:C6'	2.30	0.60
1:B:239:ARG:CZ	1:B:313:LYS:HG2	2.31	0.60
3:K:41:LYS:HE2	3:K:83:GLU:O	2.00	0.60
1:E:239:ARG:CZ	1:E:313:LYS:HG2	2.31	0.60
1:A:226:MET:HG3	4:A:348:IVM:H11A	1.82	0.60
2:G:157:GLU:HG3	2:G:184:TYR:CD2	2.37	0.60
1:C:57:GLU:OE2	1:C:90:THR:HG21	2.02	0.60
1:D:39:ILE:HD13	1:D:207:ILE:CD1	2.31	0.60
2:F:50:LEU:CD2	2:F:59:SER:HB3	2.32	0.60
1:A:39:ILE:HD13	1:A:207:ILE:CD1	2.31	0.60
1:A:226:MET:CE	1:E:253:LEU:HD11	2.32	0.60
3:K:10:LEU:HD12	3:K:20:LEU:HD23	1.84	0.60
1:A:234:SER:HA	1:A:237:PHE:HD2	1.67	0.60
1:C:242:ILE:HG22	1:C:243:PRO:HD3	1.84	0.60
3:N:39:GLN:HB2	3:N:49:LEU:HD21	1.84	0.59
1:B:88:PRO:HB3	1:B:158:ILE:HD11	1.85	0.59
1:B:325:VAL:O	1:B:329:VAL:HG23	2.03	0.59
3:L:107:THR:HG21	3:L:144:PRO:CB	2.30	0.59
1:C:39:ILE:HD13	1:C:207:ILE:CD1	2.32	0.59
2:I:50:LEU:CD2	2:I:59:SER:HB3	2.32	0.59
3:N:169:LYS:NZ	3:N:169:LYS:HB3	2.17	0.59
1:D:234:SER:HA	1:D:237:PHE:HD2	1.67	0.59
3:L:10:LEU:HD12	3:L:20:LEU:HD23	1.84	0.59
1:A:242:ILE:HG22	1:A:243:PRO:HD3	1.84	0.59
1:E:242:ILE:HG22	1:E:243:PRO:HD3	1.84	0.59
1:D:254:LEU:HD12	1:E:251:THR:HG23	1.84	0.59
1:B:57:GLU:OE2	1:B:90:THR:HG21	2.03	0.59
3:N:10:LEU:HD12	3:N:20:LEU:HD23	1.84	0.59
1:A:220:LEU:HD11	1:A:280:ILE:HD11	1.85	0.58
1:C:230:VAL:O	1:C:233:VAL:HG22	2.03	0.58
3:L:39:GLN:HB2	3:L:49:LEU:HD21	1.85	0.58
1:C:234:SER:HA	1:C:237:PHE:HD2	1.68	0.58
2:H:84:LEU:HD12	2:H:84:LEU:N	2.18	0.58
3:O:39:GLN:HB2	3:O:49:LEU:HD21	1.84	0.58
1:B:242:ILE:HG22	1:B:243:PRO:HD3	1.84	0.58
1:E:220:LEU:HD11	1:E:280:ILE:HD11	1.86	0.58
3:M:154:ASP:HA	3:M:193:SER:HB3	1.84	0.58
3:M:39:GLN:HB2	3:M:49:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:SER:HA	1:B:237:PHE:HD2	1.67	0.58
1:D:328:PHE:CE2	1:D:332:ILE:HD11	2.39	0.58
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.38	0.58
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.39	0.58
1:A:232:TRP:CH2	1:A:324:PRO:HA	2.37	0.58
1:E:234:SER:HA	1:E:237:PHE:HD2	1.67	0.58
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.38	0.58
1:C:232:TRP:CH2	1:C:324:PRO:HA	2.38	0.58
1:D:57:GLU:OE2	1:D:90:THR:HG21	2.03	0.58
2:F:110:ASP:HB3	2:F:111:TYR:CD2	2.39	0.58
2:F:46:GLU:OE1	2:F:63:LYS:HE2	2.04	0.58
2:G:84:LEU:N	2:G:84:LEU:HD12	2.19	0.58
2:J:110:ASP:HB3	2:J:111:TYR:CD2	2.39	0.58
1:A:57:GLU:OE2	1:A:90:THR:HG21	2.03	0.58
1:B:230:VAL:O	1:B:233:VAL:HG22	2.04	0.58
3:L:122:PRO:HB3	3:L:209:LEU:CD1	2.34	0.58
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.69	0.57
1:B:73:GLN:HB3	1:B:74:PRO:HD2	1.86	0.57
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.68	0.57
1:E:230:VAL:O	1:E:233:VAL:HG22	2.04	0.57
1:E:232:TRP:CH2	1:E:324:PRO:HA	2.39	0.57
2:H:110:ASP:HB3	2:H:111:TYR:CD2	2.39	0.57
2:J:179:LEU:HD13	2:J:184:TYR:CE1	2.39	0.57
2:G:110:ASP:HB3	2:G:111:TYR:CD2	2.39	0.57
2:J:46:GLU:OE1	2:J:63:LYS:HE2	2.05	0.57
3:N:41:LYS:HB3	3:N:42:PRO:HD2	1.86	0.57
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.85	0.57
1:A:299:HIS:NE2	5:A:349:LMT:H11	2.19	0.57
1:D:325:VAL:O	1:D:329:VAL:HG23	2.04	0.57
1:E:325:VAL:O	1:E:329:VAL:HG23	2.04	0.57
3:O:10:LEU:HD12	3:O:20:LEU:HD23	1.85	0.57
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.39	0.57
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.70	0.57
1:C:93:PRO:HD2	1:C:147:ASP:O	2.05	0.57
1:C:88:PRO:HB3	1:C:158:ILE:HD11	1.86	0.57
2:F:84:LEU:N	2:F:84:LEU:HD12	2.19	0.57
3:K:41:LYS:HB3	3:K:42:PRO:HD2	1.86	0.57
3:L:41:LYS:HB3	3:L:42:PRO:HD2	1.87	0.57
1:B:232:TRP:CH2	1:B:324:PRO:HA	2.39	0.57
1:C:19:ARG:HH11	1:C:157:ASP:HA	1.70	0.57
1:B:254:LEU:HD12	1:C:251:THR:CG2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLN:HB3	1:C:74:PRO:HD2	1.86	0.57
1:A:328:PHE:CE2	1:A:332:ILE:HD11	2.40	0.57
1:D:42:ILE:HD13	1:D:209:LEU:HD13	1.86	0.57
1:D:250:VAL:CG1	1:E:251:THR:HG21	2.34	0.57
2:J:164:ASN:HB3	2:J:167:SER:HB3	1.86	0.57
1:B:42:ILE:HD13	1:B:209:LEU:HD13	1.87	0.57
1:D:230:VAL:O	1:D:233:VAL:HG22	2.05	0.57
2:I:84:LEU:N	2:I:84:LEU:HD12	2.20	0.57
1:A:230:VAL:O	1:A:233:VAL:HG22	2.05	0.56
1:B:253:LEU:HD11	1:C:226:MET:HE2	1.87	0.56
1:D:17:ARG:HB3	1:E:80:THR:HB	1.86	0.56
1:A:299:HIS:HD2	5:A:349:LMT:C1	2.17	0.56
1:D:88:PRO:HB3	1:D:158:ILE:HD11	1.87	0.56
1:D:254:LEU:HD12	1:E:251:THR:CG2	2.35	0.56
1:E:93:PRO:HD2	1:E:147:ASP:O	2.06	0.56
1:E:42:ILE:HD13	1:E:209:LEU:HD13	1.87	0.56
3:M:41:LYS:HB3	3:M:42:PRO:HD2	1.87	0.56
1:B:220:LEU:HD11	1:B:280:ILE:HD11	1.86	0.56
2:H:155:PHE:CE1	2:H:156:PRO:HB3	2.40	0.56
2:I:46:GLU:OE1	2:I:63:LYS:HE2	2.05	0.56
1:A:253:LEU:HD11	1:B:226:MET:HE2	1.87	0.56
2:I:110:ASP:HB3	2:I:111:TYR:CD2	2.40	0.56
1:A:80:THR:HB	1:E:17:ARG:HB3	1.87	0.56
1:A:93:PRO:HD2	1:A:147:ASP:O	2.05	0.56
1:D:232:TRP:CH2	1:D:324:PRO:HA	2.39	0.56
1:D:73:GLN:HB3	1:D:74:PRO:HD2	1.87	0.56
2:H:46:GLU:OE1	2:H:63:LYS:HE2	2.05	0.56
1:C:325:VAL:O	1:C:329:VAL:HG23	2.05	0.56
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.39	0.56
3:O:41:LYS:HB3	3:O:42:PRO:HD2	1.86	0.56
1:D:220:LEU:HD11	1:D:280:ILE:HD11	1.87	0.56
3:K:39:GLN:HB2	3:K:49:LEU:HD21	1.87	0.56
1:A:73:GLN:HB3	1:A:74:PRO:HD2	1.87	0.56
1:D:93:PRO:HD2	1:D:147:ASP:O	2.06	0.56
2:J:84:LEU:HD12	2:J:84:LEU:N	2.21	0.56
1:B:328:PHE:CE2	1:B:332:ILE:HD11	2.41	0.56
1:E:88:PRO:HB3	1:E:158:ILE:HD11	1.86	0.56
3:M:202:GLY:O	3:M:203:HIS:HB2	2.06	0.56
1:A:88:PRO:HB3	1:A:158:ILE:HD11	1.86	0.56
1:A:42:ILE:HD13	1:A:209:LEU:HD13	1.87	0.56
1:B:93:PRO:HD2	1:B:147:ASP:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:123:PRO:HD2	3:M:188:TRP:CZ2	2.41	0.56
1:B:226:MET:HG3	4:B:348:IVM:H11A	1.87	0.55
1:C:220:LEU:HD11	1:C:280:ILE:HD11	1.87	0.55
2:G:46:GLU:OE1	2:G:63:LYS:HE2	2.06	0.55
3:M:166:GLN:HG3	3:M:167:PRO:HD2	1.87	0.55
3:N:123:PRO:HD3	3:N:135:LEU:HD13	1.88	0.55
1:D:253:LEU:HD11	1:E:226:MET:CE	2.36	0.55
3:M:105:LYS:HD2	3:M:146:VAL:CG2	2.36	0.55
1:C:328:PHE:CE2	1:C:332:ILE:HD11	2.41	0.55
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.71	0.55
1:B:90:THR:CG2	1:B:160:TYR:OH	2.47	0.55
2:F:175:PHE:CD1	3:N:178:SER:HB3	2.41	0.55
1:A:325:VAL:O	1:A:329:VAL:HG23	2.07	0.55
1:C:253:LEU:HD11	1:D:226:MET:CE	2.36	0.55
1:E:73:GLN:HB3	1:E:74:PRO:HD2	1.88	0.55
1:C:90:THR:CG2	1:C:160:TYR:OH	2.48	0.55
1:D:224:SER:HB2	1:D:279:TRP:HH2	1.72	0.55
1:A:189:THR:HG22	1:A:190:TYR:N	2.22	0.55
1:C:42:ILE:HD13	1:C:209:LEU:HD13	1.87	0.54
3:K:132:LYS:NZ	3:K:182:THR:HG23	2.21	0.54
1:E:224:SER:HB2	1:E:279:TRP:CZ3	2.43	0.54
2:H:179:LEU:HD13	2:H:184:TYR:CD1	2.42	0.54
3:K:116:PRO:HD3	3:K:200:HIS:ND1	2.21	0.54
1:D:19:ARG:HG2	1:D:20:PRO:HD2	1.89	0.54
1:E:328:PHE:CE2	1:E:332:ILE:HD11	2.43	0.54
1:C:224:SER:HB2	1:C:279:TRP:CZ3	2.43	0.54
1:D:39:ILE:HD13	1:D:207:ILE:HD13	1.90	0.54
2:J:220:VAL:HG23	2:J:221:PRO:HD2	1.90	0.54
1:A:90:THR:CG2	1:A:160:TYR:OH	2.47	0.54
1:C:189:THR:HG22	1:C:190:TYR:N	2.23	0.54
1:D:242:ILE:N	1:D:243:PRO:CD	2.71	0.54
2:J:100:GLY:HA3	2:J:108:TYR:CZ	2.43	0.54
1:A:19:ARG:HG2	1:A:20:PRO:HD2	1.88	0.54
1:B:194:VAL:HG13	2:F:52:ASN:HD22	1.73	0.54
1:C:95:GLU:HG3	1:C:98:ALA:HB2	1.90	0.54
1:D:195:THR:CA	2:I:55:ASN:HD21	2.18	0.54
3:M:152:LYS:HG2	3:M:157:PRO:HA	1.90	0.54
1:C:242:ILE:N	1:C:243:PRO:CD	2.71	0.54
1:E:39:ILE:HD13	1:E:207:ILE:HD13	1.90	0.54
1:B:100:LYS:HE2	1:C:104:ASP:H	1.72	0.54
1:E:242:ILE:N	1:E:243:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:208:HIS:CE1	2:G:210:ALA:HB3	2.42	0.54
3:N:10:LEU:HD12	3:N:20:LEU:CD2	2.38	0.54
1:B:39:ILE:HD13	1:B:207:ILE:HD13	1.88	0.54
1:C:224:SER:HB2	1:C:279:TRP:HH2	1.71	0.54
2:G:6:GLN:H	2:G:114:GLN:HE22	1.56	0.54
1:A:34:MET:HG3	1:A:53:LEU:HD12	1.90	0.53
1:B:224:SER:HB2	1:B:279:TRP:CZ3	2.43	0.53
1:D:189:THR:HG22	1:D:190:TYR:N	2.22	0.53
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.43	0.53
1:B:189:THR:HG22	1:B:190:TYR:N	2.22	0.53
2:H:156:PRO:HD2	2:H:210:ALA:HB1	1.89	0.53
3:M:10:LEU:HD12	3:M:20:LEU:CD2	2.37	0.53
1:A:39:ILE:HD13	1:A:207:ILE:HD13	1.89	0.53
1:B:250:VAL:HG12	1:C:251:THR:HG21	1.91	0.53
1:E:90:THR:CG2	1:E:160:TYR:OH	2.49	0.53
1:E:19:ARG:HG2	1:E:20:PRO:HD2	1.91	0.53
3:N:159:THR:HG23	3:N:160:GLN:HG2	1.90	0.53
1:B:242:ILE:N	1:B:243:PRO:CD	2.72	0.53
5:A:349:LMT:H6'2	5:B:350:LMT:O4'	2.09	0.53
1:E:95:GLU:HG3	1:E:98:ALA:HB2	1.91	0.53
2:F:6:GLN:H	2:F:114:GLN:HE22	1.56	0.53
2:G:186:LEU:C	2:G:186:LEU:HD12	2.28	0.53
2:F:177:ALA:HB2	2:F:186:LEU:HD23	1.90	0.53
2:F:34:MET:CE	2:F:96:CYS:HB2	2.39	0.53
2:G:100:GLY:HA3	2:G:108:TYR:CZ	2.43	0.53
2:G:69:THR:HB	2:G:82:GLU:HB2	1.91	0.53
2:I:100:GLY:HA3	2:I:108:TYR:CZ	2.44	0.53
2:I:6:GLN:H	2:I:114:GLN:HE22	1.56	0.53
3:K:10:LEU:HD12	3:K:20:LEU:CD2	2.38	0.53
1:B:316:ASP:O	1:B:320:ARG:HG3	2.09	0.53
1:E:189:THR:HG22	1:E:190:TYR:N	2.23	0.53
1:D:107:ASN:N	1:D:107:ASN:HD22	2.07	0.53
1:E:154:THR:HG23	1:E:156:LYS:H	1.74	0.53
1:E:323:PHE:HB2	1:E:324:PRO:HD3	1.91	0.53
2:G:157:GLU:HB3	2:G:158:PRO:HA	1.91	0.53
2:H:100:GLY:HA3	2:H:108:TYR:CZ	2.44	0.53
3:M:11:THR:CG2	3:M:109:LEU:HD13	2.39	0.53
3:O:42:PRO:O	3:O:43:ASP:HB2	2.09	0.53
1:A:95:GLU:HG3	1:A:98:ALA:HB2	1.90	0.53
1:B:224:SER:CB	1:B:279:TRP:CZ3	2.92	0.53
2:F:100:GLY:HA3	2:F:108:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:107:ARG:NH1	3:L:34:PHE:CZ	2.77	0.53
2:J:6:GLN:H	2:J:114:GLN:HE22	1.56	0.53
1:A:254:LEU:HD12	1:B:251:THR:CG2	2.39	0.53
1:B:19:ARG:HG2	1:B:20:PRO:HD2	1.91	0.53
1:A:107:ASN:HD22	1:A:107:ASN:N	2.06	0.52
2:F:69:THR:HB	2:F:82:GLU:HB2	1.91	0.52
2:J:206:VAL:HB	2:J:215:VAL:HG13	1.90	0.52
3:K:42:PRO:O	3:K:43:ASP:HB2	2.09	0.52
3:L:151:TRP:CE3	3:L:181:LEU:HD22	2.44	0.52
1:C:19:ARG:HG2	1:C:20:PRO:HD2	1.91	0.52
3:L:10:LEU:HD12	3:L:20:LEU:CD2	2.38	0.52
3:L:123:PRO:HD3	3:L:135:LEU:HD13	1.92	0.52
1:B:323:PHE:HB2	1:B:324:PRO:HD3	1.91	0.52
1:E:316:ASP:O	1:E:320:ARG:HG3	2.09	0.52
2:H:6:GLN:H	2:H:114:GLN:HE22	1.55	0.52
3:O:10:LEU:HD12	3:O:20:LEU:CD2	2.39	0.52
1:C:323:PHE:HB2	1:C:324:PRO:HD3	1.91	0.52
1:D:286:PHE:CZ	7:D:350:OCT:H12	2.44	0.52
1:E:234:SER:HG	1:E:294:PHE:HZ	1.57	0.52
3:O:111:GLN:HG2	3:O:112:PRO:CD	2.38	0.52
3:O:130:THR:O	3:O:131:ASN:HB3	2.10	0.52
1:A:103:ILE:HG23	1:A:103:ILE:O	2.10	0.52
1:C:39:ILE:HD13	1:C:207:ILE:HD13	1.91	0.52
1:A:224:SER:HB2	1:A:279:TRP:CZ3	2.44	0.52
1:A:323:PHE:HB2	1:A:324:PRO:HD3	1.91	0.52
1:B:95:GLU:HG3	1:B:98:ALA:HB2	1.91	0.52
1:E:34:MET:HG3	1:E:53:LEU:HD12	1.92	0.52
5:B:350:LMT:H1B	5:B:350:LMT:C6'	2.40	0.52
1:D:224:SER:CB	1:D:279:TRP:CZ3	2.92	0.52
1:D:323:PHE:HB2	1:D:324:PRO:HD3	1.91	0.52
1:D:34:MET:HG3	1:D:53:LEU:HD12	1.92	0.52
1:D:95:GLU:HG3	1:D:98:ALA:HB2	1.90	0.52
3:L:42:PRO:O	3:L:43:ASP:HB2	2.10	0.52
1:C:107:ASN:HD22	1:C:107:ASN:N	2.08	0.52
1:D:90:THR:CG2	1:D:160:TYR:OH	2.48	0.52
1:A:251:THR:CG2	1:E:254:LEU:HD12	2.40	0.52
1:E:313:LYS:O	1:E:317:LEU:HD13	2.10	0.52
1:D:194:VAL:HG13	2:I:52:ASN:HD22	1.75	0.52
1:A:242:ILE:N	1:A:243:PRO:CD	2.72	0.52
2:I:69:THR:HB	2:I:82:GLU:HB2	1.91	0.52
3:O:170:GLN:HG2	3:O:176:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:SER:HB2	1:B:279:TRP:HH2	1.73	0.51
1:E:102:THR:HA	1:E:106:PRO:HA	1.92	0.51
2:H:69:THR:HB	2:H:82:GLU:HB2	1.92	0.51
2:J:34:MET:CE	2:J:96:CYS:HB2	2.40	0.51
1:A:224:SER:HB2	1:A:279:TRP:HH2	1.73	0.51
1:A:67:GLY:O	1:A:70:GLY:N	2.43	0.51
1:C:34:MET:HG3	1:C:53:LEU:HD12	1.91	0.51
1:D:102:THR:HA	1:D:106:PRO:HA	1.92	0.51
1:D:316:ASP:O	1:D:320:ARG:HG3	2.09	0.51
1:E:185:ASN:ND2	6:E:400:NAG:O7	2.43	0.51
1:E:67:GLY:O	1:E:70:GLY:N	2.43	0.51
2:F:203:THR:HG22	2:F:204:CYS:N	2.26	0.51
3:M:42:PRO:O	3:M:43:ASP:HB2	2.10	0.51
3:O:151:TRP:CD2	3:O:181:LEU:HD12	2.45	0.51
1:B:313:LYS:O	1:B:317:LEU:HD13	2.10	0.51
1:C:67:GLY:O	1:C:70:GLY:N	2.44	0.51
1:E:107:ASN:N	1:E:107:ASN:HD22	2.07	0.51
2:I:131:TYR:CD2	3:O:127:GLU:HG2	2.45	0.51
3:M:172:ASN:OD1	3:M:174:LYS:HD3	2.10	0.51
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.91	0.51
1:A:224:SER:CB	1:A:279:TRP:CZ3	2.94	0.51
1:E:103:ILE:HG23	1:E:103:ILE:O	2.11	0.51
1:E:36:LEU:HD13	1:E:168:LEU:HD11	1.91	0.51
2:G:213:THR:HG22	2:G:215:VAL:HG23	1.93	0.51
2:J:162:THR:OG1	2:J:205:ASN:HB2	2.09	0.51
1:C:316:ASP:O	1:C:320:ARG:HG3	2.11	0.51
2:G:201:THR:O	2:G:202:VAL:HG23	2.10	0.51
2:H:34:MET:CE	2:H:96:CYS:HB2	2.41	0.51
2:I:34:MET:CE	2:I:96:CYS:HB2	2.40	0.51
1:A:254:LEU:HD12	1:B:251:THR:HG23	1.91	0.51
1:B:34:MET:HG3	1:B:53:LEU:HD12	1.92	0.51
1:C:36:LEU:HD13	1:C:168:LEU:HD11	1.93	0.51
2:J:69:THR:HB	2:J:82:GLU:HB2	1.91	0.51
3:M:122:PRO:HG3	3:M:209:LEU:HD11	1.93	0.51
3:N:42:PRO:O	3:N:43:ASP:HB2	2.10	0.51
1:A:102:THR:HA	1:A:106:PRO:HA	1.92	0.51
1:B:67:GLY:O	1:B:70:GLY:N	2.43	0.51
1:D:286:PHE:CE2	7:D:350:OCT:H32	2.46	0.51
1:A:154:THR:HG23	1:A:156:LYS:H	1.76	0.51
1:A:313:LYS:O	1:A:317:LEU:HD13	2.11	0.51
1:C:154:THR:HG23	1:C:156:LYS:H	1.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:CB	1:C:279:TRP:CZ3	2.93	0.51
1:D:36:LEU:HD13	1:D:168:LEU:HD11	1.93	0.51
3:L:152:LYS:HD3	3:L:197:GLN:NE2	2.25	0.51
1:B:102:THR:HA	1:B:106:PRO:HA	1.93	0.50
2:F:164:ASN:HB2	2:F:167:SER:HB2	1.93	0.50
3:M:9:ALA:HB2	3:M:146:VAL:HG21	1.94	0.50
3:N:170:GLN:O	3:N:171:SER:C	2.49	0.50
1:D:67:GLY:O	1:D:70:GLY:N	2.44	0.50
2:G:133:LEU:HB2	2:G:148:GLY:O	2.10	0.50
1:B:253:LEU:HD11	1:C:226:MET:HE1	1.93	0.50
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.92	0.50
1:C:254:LEU:HD12	1:D:251:THR:HG23	1.93	0.50
2:H:163:TRP:HZ2	2:H:188:SER:O	1.93	0.50
3:N:142:PHE:HE1	3:N:145:GLY:HA2	1.76	0.50
1:B:103:ILE:HG23	1:B:103:ILE:O	2.10	0.50
1:E:48:GLU:OE1	1:E:96:LYS:HE2	2.11	0.50
2:H:128:PRO:HB3	2:H:151:VAL:HG12	1.94	0.50
2:J:179:LEU:HD13	2:J:184:TYR:CZ	2.47	0.50
1:C:48:GLU:OE1	1:C:96:LYS:HE2	2.12	0.50
1:E:224:SER:HB2	1:E:279:TRP:HH2	1.74	0.50
2:I:125:THR:HG21	2:I:210:ALA:O	2.12	0.50
1:C:49:TYR:CE2	1:C:144:CYS:HB3	2.47	0.50
1:E:49:TYR:CE2	1:E:144:CYS:HB3	2.47	0.50
1:C:313:LYS:O	1:C:317:LEU:HD13	2.11	0.50
3:O:151:TRP:CE3	3:O:181:LEU:HD12	2.47	0.50
2:G:151:VAL:HG12	2:G:154:TYR:CD1	2.47	0.49
1:A:226:MET:HE2	1:E:253:LEU:HD11	1.92	0.49
2:F:203:THR:HG22	2:F:204:CYS:H	1.77	0.49
2:G:107:ARG:NH1	3:K:34:PHE:CZ	2.80	0.49
1:A:316:ASP:O	1:A:320:ARG:HG3	2.12	0.49
1:C:222:ILE:N	1:C:223:PRO:HD2	2.28	0.49
1:E:224:SER:CB	1:E:279:TRP:CZ3	2.95	0.49
2:I:186:LEU:HD12	2:I:186:LEU:O	2.13	0.49
2:J:128:PRO:HD3	2:J:208:HIS:ND1	2.26	0.49
1:B:154:THR:HG23	1:B:156:LYS:H	1.76	0.49
1:D:103:ILE:HG23	1:D:103:ILE:O	2.12	0.49
1:D:313:LYS:O	1:D:317:LEU:HD13	2.11	0.49
2:H:186:LEU:C	2:H:186:LEU:HD12	2.32	0.49
3:K:197:GLN:HB3	3:K:206:GLU:HG2	1.94	0.49
1:B:48:GLU:OE1	1:B:96:LYS:HE2	2.13	0.49
1:D:154:THR:HG23	1:D:156:LYS:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:THR:HG23	1:E:254:LEU:HD12	1.94	0.49
2:G:12:VAL:HG21	2:G:86:LEU:HD13	1.95	0.49
2:J:36:TRP:CD1	2:J:70:LEU:HD22	2.48	0.49
3:L:118:VAL:HG13	3:L:207:LYS:HD3	1.93	0.49
1:B:107:ASN:N	1:B:107:ASN:HD22	2.10	0.49
1:C:100:LYS:HE2	1:D:104:ASP:H	1.78	0.49
1:E:128:LEU:HD13	1:E:146:ILE:HG12	1.94	0.49
1:C:254:LEU:HD12	1:D:251:THR:CG2	2.42	0.49
2:F:36:TRP:CD1	2:F:70:LEU:HD22	2.48	0.49
1:C:103:ILE:HG23	1:C:103:ILE:O	2.12	0.49
2:G:30:THR:HA	2:G:53:PRO:HB2	1.95	0.49
3:M:111:GLN:HB2	3:M:112:PRO:HD2	1.94	0.49
1:C:137:TYR:CE1	1:C:267:LEU:HD21	2.48	0.49
1:B:286:PHE:CZ	7:B:351:OCT:H42	2.47	0.48
1:B:49:TYR:CE2	1:B:144:CYS:HB3	2.48	0.48
1:D:234:SER:HG	1:D:294:PHE:HZ	1.59	0.48
2:I:36:TRP:CD1	2:I:70:LEU:HD22	2.48	0.48
3:N:123:PRO:HD3	3:N:135:LEU:CD1	2.43	0.48
1:A:48:GLU:OE1	1:A:96:LYS:HE2	2.13	0.48
1:D:141:VAL:HG12	1:D:210:LYS:HA	1.96	0.48
3:L:120:LEU:HD23	3:L:120:LEU:C	2.33	0.48
3:L:166:GLN:HG3	3:L:167:PRO:HD2	1.95	0.48
3:O:164:THR:HG22	3:O:179:SER:OG	2.13	0.48
2:I:30:THR:HA	2:I:53:PRO:HB2	1.95	0.48
3:M:143:TYR:HA	3:M:144:PRO:C	2.34	0.48
2:F:30:THR:HA	2:F:53:PRO:HB2	1.95	0.48
1:A:250:VAL:CG1	1:B:251:THR:HG21	2.44	0.48
1:D:49:TYR:CE2	1:D:144:CYS:HB3	2.49	0.48
2:J:12:VAL:HG21	2:J:86:LEU:HD13	1.95	0.48
5:B:350:LMT:H6D	5:B:350:LMT:H1B	1.95	0.48
1:C:234:SER:HG	1:C:294:PHE:HZ	1.59	0.48
1:D:48:GLU:OE1	1:D:96:LYS:HE2	2.14	0.48
2:F:128:PRO:HB3	2:F:154:TYR:HB3	1.95	0.48
1:B:195:THR:CA	2:F:55:ASN:HD21	2.20	0.48
2:I:100:GLY:HA3	2:I:108:TYR:CE1	2.49	0.48
1:A:70:GLY:C	1:A:72:GLY:H	2.17	0.48
1:C:128:LEU:HD13	1:C:146:ILE:HG12	1.95	0.48
1:D:222:ILE:N	1:D:223:PRO:HD2	2.29	0.48
2:G:155:PHE:CD2	2:G:156:PRO:HA	2.49	0.48
1:A:79:LEU:HD13	1:A:112:ILE:HD11	1.96	0.48
2:F:12:VAL:HG21	2:F:86:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:157:GLU:HG3	2:G:184:TYR:CE2	2.49	0.48
2:J:101:ASP:HB3	2:J:104:ARG:HG3	1.96	0.48
4:D:349:IVM:H4B	1:E:226:MET:HB2	1.95	0.48
1:A:49:TYR:CE2	1:A:144:CYS:HB3	2.49	0.48
1:A:17:ARG:HB3	1:B:80:THR:HB	1.96	0.48
1:D:253:LEU:HD11	1:E:226:MET:HE2	1.96	0.48
1:E:70:GLY:C	1:E:72:GLY:H	2.17	0.48
2:F:100:GLY:HA3	2:F:108:TYR:CE1	2.49	0.48
2:G:2:VAL:HG21	2:G:111:TYR:CE2	2.49	0.48
3:N:142:PHE:CE1	3:N:145:GLY:HA2	2.47	0.48
1:A:141:VAL:HG12	1:A:210:LYS:HA	1.96	0.47
2:J:159:VAL:HG23	2:J:186:LEU:HD21	1.95	0.47
3:O:120:LEU:HD13	3:O:120:LEU:C	2.34	0.47
1:D:128:LEU:HD13	1:D:146:ILE:HG12	1.95	0.47
1:E:141:VAL:HG12	1:E:210:LYS:HA	1.96	0.47
2:F:101:ASP:HB3	2:F:104:ARG:HG3	1.96	0.47
2:H:30:THR:HA	2:H:53:PRO:HB2	1.95	0.47
1:B:128:LEU:HD13	1:B:146:ILE:HG12	1.94	0.47
2:J:30:THR:HA	2:J:53:PRO:HB2	1.95	0.47
3:L:56:ARG:NH2	3:L:64:PHE:O	2.47	0.47
1:A:128:LEU:HD13	1:A:146:ILE:HG12	1.95	0.47
1:A:222:ILE:N	1:A:223:PRO:HD2	2.30	0.47
1:A:137:TYR:CE1	1:A:267:LEU:HD21	2.50	0.47
2:G:100:GLY:HA3	2:G:108:TYR:CE1	2.50	0.47
2:G:34:MET:CE	2:G:96:CYS:HB2	2.43	0.47
1:A:20:PRO:HD3	1:A:86:TRP:CD2	2.49	0.47
4:B:349:IVM:H4B	1:C:226:MET:HB2	1.97	0.47
1:B:20:PRO:HD3	1:B:86:TRP:CD2	2.49	0.47
2:H:100:GLY:HA3	2:H:108:TYR:CE1	2.50	0.47
2:H:2:VAL:HG21	2:H:111:TYR:CE2	2.50	0.47
2:J:157:GLU:HB3	2:J:158:PRO:HA	1.97	0.47
1:B:284:MET:HG3	1:C:226:MET:HE3	1.95	0.47
1:D:20:PRO:HD3	1:D:86:TRP:CD2	2.49	0.47
1:E:163:LYS:O	1:E:167:PRO:HG3	2.15	0.47
3:K:130:THR:HG22	3:K:130:THR:O	2.14	0.47
1:C:73:GLN:CB	1:C:74:PRO:HD2	2.45	0.47
1:E:128:LEU:CD1	1:E:146:ILE:HG12	2.45	0.47
2:G:108:TYR:HA	3:K:36:ASN:OD1	2.15	0.47
3:M:56:ARG:NH2	3:M:64:PHE:O	2.48	0.47
1:B:70:GLY:C	1:B:72:GLY:H	2.18	0.47
1:D:267:LEU:HD13	1:D:274:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:TYR:CE1	1:D:267:LEU:HD21	2.50	0.47
2:G:33:THR:HA	2:G:53:PRO:HD3	1.97	0.47
2:G:36:TRP:CD1	2:G:70:LEU:HD22	2.49	0.47
2:J:100:GLY:HA3	2:J:108:TYR:CE1	2.49	0.47
2:J:33:THR:HA	2:J:53:PRO:HD3	1.97	0.47
1:C:102:THR:HA	1:C:106:PRO:HA	1.95	0.47
1:A:251:THR:HG21	1:E:250:VAL:CG1	2.44	0.47
3:O:127:GLU:OE1	3:O:134:THR:N	2.48	0.47
1:C:20:PRO:HD3	1:C:86:TRP:CD2	2.50	0.47
1:D:70:GLY:C	1:D:72:GLY:H	2.18	0.47
1:E:20:PRO:HD3	1:E:86:TRP:CD2	2.49	0.47
2:F:2:VAL:HG21	2:F:111:TYR:CE2	2.50	0.47
2:I:101:ASP:HB3	2:I:104:ARG:HG3	1.97	0.47
2:I:2:VAL:HG21	2:I:111:TYR:CE2	2.50	0.47
2:J:2:VAL:HG21	2:J:111:TYR:CE2	2.50	0.47
3:K:169:LYS:HG2	3:K:175:TYR:CE2	2.49	0.47
3:K:56:ARG:NH2	3:K:64:PHE:O	2.48	0.47
3:L:122:PRO:HA	3:L:135:LEU:HD13	1.96	0.47
3:N:56:ARG:NH2	3:N:64:PHE:O	2.48	0.47
1:C:141:VAL:HG12	1:C:210:LYS:HA	1.97	0.46
1:D:242:ILE:HD11	1:D:294:PHE:HB3	1.97	0.46
2:I:12:VAL:HG21	2:I:86:LEU:HD13	1.95	0.46
1:C:163:LYS:O	1:C:167:PRO:HG3	2.15	0.46
1:E:222:ILE:N	1:E:223:PRO:HD2	2.30	0.46
1:C:267:LEU:HD13	1:C:274:LYS:HE3	1.98	0.46
2:H:157:GLU:HG3	2:H:184:TYR:CD2	2.51	0.46
1:B:128:LEU:CD1	1:B:146:ILE:HG12	2.45	0.46
1:E:73:GLN:CB	1:E:74:PRO:HD2	2.46	0.46
3:K:148:THR:HB	3:K:199:THR:HB	1.97	0.46
1:A:130:CYS:O	1:A:132:MET:HG3	2.15	0.46
1:A:138:PRO:HB2	1:A:139:MET:SD	2.56	0.46
1:B:222:ILE:N	1:B:223:PRO:HD2	2.31	0.46
1:B:267:LEU:HD13	1:B:274:LYS:HE3	1.97	0.46
2:H:101:ASP:HB3	2:H:104:ARG:HG3	1.97	0.46
1:A:300:ILE:HG22	5:A:349:LMT:H12	1.97	0.46
1:A:303:ALA:HB2	5:A:349:LMT:C6'	2.37	0.46
1:D:73:GLN:CB	1:D:74:PRO:HD2	2.45	0.46
2:F:33:THR:HA	2:F:53:PRO:HD3	1.98	0.46
2:H:36:TRP:CD1	2:H:70:LEU:HD22	2.50	0.46
3:L:166:GLN:CG	3:L:167:PRO:HD2	2.46	0.46
1:A:73:GLN:CB	1:A:74:PRO:HD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:VAL:HG12	1:B:210:LYS:HA	1.96	0.46
1:C:70:GLY:C	1:C:72:GLY:H	2.17	0.46
2:G:101:ASP:HB3	2:G:104:ARG:HG3	1.97	0.46
3:O:56:ARG:NH2	3:O:64:PHE:O	2.48	0.46
5:A:349:LMT:H1'	5:B:350:LMT:O3'	2.16	0.46
1:B:130:CYS:O	1:B:132:MET:HG3	2.16	0.46
2:G:131:TYR:HE2	2:G:152:LYS:HD3	1.82	0.46
3:K:105:LYS:HD2	3:K:146:VAL:CG1	2.46	0.46
2:J:107:ARG:NH1	3:M:34:PHE:CZ	2.83	0.46
1:A:128:LEU:CD1	1:A:146:ILE:HG12	2.47	0.45
1:A:267:LEU:HD13	1:A:274:LYS:HE3	1.98	0.45
1:B:137:TYR:CE1	1:B:267:LEU:HD21	2.51	0.45
1:B:73:GLN:CB	1:B:74:PRO:HD2	2.45	0.45
1:D:128:LEU:CD1	1:D:146:ILE:HG12	2.46	0.45
1:D:163:LYS:O	1:D:167:PRO:HG3	2.16	0.45
3:K:209:LEU:HD23	3:K:209:LEU:N	2.31	0.45
1:D:130:CYS:O	1:D:132:MET:HG3	2.16	0.45
1:E:79:LEU:HD11	1:E:83:HIS:HB2	1.98	0.45
1:B:234:SER:HG	1:B:294:PHE:HZ	1.57	0.45
1:C:224:SER:CB	1:C:279:TRP:CH2	2.99	0.45
1:D:134:LEU:HB3	1:D:137:TYR:HB2	1.98	0.45
1:E:137:TYR:CE1	1:E:267:LEU:HD21	2.51	0.45
2:H:33:THR:HA	2:H:53:PRO:HD3	1.98	0.45
3:K:41:LYS:HD3	3:K:86:ALA:HB2	1.98	0.45
3:O:111:GLN:HE22	3:O:174:LYS:HE3	1.81	0.45
1:B:138:PRO:HB2	1:B:139:MET:SD	2.57	0.45
2:G:131:TYR:CE2	2:G:152:LYS:HD3	2.52	0.45
2:H:12:VAL:HG21	2:H:86:LEU:HD13	1.97	0.45
3:K:120:LEU:HD23	3:K:121:PHE:N	2.31	0.45
3:O:41:LYS:HD3	3:O:86:ALA:HB2	1.98	0.45
1:A:163:LYS:O	1:A:167:PRO:HG3	2.15	0.45
1:A:234:SER:HG	1:A:294:PHE:HZ	1.59	0.45
1:A:242:ILE:HD11	1:A:294:PHE:HB3	1.98	0.45
1:B:185:ASN:ND2	6:B:400:NAG:O7	2.49	0.45
1:C:134:LEU:HB3	1:C:137:TYR:HB2	1.99	0.45
1:D:138:PRO:HB2	1:D:139:MET:SD	2.57	0.45
2:F:11:LEU:HD21	2:F:155:PHE:CZ	2.52	0.45
2:G:168:LEU:HD21	2:G:190:VAL:HG21	1.99	0.45
3:N:41:LYS:HD3	3:N:86:ALA:HB2	1.98	0.45
1:B:79:LEU:HD11	1:B:83:HIS:HB2	1.98	0.45
1:E:242:ILE:HD11	1:E:294:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ILE:HD11	1:E:112:ILE:CD1	2.46	0.45
2:H:203:THR:HA	2:H:218:LYS:HA	1.98	0.45
3:L:41:LYS:HD3	3:L:86:ALA:HB2	1.99	0.45
3:M:41:LYS:HD3	3:M:86:ALA:HB2	1.97	0.45
5:A:349:LMT:H1B	5:A:349:LMT:H6E	1.96	0.45
1:C:91:PHE:HD1	1:D:123:ARG:NH1	2.15	0.45
1:D:79:LEU:HD13	1:D:112:ILE:HD11	1.99	0.45
1:B:192:THR:HG23	1:B:200:TYR:O	2.16	0.45
1:C:253:LEU:HD11	1:D:226:MET:HE2	1.98	0.45
1:E:79:LEU:HD13	1:E:112:ILE:HD11	1.99	0.45
1:E:130:CYS:O	1:E:132:MET:HG3	2.16	0.45
3:L:108:VAL:O	3:L:143:TYR:OH	2.34	0.45
1:B:224:SER:CB	1:B:279:TRP:CH2	2.99	0.45
1:D:224:SER:CB	1:D:279:TRP:CH2	2.98	0.45
2:J:29:PHE:HZ	2:J:72:VAL:HG23	1.82	0.45
1:A:224:SER:CB	1:A:279:TRP:CH2	2.99	0.45
1:A:79:LEU:HD11	1:A:83:HIS:HB2	1.99	0.45
1:E:134:LEU:HB3	1:E:137:TYR:HB2	1.98	0.45
1:E:138:PRO:HB2	1:E:139:MET:SD	2.57	0.45
1:E:20:PRO:HA	1:E:21:PRO:HD3	1.87	0.45
1:E:66:TYR:CG	1:E:67:GLY:N	2.85	0.45
2:I:33:THR:HA	2:I:53:PRO:HD3	1.98	0.45
3:O:130:THR:O	3:O:131:ASN:CB	2.65	0.45
1:E:267:LEU:HD13	1:E:274:LYS:HE3	1.98	0.44
3:L:154:ASP:OD2	3:L:191:HIS:HB3	2.17	0.44
3:O:123:PRO:HD2	3:O:188:TRP:CH2	2.52	0.44
1:B:163:LYS:O	1:B:167:PRO:HG3	2.18	0.44
1:C:79:LEU:HD13	1:C:112:ILE:HD11	1.99	0.44
1:C:130:CYS:O	1:C:132:MET:HG3	2.16	0.44
1:A:56:ARG:HA	1:A:120:TYR:O	2.17	0.44
1:B:134:LEU:HB3	1:B:137:TYR:HB2	1.99	0.44
1:B:242:ILE:HD11	1:B:294:PHE:HB3	1.99	0.44
1:B:79:LEU:HD13	1:B:112:ILE:HD11	1.99	0.44
1:D:79:LEU:HD11	1:D:83:HIS:HB2	1.99	0.44
3:M:147:VAL:HG12	3:M:200:HIS:HB2	1.98	0.44
1:A:66:TYR:CG	1:A:67:GLY:N	2.85	0.44
1:C:128:LEU:CD1	1:C:146:ILE:HG12	2.46	0.44
1:C:66:TYR:CG	1:C:67:GLY:N	2.85	0.44
1:C:79:LEU:HD11	1:C:83:HIS:HB2	2.00	0.44
1:C:17:ARG:HD2	1:D:81:VAL:O	2.16	0.44
2:J:6:GLN:N	2:J:114:GLN:HE22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:81:GLN:O	3:M:108:VAL:HG21	2.18	0.44
1:B:103:ILE:CG2	1:B:103:ILE:O	2.66	0.44
1:D:192:THR:HG23	1:D:200:TYR:O	2.18	0.44
1:D:9:LEU:HD21	1:D:66:TYR:HB3	1.99	0.44
2:I:131:TYR:CE2	3:O:127:GLU:HG2	2.52	0.44
2:I:6:GLN:N	2:I:114:GLN:HE22	2.16	0.44
3:L:153:VAL:HG23	3:L:193:SER:O	2.17	0.44
3:M:188:TRP:CZ3	3:M:194:TYR:CE1	3.05	0.44
1:C:104:ASP:HB3	1:C:105:LYS:H	1.61	0.44
1:C:242:ILE:HD11	1:C:294:PHE:HB3	2.00	0.44
1:D:66:TYR:CG	1:D:67:GLY:N	2.85	0.44
2:G:133:LEU:HB2	2:G:148:GLY:C	2.38	0.44
1:A:134:LEU:HB3	1:A:137:TYR:HB2	1.99	0.44
1:C:103:ILE:HA	1:C:103:ILE:HD12	1.84	0.44
2:F:163:TRP:CZ3	2:F:204:CYS:HB3	2.53	0.44
1:B:9:LEU:HD21	1:B:66:TYR:HB3	1.99	0.44
3:K:206:GLU:O	3:K:207:LYS:HD3	2.18	0.44
3:K:81:GLN:O	3:K:108:VAL:HG21	2.18	0.44
3:L:81:GLN:O	3:L:108:VAL:HG21	2.18	0.44
1:A:103:ILE:O	1:A:103:ILE:CG2	2.66	0.44
1:B:66:TYR:CG	1:B:67:GLY:N	2.85	0.44
2:F:131:TYR:HB3	3:N:124:SER:OG	2.18	0.44
3:O:81:GLN:O	3:O:108:VAL:HG21	2.18	0.44
1:A:162:TRP:CE2	1:A:203:LEU:HB3	2.53	0.43
2:F:215:VAL:HG12	2:F:216:ASP:N	2.33	0.43
2:H:131:TYR:CD2	3:L:127:GLU:HB3	2.53	0.43
2:H:197:TRP:CG	2:H:198:PRO:HA	2.53	0.43
2:H:6:GLN:N	2:H:114:GLN:HE22	2.16	0.43
3:K:132:LYS:HD2	3:K:183:LEU:O	2.18	0.43
1:A:107:ASN:ND2	1:A:107:ASN:N	2.66	0.43
1:B:234:SER:HA	1:B:237:PHE:CD2	2.50	0.43
1:D:95:GLU:HA	1:D:128:LEU:HD23	2.01	0.43
2:G:181:SER:O	2:G:182:ASP:CB	2.66	0.43
2:G:177:ALA:HA	2:G:186:LEU:HB3	1.99	0.43
2:G:29:PHE:HZ	2:G:72:VAL:HG23	1.84	0.43
2:H:29:PHE:HZ	2:H:72:VAL:HG23	1.83	0.43
2:I:216:ASP:O	2:I:217:LYS:HD2	2.18	0.43
1:B:95:GLU:HA	1:B:128:LEU:HD23	2.01	0.43
1:B:286:PHE:CE2	7:B:351:OCT:H42	2.53	0.43
2:F:30:THR:O	2:F:54:TYR:HB2	2.19	0.43
3:L:111:GLN:HB2	3:L:112:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ARG:HA	1:C:120:TYR:O	2.19	0.43
1:E:274:LYS:HB2	1:E:276:ILE:HG22	2.01	0.43
1:E:309:ASN:O	1:E:312:SER:HB3	2.18	0.43
3:K:105:LYS:HD2	3:K:146:VAL:HG13	2.00	0.43
3:M:123:PRO:HD2	3:M:188:TRP:CH2	2.53	0.43
2:F:133:LEU:HD11	3:N:136:VAL:HG21	1.99	0.43
3:O:137:CYS:HB2	3:O:151:TRP:CH2	2.54	0.43
1:C:274:LYS:HB2	1:C:276:ILE:HG22	2.00	0.43
1:D:100:LYS:HE2	1:E:104:ASP:H	1.84	0.43
1:E:234:SER:HA	1:E:237:PHE:CD2	2.51	0.43
2:F:29:PHE:HZ	2:F:72:VAL:HG23	1.83	0.43
2:F:6:GLN:N	2:F:114:GLN:HE22	2.16	0.43
2:I:30:THR:O	2:I:54:TYR:HB2	2.19	0.43
1:A:20:PRO:HA	1:A:21:PRO:HD3	1.89	0.43
1:C:9:LEU:HD21	1:C:66:TYR:HB3	2.00	0.43
1:D:234:SER:HA	1:D:237:PHE:CD2	2.51	0.43
2:G:14:PRO:HD2	2:G:122:SER:HB3	2.00	0.43
3:K:111:GLN:CG	3:K:112:PRO:HD2	2.47	0.43
2:J:133:LEU:HB3	3:M:121:PHE:CD1	2.53	0.43
2:I:131:TYR:CD2	3:O:127:GLU:CG	3.02	0.43
1:A:274:LYS:HB2	1:A:276:ILE:HG22	2.01	0.43
1:A:9:LEU:HD21	1:A:66:TYR:HB3	2.00	0.43
1:B:274:LYS:HB2	1:B:276:ILE:HG22	2.00	0.43
1:C:234:SER:HA	1:C:237:PHE:CD2	2.51	0.43
1:D:274:LYS:HB2	1:D:276:ILE:HG22	2.00	0.43
1:D:195:THR:CA	2:I:55:ASN:ND2	2.71	0.43
3:L:118:VAL:O	3:L:207:LYS:HE3	2.19	0.43
3:N:81:GLN:O	3:N:108:VAL:HG21	2.18	0.43
3:O:164:THR:HG22	3:O:179:SER:CB	2.49	0.43
1:B:239:ARG:HD2	1:B:312:SER:OG	2.19	0.43
2:H:30:THR:O	2:H:54:TYR:HB2	2.19	0.43
1:D:213:PHE:CE2	1:D:217:LEU:HB2	2.53	0.42
1:E:192:THR:HG23	1:E:200:TYR:O	2.19	0.42
2:H:155:PHE:CD1	2:H:156:PRO:N	2.87	0.42
3:K:182:THR:O	3:K:183:LEU:HD23	2.18	0.42
3:M:123:PRO:HG2	3:M:188:TRP:CD2	2.54	0.42
1:C:213:PHE:CE2	1:C:217:LEU:HB2	2.54	0.42
1:C:309:ASN:O	1:C:312:SER:HB3	2.19	0.42
2:I:178:VAL:HG22	2:I:185:THR:O	2.19	0.42
1:B:309:ASN:O	1:B:312:SER:HB3	2.20	0.42
1:C:85:ILE:HD11	1:C:112:ILE:CD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:133:LEU:HD12	2:G:149:CYS:O	2.19	0.42
2:G:6:GLN:N	2:G:114:GLN:HE22	2.16	0.42
2:J:30:THR:O	2:J:54:TYR:HB2	2.19	0.42
1:A:192:THR:HG23	1:A:200:TYR:O	2.19	0.42
1:B:56:ARG:HA	1:B:120:TYR:O	2.19	0.42
1:C:138:PRO:HB2	1:C:139:MET:SD	2.59	0.42
1:C:239:ARG:HD2	1:C:312:SER:OG	2.19	0.42
1:E:9:LEU:HD21	1:E:66:TYR:HB3	2.00	0.42
2:G:157:GLU:CB	2:G:158:PRO:HA	2.49	0.42
2:H:175:PHE:HB3	2:H:176:PRO:HD2	2.01	0.42
1:B:314:ARG:O	1:B:318:ILE:HG13	2.20	0.42
1:D:239:ARG:HD2	1:D:312:SER:OG	2.19	0.42
1:D:226:MET:HB2	4:D:348:IVM:H4B	2.01	0.42
2:F:164:ASN:CB	2:F:167:SER:HB2	2.50	0.42
3:K:142:PHE:HB2	3:K:200:HIS:CE1	2.54	0.42
2:G:126:THR:HG22	2:G:127:PRO:O	2.19	0.42
2:J:147:LEU:HD22	2:J:219:ILE:HG21	2.01	0.42
3:L:130:THR:O	3:L:130:THR:HG22	2.20	0.42
1:B:174:LEU:C	1:B:174:LEU:HD23	2.40	0.42
1:B:213:PHE:CE2	1:B:217:LEU:HB2	2.55	0.42
1:C:192:THR:HG23	1:C:200:TYR:O	2.19	0.42
1:E:103:ILE:CG2	1:E:103:ILE:O	2.67	0.42
1:B:36:LEU:HB2	1:B:170:LEU:HD23	2.02	0.42
1:C:103:ILE:CG2	1:C:103:ILE:O	2.67	0.42
1:D:103:ILE:CG2	1:D:103:ILE:O	2.68	0.42
1:D:162:TRP:CE2	1:D:203:LEU:HB3	2.55	0.42
1:E:286:PHE:CE2	7:E:348:OCT:H12	2.55	0.42
2:I:177:ALA:HB2	2:I:186:LEU:HD23	2.02	0.42
2:J:152:LYS:HA	2:J:185:THR:HG23	2.02	0.42
2:J:174:THR:O	3:M:176:MET:HE1	2.20	0.42
2:G:30:THR:O	2:G:54:TYR:HB2	2.20	0.42
1:D:172:VAL:HA	2:G:54:TYR:OH	2.20	0.41
1:D:309:ASN:O	1:D:312:SER:HB3	2.19	0.41
1:E:292:LEU:HA	1:E:292:LEU:HD12	1.90	0.41
2:H:135:PRO:HD3	2:H:147:LEU:CD2	2.50	0.41
2:H:128:PRO:HB3	2:H:151:VAL:CG1	2.50	0.41
2:J:39:GLN:HG3	2:J:45:LEU:HD23	2.01	0.41
1:D:302:ASN:HD22	1:E:238:ASP:HB3	1.84	0.41
1:E:314:ARG:O	1:E:318:ILE:HG13	2.20	0.41
1:E:286:PHE:CE2	7:E:348:OCT:C1	3.04	0.41
1:E:56:ARG:HA	1:E:120:TYR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:107:ARG:NH1	3:O:34:PHE:CZ	2.88	0.41
2:J:163:TRP:CZ3	2:J:204:CYS:HB3	2.55	0.41
1:A:213:PHE:CE2	1:A:217:LEU:HB2	2.55	0.41
1:B:162:TRP:CE2	1:B:203:LEU:HB3	2.55	0.41
2:I:29:PHE:HZ	2:I:72:VAL:HG23	1.83	0.41
2:J:10:GLU:HG3	2:J:18:MET:CE	2.51	0.41
2:J:197:TRP:CZ2	2:J:221:PRO:HD3	2.56	0.41
3:L:158:VAL:HG11	3:L:181:LEU:CD1	2.51	0.41
2:I:108:TYR:HA	3:O:36:ASN:OD1	2.19	0.41
1:C:36:LEU:HB2	1:C:170:LEU:HD23	2.02	0.41
1:D:302:ASN:ND2	1:E:238:ASP:HB3	2.36	0.41
1:E:107:ASN:N	1:E:107:ASN:ND2	2.68	0.41
2:G:161:VAL:HG22	2:G:206:VAL:HG22	2.02	0.41
1:A:95:GLU:HA	1:A:128:LEU:HD23	2.02	0.41
1:A:20:PRO:HD2	1:A:28:VAL:HG21	2.01	0.41
1:C:269:PRO:HB3	1:D:215:PHE:CG	2.55	0.41
1:C:95:GLU:HA	1:C:128:LEU:HD23	2.02	0.41
1:D:56:ARG:HA	1:D:120:TYR:O	2.20	0.41
2:H:10:GLU:HG3	2:H:18:MET:CE	2.51	0.41
1:A:85:ILE:HD11	1:A:112:ILE:CD1	2.49	0.41
4:D:349:IVM:H1B	4:D:349:IVM:H5	1.91	0.41
1:E:162:TRP:CE2	1:E:203:LEU:HB3	2.55	0.41
1:E:239:ARG:HD2	1:E:312:SER:OG	2.20	0.41
2:H:172:VAL:HG12	2:H:173:HIS:N	2.36	0.41
2:H:39:GLN:HG3	2:H:45:LEU:HD23	2.01	0.41
3:M:145:GLY:HA3	3:M:175:TYR:CG	2.55	0.41
1:A:89:ASP:HB2	1:B:105:LYS:CB	2.50	0.41
1:D:174:LEU:C	1:D:174:LEU:HD23	2.41	0.41
2:I:10:GLU:HG3	2:I:18:MET:CE	2.51	0.41
2:I:198:PRO:HG3	2:I:221:PRO:HG3	2.03	0.41
3:K:120:LEU:HD12	3:K:196:CYS:HB3	2.02	0.41
3:K:28:ALA:CB	3:K:71:ASP:HB2	2.51	0.41
3:L:124:SER:C	3:L:126:GLU:H	2.23	0.41
3:O:118:VAL:HB	3:O:207:LYS:HZ1	1.86	0.41
1:A:234:SER:HA	1:A:237:PHE:CD2	2.50	0.41
1:C:107:ASN:ND2	1:C:107:ASN:N	2.68	0.41
1:E:104:ASP:HB3	1:E:105:LYS:H	1.61	0.41
2:J:149:CYS:O	2:J:187:SER:HB2	2.20	0.41
1:A:104:ASP:HB3	1:A:105:LYS:H	1.61	0.41
1:A:309:ASN:O	1:A:312:SER:HB3	2.21	0.41
1:C:162:TRP:CE2	1:C:203:LEU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:SER:CB	1:D:279:TRP:HZ3	2.34	0.41
1:E:213:PHE:CE2	1:E:217:LEU:HB2	2.56	0.41
3:N:41:LYS:HB2	3:N:45:LEU:HB2	2.02	0.41
3:O:127:GLU:HB3	3:O:132:LYS:O	2.21	0.41
1:C:174:LEU:C	1:C:174:LEU:HD23	2.41	0.41
1:A:239:ARG:HD2	1:A:312:SER:OG	2.21	0.41
1:C:314:ARG:O	1:C:318:ILE:HG13	2.21	0.41
1:A:104:ASP:H	1:E:100:LYS:HE2	1.85	0.41
2:H:171:GLY:HA3	2:H:191:THR:HG22	2.02	0.41
2:I:131:TYR:CD1	3:O:126:GLU:OE1	2.74	0.41
3:O:49:LEU:C	3:O:50:ILE:HD13	2.41	0.41
1:A:126:LEU:HD13	1:A:128:LEU:HD21	2.03	0.40
1:B:104:ASP:HB3	1:B:105:LYS:H	1.61	0.40
1:B:85:ILE:HD11	1:B:112:ILE:CD1	2.46	0.40
1:D:107:ASN:ND2	1:D:107:ASN:N	2.68	0.40
2:F:156:PRO:O	2:F:208:HIS:CE1	2.74	0.40
2:I:39:GLN:HG3	2:I:45:LEU:HD23	2.03	0.40
1:A:174:LEU:C	1:A:174:LEU:HD23	2.40	0.40
1:A:302:ASN:HD22	1:B:238:ASP:HB3	1.86	0.40
1:A:36:LEU:HB2	1:A:170:LEU:HD23	2.03	0.40
1:D:126:LEU:HD13	1:D:128:LEU:HD21	2.03	0.40
2:G:10:GLU:HG3	2:G:18:MET:CE	2.51	0.40
2:J:186:LEU:HD12	2:J:186:LEU:C	2.42	0.40
3:M:109:LEU:HD12	3:M:109:LEU:HA	1.95	0.40
1:E:36:LEU:HB2	1:E:170:LEU:HD23	2.03	0.40
1:E:174:LEU:HD23	1:E:174:LEU:C	2.41	0.40
1:E:20:PRO:HD2	1:E:28:VAL:HG21	2.03	0.40
2:H:160:THR:OG1	2:H:207:ALA:HB3	2.21	0.40
2:I:207:ALA:HB1	2:I:214:LYS:HE2	2.03	0.40
1:B:20:PRO:HD2	1:B:28:VAL:HG21	2.03	0.40
2:G:178:VAL:HG22	2:G:185:THR:O	2.21	0.40
3:O:169:LYS:CG	3:O:173:ASN:HA	2.51	0.40
1:C:292:LEU:HA	1:C:292:LEU:HD12	1.91	0.40
1:D:314:ARG:O	1:D:318:ILE:HG13	2.22	0.40
2:G:208:HIS:HA	2:G:209:PRO:HD3	1.87	0.40
2:I:207:ALA:CB	2:I:214:LYS:HG2	2.51	0.40
2:J:134:ALA:HB1	2:J:135:PRO:HD2	2.03	0.40
3:K:41:LYS:HB2	3:K:45:LEU:HB2	2.04	0.40
2:H:108:TYR:CE2	3:L:55:ASN:ND2	2.90	0.40
1:D:161:LEU:HD11	3:O:32:ILE:HG23	2.03	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	338/347 (97%)	321 (95%)	16 (5%)	1 (0%)	41	72
1	B	338/347 (97%)	320 (95%)	17 (5%)	1 (0%)	41	72
1	C	337/347 (97%)	320 (95%)	16 (5%)	1 (0%)	41	72
1	D	338/347 (97%)	321 (95%)	16 (5%)	1 (0%)	41	72
1	E	338/347 (97%)	322 (95%)	15 (4%)	1 (0%)	41	72
2	F	185/221 (84%)	171 (92%)	12 (6%)	2 (1%)	14	46
2	G	194/221 (88%)	176 (91%)	18 (9%)	0	100	100
2	H	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
2	I	193/221 (87%)	181 (94%)	10 (5%)	2 (1%)	15	47
2	J	211/221 (96%)	199 (94%)	12 (6%)	0	100	100
3	K	195/210 (93%)	173 (89%)	21 (11%)	1 (0%)	29	62
3	L	208/210 (99%)	186 (89%)	20 (10%)	2 (1%)	15	47
3	M	208/210 (99%)	189 (91%)	19 (9%)	0	100	100
3	N	148/210 (70%)	131 (88%)	16 (11%)	1 (1%)	22	56
3	O	189/210 (90%)	166 (88%)	23 (12%)	0	100	100
All	All	3639/3890 (94%)	3378 (93%)	248 (7%)	13 (0%)	34	67

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	190	VAL
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
3	L	109	LEU
3	L	190	ARG

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Mol	Chain	Res	Type
3	N	165	THR
2	F	167	SER
2	F	178	VAL
2	I	178	VAL
3	K	146	VAL

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	307/316 (97%)	306 (100%)	1 (0%)	92	96
1	B	307/316 (97%)	306 (100%)	1 (0%)	92	96
1	C	306/316 (97%)	305 (100%)	1 (0%)	92	96
1	D	307/316 (97%)	306 (100%)	1 (0%)	92	96
1	E	307/316 (97%)	306 (100%)	1 (0%)	92	96
2	F	165/190 (87%)	165 (100%)	0	100	100
2	G	171/190 (90%)	170 (99%)	1 (1%)	86	91
2	H	190/190 (100%)	190 (100%)	0	100	100
2	I	172/190 (90%)	172 (100%)	0	100	100
2	J	185/190 (97%)	184 (100%)	1 (0%)	88	93
3	K	169/178 (95%)	169 (100%)	0	100	100
3	L	178/178 (100%)	178 (100%)	0	100	100
3	M	177/178 (99%)	177 (100%)	0	100	100
3	N	130/178 (73%)	130 (100%)	0	100	100
3	O	162/178 (91%)	161 (99%)	1 (1%)	86	91
All	All	3233/3420 (94%)	3225 (100%)	8 (0%)	93	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASP

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Mol	Chain	Res	Type
1	B	104	ASP
1	C	104	ASP
1	D	104	ASP
1	E	104	ASP
2	G	45	LEU
2	J	205	ASN
3	O	3	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	169	GLN
1	A	299	HIS
1	B	46	ASN
1	B	84	GLN
1	C	84	GLN
1	C	169	GLN
1	D	84	GLN
1	D	169	GLN
1	E	84	GLN
1	E	169	GLN
2	F	5	GLN
2	F	55	ASN
2	F	180	GLN
2	F	208	HIS
2	G	5	GLN
2	G	55	ASN
2	G	180	GLN
2	H	5	GLN
2	H	180	GLN
2	I	5	GLN
2	I	55	ASN
2	I	180	GLN
2	J	5	GLN
2	J	55	ASN
3	K	111	GLN
3	K	197	GLN
3	M	160	GLN
3	N	166	GLN
3	N	170	GLN
3	O	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	LMT	A	350	-	28,28,36	1.52	4 (14%)	39,39,47	1.32	4 (10%)
8	UND	B	352	-	10,10,10	0.42	0	9,9,9	0.43	0
6	NAG	B	400	1	14,14,15	0.57	0	17,19,21	1.70	3 (17%)
4	IVM	D	348	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
5	LMT	A	349	-	27,27,36	1.59	6 (22%)	37,38,47	2.05	12 (32%)
4	IVM	B	349	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
4	IVM	B	348	-	65,68,68	0.80	1 (1%)	82,102,102	1.63	17 (20%)
4	IVM	A	348	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	15 (18%)
6	NAG	C	400	1	14,14,15	0.60	0	17,19,21	2.60	3 (17%)
5	LMT	B	350	-	27,27,36	1.54	4 (14%)	37,38,47	1.44	7 (18%)
4	IVM	D	349	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
6	NAG	E	400	1	14,14,15	1.39	2 (14%)	17,19,21	1.90	5 (29%)
7	OCT	D	350	-	7,7,7	0.17	0	6,6,6	0.36	0
7	OCT	E	348	-	7,7,7	0.13	0	6,6,6	0.48	0
7	OCT	B	351	-	7,7,7	0.13	0	6,6,6	0.44	0

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	LMT	A	350	-	-	6/13/53/61	0/2/2/2
8	UND	B	352	-	-	0/8/8/8	-
6	NAG	B	400	1	-	2/6/23/26	0/1/1/1
4	IVM	D	348	-	-	3/45/141/141	0/6/7/7
5	LMT	A	349	-	-	6/12/52/61	0/2/2/2
4	IVM	B	349	-	-	3/45/141/141	0/6/7/7
4	IVM	B	348	-	-	3/45/141/141	0/6/7/7
4	IVM	A	348	-	-	3/45/141/141	0/6/7/7
6	NAG	C	400	1	-	2/6/23/26	0/1/1/1
5	LMT	B	350	-	-	6/12/52/61	0/2/2/2
4	IVM	D	349	-	-	3/45/141/141	0/6/7/7
6	NAG	E	400	1	-	2/6/23/26	0/1/1/1
7	OCT	D	350	-	-	0/5/5/5	-
7	OCT	E	348	-	-	0/5/5/5	-
7	OCT	B	351	-	-	0/5/5/5	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	349	IVM	O12-C46	4.93	1.45	1.34
4	D	349	IVM	O12-C46	4.87	1.45	1.34
4	A	348	IVM	O12-C46	4.85	1.45	1.34
4	B	348	IVM	O12-C46	4.84	1.45	1.34
4	D	348	IVM	O12-C46	4.78	1.45	1.34
6	E	400	NAG	C1-C2	4.21	1.58	1.52
5	A	349	LMT	C3'-C4'	-4.16	1.41	1.52
5	A	350	LMT	C3'-C4'	-4.09	1.41	1.52
5	B	350	LMT	C3'-C4'	-4.01	1.41	1.52
5	B	350	LMT	C4B-C3B	-3.78	1.42	1.52
5	A	350	LMT	C4B-C3B	-3.71	1.42	1.52
5	A	349	LMT	C4B-C3B	-3.65	1.43	1.52
5	A	350	LMT	C3B-C2B	-2.88	1.45	1.52
5	B	350	LMT	C3B-C2B	-2.84	1.45	1.52
5	A	349	LMT	C3B-C2B	-2.69	1.45	1.52
5	A	349	LMT	C3'-C2'	-2.27	1.46	1.52
5	A	349	LMT	O2'-C2'	-2.22	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	349	LMT	O5'-C5'	2.21	1.49	1.44
5	B	350	LMT	O2'-C2'	-2.20	1.37	1.43
5	A	350	LMT	O2'-C2'	-2.16	1.37	1.43
6	E	400	NAG	C3-C2	2.03	1.56	1.52

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	400	NAG	O5-C1-C2	8.34	124.45	111.29
4	D	349	IVM	O12-C46-C45	6.93	121.00	110.97
4	A	348	IVM	O12-C46-C45	6.79	120.79	110.97
4	D	348	IVM	O12-C46-C45	6.72	120.69	110.97
4	B	349	IVM	O12-C46-C45	6.70	120.67	110.97
4	B	348	IVM	O12-C46-C45	6.62	120.56	110.97
5	A	349	LMT	C1-O1'-C1'	6.36	124.39	113.84
6	C	400	NAG	C1-O5-C5	5.62	119.81	112.19
6	B	400	NAG	C1-O5-C5	5.24	119.30	112.19
4	D	348	IVM	C13-C14-C15	-4.94	106.60	113.21
4	B	349	IVM	C13-C14-C15	-4.89	106.66	113.21
4	D	349	IVM	C13-C14-C15	-4.67	106.95	113.21
4	A	348	IVM	C13-C14-C15	-4.67	106.95	113.21
4	B	348	IVM	C13-C14-C15	-4.47	107.22	113.21
6	E	400	NAG	O5-C1-C2	-4.37	104.38	111.29
4	A	348	IVM	O9-C40-C39	-3.76	102.26	105.73
4	D	348	IVM	O9-C40-C39	-3.71	102.30	105.73
4	B	348	IVM	O9-C40-C39	-3.64	102.37	105.73
4	B	349	IVM	O9-C40-C39	-3.56	102.44	105.73
4	D	349	IVM	O9-C40-C39	-3.51	102.49	105.73
5	A	349	LMT	O1B-C4'-C5'	3.50	119.05	109.45
5	B	350	LMT	C1-O1'-C1'	3.48	119.62	113.84
4	D	349	IVM	C12-O12-C46	-3.29	112.31	117.69
4	D	348	IVM	C12-O12-C46	-3.26	112.34	117.69
4	B	349	IVM	O14-C14-C15	3.19	108.89	105.82
4	A	348	IVM	C12-O12-C46	-3.18	112.47	117.69
4	B	348	IVM	C12-O12-C46	-3.18	112.47	117.69
4	B	349	IVM	C12-O12-C46	-3.13	112.56	117.69
4	B	348	IVM	O14-C14-C15	3.11	108.82	105.82
4	D	349	IVM	O14-C14-C15	3.05	108.76	105.82
5	A	349	LMT	O1'-C1'-C2'	-3.05	103.54	108.30
5	A	350	LMT	O3'-C3'-C2'	-3.05	103.30	110.35
4	D	348	IVM	O14-C14-C15	2.99	108.70	105.82
4	D	349	IVM	C37-C38-C39	-2.99	120.62	130.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	348	IVM	O14-C14-C15	2.96	108.67	105.82
4	D	349	IVM	O11-C46-C45	-2.94	120.01	125.05
6	E	400	NAG	O7-C7-N2	2.92	127.32	121.95
4	B	348	IVM	C37-C38-C39	-2.91	120.86	130.07
4	A	348	IVM	C37-C38-C39	-2.90	120.90	130.07
4	D	348	IVM	C37-C38-C39	-2.90	120.91	130.07
6	E	400	NAG	O7-C7-C8	-2.88	116.71	122.06
6	E	400	NAG	C2-N2-C7	2.87	126.99	122.90
5	A	349	LMT	C3B-C4B-C5B	2.87	115.36	110.24
4	B	349	IVM	C37-C38-C39	-2.86	121.03	130.07
4	D	348	IVM	O11-C46-C45	-2.85	120.17	125.05
4	B	349	IVM	C34-C19-C17	-2.85	108.22	113.89
4	D	348	IVM	C34-C19-C17	-2.85	108.22	113.89
5	A	349	LMT	O3'-C3'-C2'	-2.84	103.79	110.35
5	B	350	LMT	O3'-C3'-C2'	-2.80	103.88	110.35
5	A	349	LMT	C1B-O5B-C5B	-2.79	108.20	113.69
4	B	348	IVM	O11-C46-C45	-2.79	120.28	125.05
4	B	349	IVM	O11-C46-C45	-2.78	120.28	125.05
4	A	348	IVM	O11-C46-C45	-2.78	120.30	125.05
4	D	349	IVM	C34-C19-C17	-2.78	108.36	113.89
5	A	349	LMT	O1B-C4'-C3'	-2.74	99.98	107.28
4	B	348	IVM	C34-C19-C17	-2.74	108.43	113.89
4	A	348	IVM	O12-C46-O11	-2.70	118.89	123.94
6	C	400	NAG	O5-C5-C4	2.70	117.39	110.83
4	A	348	IVM	C34-C19-C17	-2.69	108.52	113.89
5	B	350	LMT	O1B-C1B-C2B	2.69	115.06	108.10
4	D	349	IVM	O12-C46-O11	-2.66	118.97	123.94
5	A	350	LMT	O1'-C1-C2	2.64	118.82	109.56
4	B	349	IVM	O12-C46-O11	-2.63	119.02	123.94
4	B	348	IVM	C15-C16-C17	-2.63	121.03	127.56
4	B	349	IVM	C15-C16-C17	-2.60	121.11	127.56
4	D	348	IVM	C15-C16-C17	-2.59	121.12	127.56
4	D	348	IVM	O12-C46-O11	-2.59	119.11	123.94
4	A	348	IVM	C15-C16-C17	-2.57	121.18	127.56
4	B	348	IVM	O12-C46-O11	-2.57	119.14	123.94
6	E	400	NAG	C1-C2-N2	2.55	114.84	110.49
4	D	349	IVM	C15-C16-C17	-2.54	121.26	127.56
5	A	350	LMT	C1B-O1B-C4'	-2.51	111.76	117.96
4	D	348	IVM	C3-C5-C9	-2.44	112.14	116.50
5	A	349	LMT	O5B-C5B-C4B	2.42	114.09	109.69
4	B	349	IVM	C3-C5-C9	-2.41	112.19	116.50
5	B	350	LMT	O5B-C5B-C4B	2.39	114.04	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	349	IVM	C3-C5-C9	-2.37	112.26	116.50
4	B	348	IVM	C38-C37-C36	-2.36	118.80	124.53
4	B	348	IVM	C3-C5-C9	-2.36	112.28	116.50
4	A	348	IVM	C3-C5-C9	-2.35	112.30	116.50
4	A	348	IVM	C38-C37-C36	-2.35	118.84	124.53
5	A	349	LMT	O3B-C3B-C4B	-2.32	104.97	110.35
5	A	350	LMT	C1-O1'-C1'	2.31	117.68	113.84
4	D	348	IVM	C38-C37-C36	-2.31	118.92	124.53
4	D	349	IVM	C38-C37-C36	-2.28	119.00	124.53
5	B	350	LMT	C3B-C4B-C5B	2.25	114.25	110.24
5	A	349	LMT	O1B-C1B-O5B	-2.25	104.39	110.67
4	B	349	IVM	C38-C37-C36	-2.24	119.09	124.53
4	A	348	IVM	C18-C17-C19	2.24	119.55	115.68
5	B	350	LMT	O3B-C3B-C4B	-2.24	105.18	110.35
4	D	348	IVM	O1-C5-C3	2.23	109.51	106.12
4	B	348	IVM	C18-C17-C19	2.20	119.48	115.68
4	B	348	IVM	C34-C36-C37	-2.18	121.57	126.16
4	B	349	IVM	C8-C9-C5	2.17	111.69	108.41
4	B	349	IVM	C18-C17-C19	2.17	119.43	115.68
5	A	349	LMT	C1B-O1B-C4'	2.17	123.32	117.96
6	B	400	NAG	O7-C7-C8	-2.13	118.09	122.06
4	B	349	IVM	O1-C5-C3	2.13	109.36	106.12
4	D	348	IVM	C34-C36-C37	-2.12	121.70	126.16
4	D	348	IVM	C18-C17-C19	2.10	119.31	115.68
4	D	349	IVM	C8-C9-C5	2.10	111.58	108.41
4	B	349	IVM	C34-C36-C37	-2.08	121.78	126.16
4	D	349	IVM	C18-C17-C19	2.08	119.27	115.68
4	D	349	IVM	O1-C5-C3	2.08	109.29	106.12
4	A	348	IVM	C34-C36-C37	-2.06	121.83	126.16
5	A	349	LMT	O5'-C1'-O1'	2.05	114.83	109.97
4	B	348	IVM	O1-C5-C3	2.05	109.24	106.12
4	B	348	IVM	C8-C9-C5	2.05	111.50	108.41
4	D	348	IVM	C8-C9-C5	2.04	111.50	108.41
4	A	348	IVM	O1-C5-C3	2.02	109.20	106.12
6	B	400	NAG	C4-C3-C2	2.01	113.96	111.02
4	B	348	IVM	O10-C42-C43	-2.00	106.75	110.48
4	D	349	IVM	C6-O1-C5	-2.00	111.50	114.27
5	B	350	LMT	O6B-C6B-C5B	2.00	118.16	111.29

There are no chirality outliers.

All (39) torsion outliers are listed below:

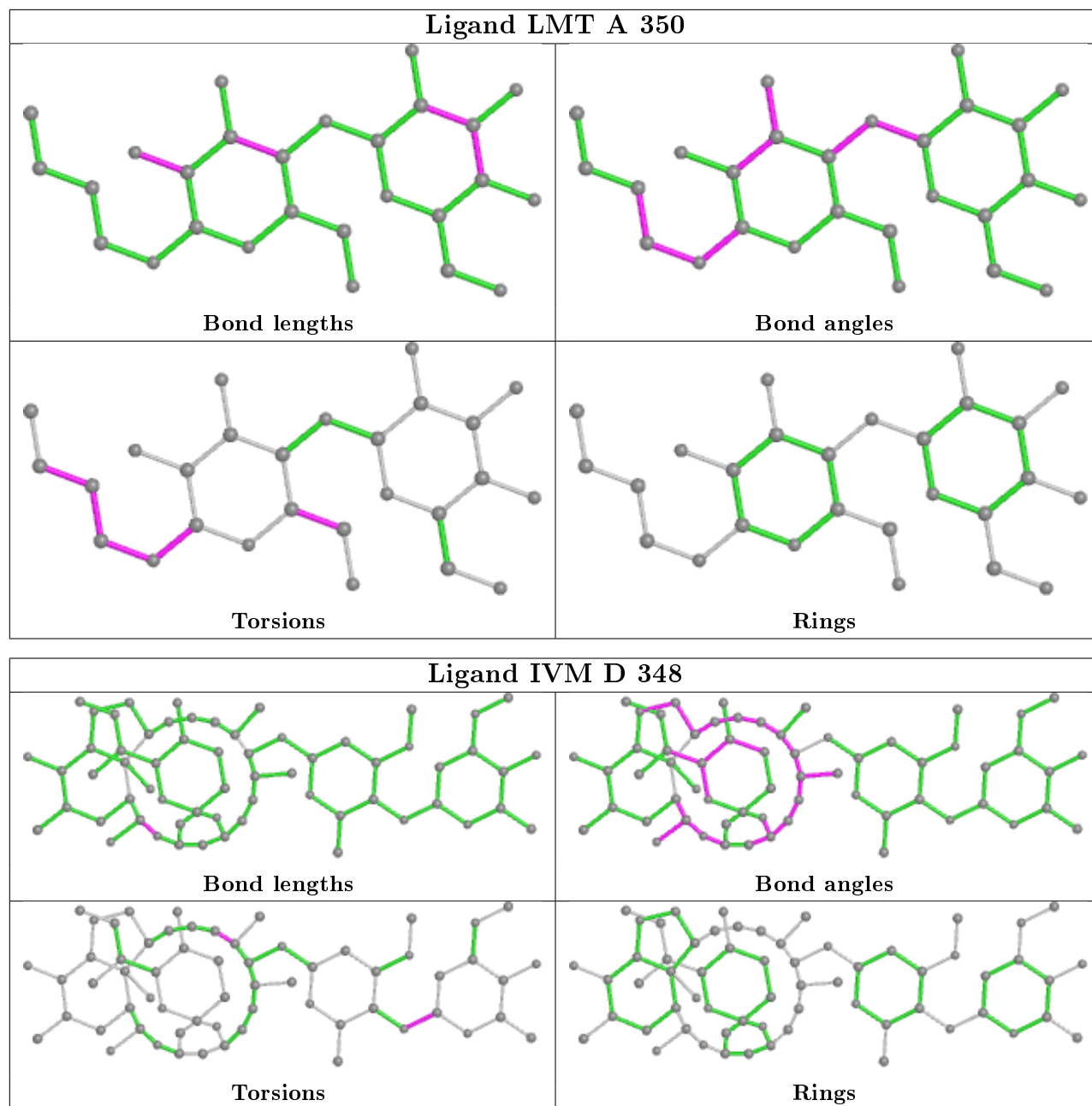
Mol	Chain	Res	Type	Atoms
5	A	350	LMT	C2'-C1'-O1'-C1
5	A	350	LMT	O5'-C1'-O1'-C1
4	D	348	IVM	O7-C25-O4-C24
4	D	348	IVM	C26-C25-O4-C24
5	A	349	LMT	O5'-C1'-O1'-C1
4	B	349	IVM	O7-C25-O4-C24
4	B	349	IVM	C26-C25-O4-C24
4	B	348	IVM	O7-C25-O4-C24
4	B	348	IVM	C26-C25-O4-C24
4	A	348	IVM	O7-C25-O4-C24
4	A	348	IVM	C26-C25-O4-C24
4	D	349	IVM	O7-C25-O4-C24
4	D	349	IVM	C26-C25-O4-C24
6	E	400	NAG	C1-C2-N2-C7
5	A	349	LMT	C5'-C4'-O1B-C1B
6	B	400	NAG	C4-C5-C6-O6
5	B	350	LMT	C2B-C1B-O1B-C4'
5	B	350	LMT	O5B-C1B-O1B-C4'
6	B	400	NAG	O5-C5-C6-O6
5	A	349	LMT	O5'-C5'-C6'-O6'
5	A	349	LMT	C4'-C5'-C6'-O6'
5	A	349	LMT	O1'-C1-C2-C3
5	B	350	LMT	O1'-C1-C2-C3
5	A	350	LMT	O5'-C5'-C6'-O6'
5	A	349	LMT	O5B-C5B-C6B-O6B
6	C	400	NAG	O5-C5-C6-O6
5	B	350	LMT	C2-C1-O1'-C1'
5	B	350	LMT	O5'-C5'-C6'-O6'
6	E	400	NAG	O5-C5-C6-O6
5	B	350	LMT	O5B-C5B-C6B-O6B
5	A	350	LMT	C2-C1-O1'-C1'
4	D	348	IVM	C19-C34-C36-C37
4	B	349	IVM	C19-C34-C36-C37
4	B	348	IVM	C19-C34-C36-C37
4	A	348	IVM	C19-C34-C36-C37
4	D	349	IVM	C19-C34-C36-C37
6	C	400	NAG	C4-C5-C6-O6
5	A	350	LMT	O1'-C1-C2-C3
5	A	350	LMT	C1-C2-C3-C4

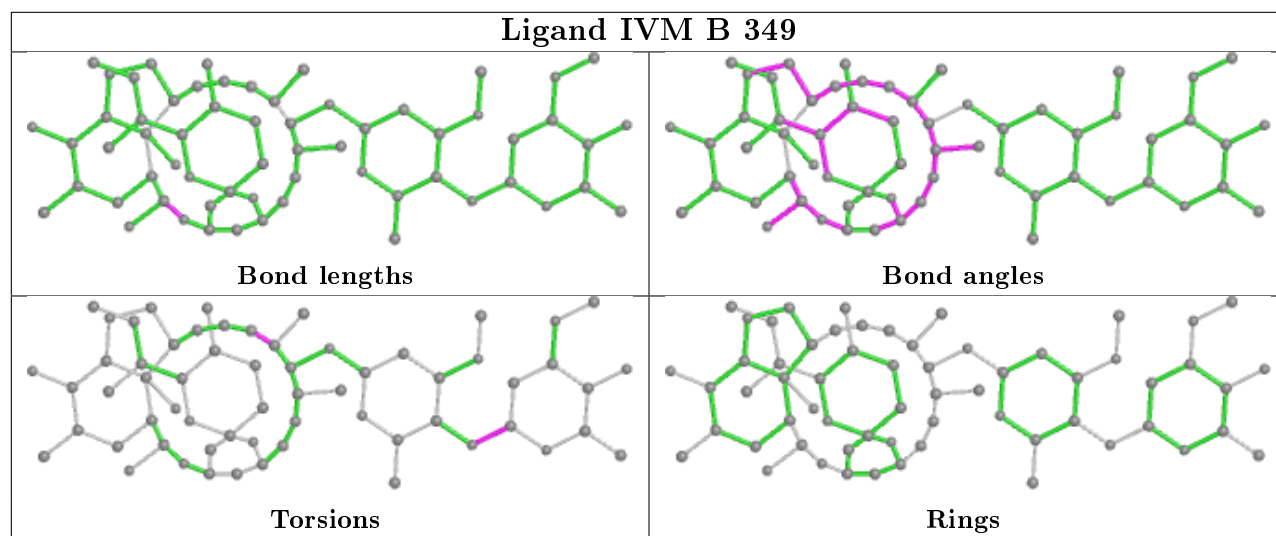
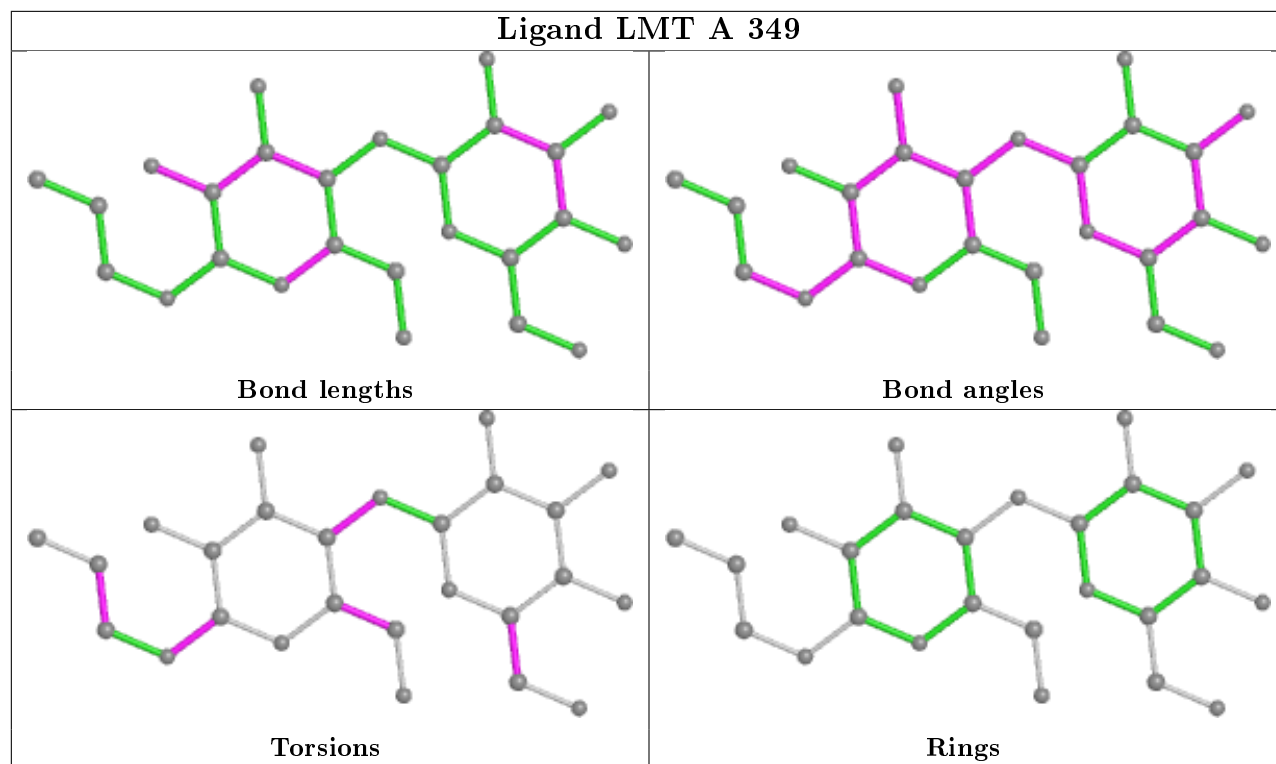
There are no ring outliers.

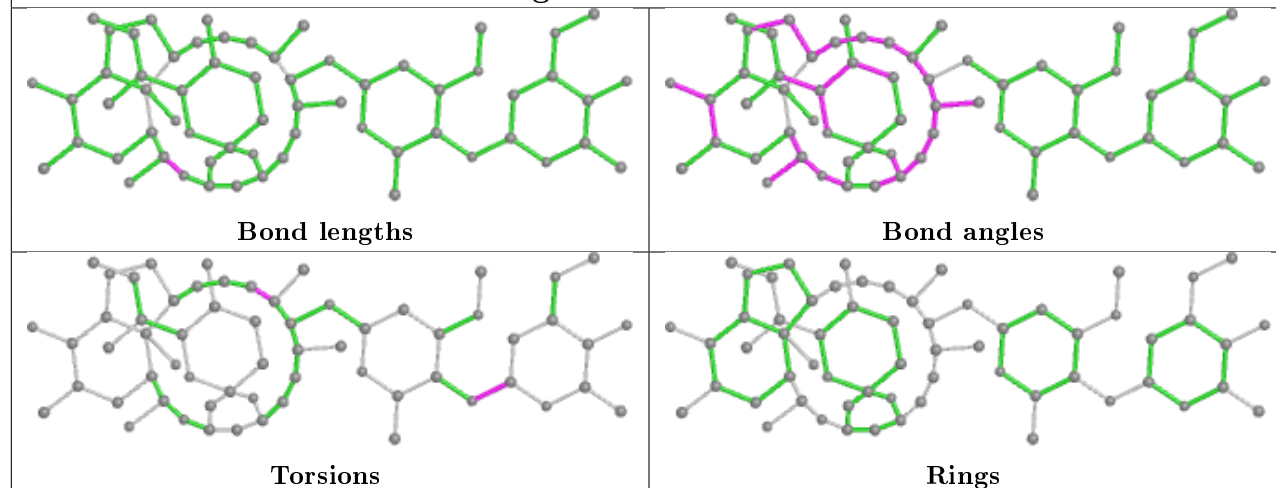
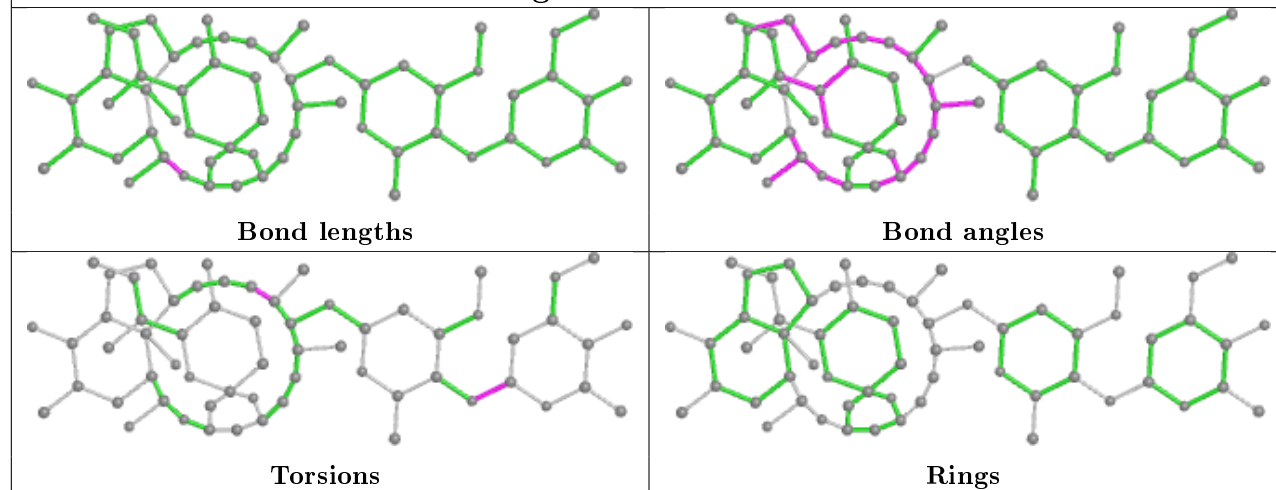
13 monomers are involved in 32 short contacts:

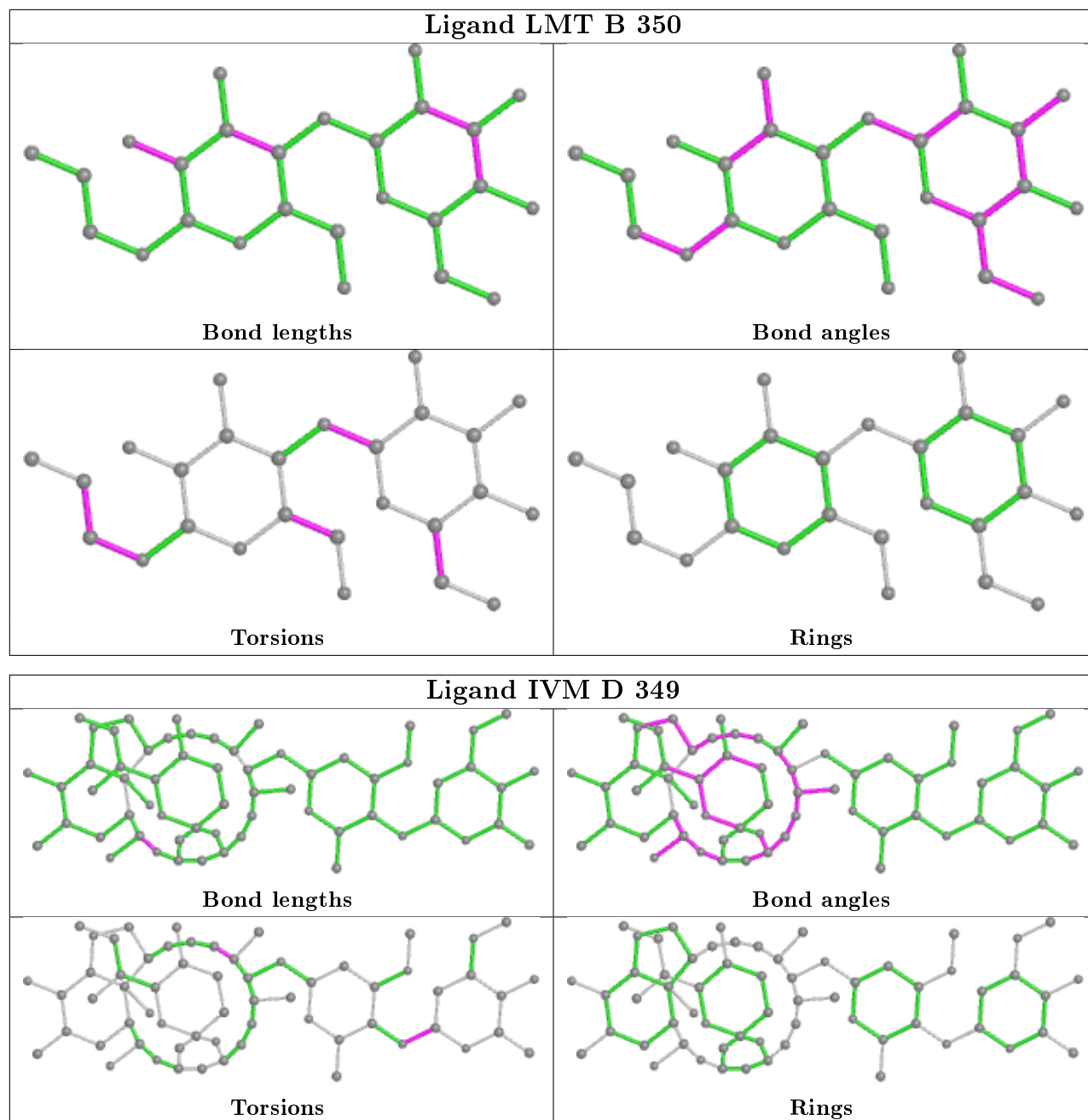
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	400	NAG	1	0
4	D	348	IVM	2	0
5	A	349	LMT	12	0
4	B	349	IVM	2	0
4	B	348	IVM	1	0
4	A	348	IVM	1	0
6	C	400	NAG	1	0
5	B	350	LMT	4	0
4	D	349	IVM	3	0
6	E	400	NAG	1	0
7	D	350	OCT	2	0
7	E	348	OCT	2	0
7	B	351	OCT	2	0

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.





Ligand IVM B 348**Ligand IVM A 348**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/347 (97%)	0.38	8 (2%) 59 55	35, 64, 128, 174	0
1	B	340/347 (97%)	0.45	19 (5%) 24 22	39, 66, 119, 196	0
1	C	339/347 (97%)	0.48	16 (4%) 31 28	44, 72, 144, 238	0
1	D	340/347 (97%)	0.42	9 (2%) 56 52	42, 73, 142, 215	0
1	E	340/347 (97%)	0.38	10 (2%) 51 50	38, 70, 138, 207	0
2	F	191/221 (86%)	1.06	32 (16%) 1 1	49, 102, 161, 181	0
2	G	200/221 (90%)	0.56	11 (5%) 25 23	52, 94, 146, 181	0
2	H	221/221 (100%)	0.52	13 (5%) 22 21	40, 77, 131, 280	0
2	I	199/221 (90%)	1.29	53 (26%) 0 0	56, 106, 170, 206	0
2	J	215/221 (97%)	0.36	4 (1%) 66 64	47, 80, 150, 240	0
3	K	199/210 (94%)	0.32	4 (2%) 65 63	61, 102, 149, 201	0
3	L	210/210 (100%)	0.42	7 (3%) 46 43	43, 74, 119, 157	0
3	M	210/210 (100%)	0.41	6 (2%) 51 50	46, 82, 126, 150	0
3	N	158/210 (75%)	0.82	19 (12%) 4 4	60, 106, 170, 198	0
3	O	195/210 (92%)	1.44	56 (28%) 0 0	61, 109, 160, 189	0
All	All	3697/3890 (95%)	0.58	267 (7%) 15 15	35, 80, 150, 280	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	188	SER	9.1
1	B	302	ASN	8.7
2	H	136	GLY	8.1
2	I	189	SER	7.3
3	O	208	SER	7.3
2	I	187	SER	5.5
2	I	207	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
3	O	207	LYS	5.3
2	I	173	HIS	5.2
3	O	206	GLU	5.1
2	H	139	ALA	5.1
2	F	168	LEU	4.9
3	O	175	TYR	4.9
1	E	340	HIS	4.8
3	O	136	VAL	4.8
1	B	304	GLY	4.8
3	O	197	GLN	4.8
2	H	138	ALA	4.7
1	C	305	THR	4.7
2	I	213	THR	4.7
2	F	217	LYS	4.6
2	F	216	ASP	4.6
3	O	176	MET	4.5
1	C	304	GLY	4.5
2	I	215	VAL	4.5
3	O	195	SER	4.4
1	D	242	ILE	4.3
2	I	147	LEU	4.3
3	O	116	PRO	4.3
3	O	100	PHE	4.3
2	I	174	THR	4.3
2	H	140	GLN	4.3
2	I	212	SER	4.2
1	B	301	ALA	4.2
2	I	219	ILE	4.1
2	I	178	VAL	4.1
1	B	298	ASN	4.1
1	C	303	ALA	4.1
3	O	179	SER	4.1
3	N	109	LEU	4.0
3	O	117	SER	4.0
3	O	151	TRP	3.9
1	A	340	HIS	3.9
2	I	37	VAL	3.9
3	O	121	PHE	3.9
2	F	215	VAL	3.9
2	F	151	VAL	3.8
2	F	176	PRO	3.8
2	F	170	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	I	97	ALA	3.7
1	B	308	TRP	3.7
1	C	239	ARG	3.7
2	I	214	LYS	3.7
3	O	138	THR	3.7
3	O	203	HIS	3.6
1	D	246	VAL	3.6
3	O	89	PHE	3.6
3	N	165	THR	3.5
3	O	88	TYR	3.5
3	O	120	LEU	3.5
1	D	83	HIS	3.5
2	H	141	THR	3.5
3	M	173	ASN	3.5
2	I	206	VAL	3.5
3	N	82	THR	3.4
1	C	259	GLN	3.4
2	I	45	LEU	3.4
2	I	176	PRO	3.4
3	K	197	GLN	3.4
1	E	307	GLU	3.4
2	F	178	VAL	3.3
2	I	4	LEU	3.3
2	I	191	THR	3.3
2	J	194	SER	3.3
2	H	137	SER	3.3
2	G	168	LEU	3.3
2	I	175	PHE	3.3
3	O	99	VAL	3.3
3	O	205	VAL	3.3
2	J	137	SER	3.3
2	F	169	SER	3.3
2	I	134	ALA	3.3
3	O	178	SER	3.2
2	I	172	VAL	3.2
1	A	306	THR	3.2
3	O	177	ALA	3.2
2	G	180	GLN	3.2
3	O	45	LEU	3.2
3	O	198	VAL	3.2
2	I	34	MET	3.1
2	I	190	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	338	PHE	3.1
2	H	1	GLU	3.1
3	O	135	LEU	3.1
3	O	41	LYS	3.1
3	L	194	TYR	3.0
3	O	113	LYS	3.0
2	F	206	VAL	3.0
1	A	309	ASN	3.0
3	O	196	CYS	3.0
2	I	133	LEU	3.0
3	O	18	VAL	3.0
1	B	305	THR	3.0
1	C	247	THR	3.0
2	F	221	PRO	2.9
1	E	68	VAL	2.9
3	N	108	VAL	2.9
2	J	195	SER	2.9
3	O	139	ILE	2.9
2	F	150	LEU	2.9
2	H	42	GLY	2.9
2	F	161	VAL	2.9
3	O	194	TYR	2.9
2	I	148	GLY	2.9
3	O	168	SER	2.8
3	O	150	ASP	2.8
3	L	203	HIS	2.8
3	N	136	VAL	2.8
3	L	1	GLN	2.8
1	A	305	THR	2.8
2	F	177	ALA	2.8
2	F	175	PHE	2.7
3	N	178	SER	2.7
3	N	106	LEU	2.7
2	F	219	ILE	2.7
1	C	308	TRP	2.7
2	I	198	PRO	2.7
2	F	210	ALA	2.7
3	O	170	GLN	2.7
3	N	171	SER	2.7
1	B	294	PHE	2.7
3	O	149	VAL	2.7
2	I	24	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	124	LYS	2.7
1	D	304	GLY	2.7
3	N	167	PRO	2.7
2	F	211	SER	2.6
2	I	112	TRP	2.6
2	I	39	GLN	2.6
2	I	221	PRO	2.6
2	I	197	TRP	2.6
2	I	35	ASN	2.6
3	O	144	PRO	2.6
1	D	79	LEU	2.6
3	N	144	PRO	2.6
3	N	162	MET	2.6
3	O	104	THR	2.6
2	G	4	LEU	2.6
2	H	144	MET	2.5
3	O	101	GLY	2.5
2	F	156	PRO	2.5
3	O	46	PHE	2.5
2	F	164	ASN	2.5
3	K	206	GLU	2.5
1	B	309	ASN	2.5
2	F	204	CYS	2.5
1	D	237	PHE	2.5
3	N	169	LYS	2.5
3	O	142	PHE	2.5
3	O	39	GLN	2.5
1	E	104	ASP	2.5
3	L	178	SER	2.5
2	H	168	LEU	2.4
2	F	11	LEU	2.4
1	E	338	PHE	2.4
3	L	181	LEU	2.4
1	C	237	PHE	2.4
1	E	291	LEU	2.4
3	N	135	LEU	2.4
2	I	25	SER	2.4
1	B	244	ALA	2.4
1	B	139	MET	2.4
3	O	1	GLN	2.4
3	M	53	ILE	2.4
3	O	171	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	303	ALA	2.4
2	I	216	ASP	2.4
2	I	220	VAL	2.4
3	O	49	LEU	2.4
1	B	338	PHE	2.4
2	I	195	SER	2.4
3	O	92	LEU	2.4
2	I	94	TYR	2.4
2	G	29	PHE	2.3
2	F	12	VAL	2.3
2	I	1	GLU	2.3
1	A	237	PHE	2.3
2	I	23	LYS	2.3
1	C	233	VAL	2.3
2	I	3	GLN	2.3
3	O	19	THR	2.3
3	O	108	VAL	2.3
2	H	43	LYS	2.3
2	F	172	VAL	2.3
3	O	111	GLN	2.3
2	I	127	PRO	2.3
2	F	186	LEU	2.3
2	I	110	ASP	2.3
1	B	311	ILE	2.3
3	M	175	TYR	2.3
2	F	205	ASN	2.2
3	O	109	LEU	2.2
3	M	52	GLY	2.2
1	E	304	GLY	2.2
2	F	31	GLY	2.2
3	N	166	GLN	2.2
2	J	183	LEU	2.2
3	O	105	LYS	2.2
2	I	185	THR	2.2
2	F	213	THR	2.2
2	G	160	THR	2.2
1	B	193	SER	2.2
1	E	193	SER	2.2
1	B	259	GLN	2.2
1	B	260	SER	2.2
1	D	254	LEU	2.2
1	A	241	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	243	PRO	2.2
2	F	220	VAL	2.2
2	I	33	THR	2.2
3	K	70	GLY	2.2
1	B	307	GLU	2.2
1	A	308	TRP	2.1
1	C	248	LEU	2.1
2	G	95	TYR	2.1
2	I	209	PRO	2.1
1	C	298	ASN	2.1
3	M	35	ALA	2.1
2	G	155	PHE	2.1
2	I	149	CYS	2.1
2	G	165	SER	2.1
3	O	202	GLY	2.1
1	B	300	ILE	2.1
2	F	128	PRO	2.1
2	I	46	GLU	2.1
3	O	38	VAL	2.1
2	H	28	SER	2.1
3	L	53	ILE	2.1
3	N	120	LEU	2.1
3	L	135	LEU	2.1
3	K	196	CYS	2.1
1	E	155	THR	2.1
2	F	32	TYR	2.1
1	C	334	TYR	2.0
2	G	32	TYR	2.0
2	H	145	VAL	2.0
3	M	54	ASN	2.0
2	I	20	ILE	2.0
3	O	167	PRO	2.0
3	O	183	LEU	2.0
1	D	104	ASP	2.0
3	N	179	SER	2.0
2	I	36	TRP	2.0
1	C	194	VAL	2.0
1	E	199	ILE	2.0
2	I	171	GLY	2.0
2	G	102	TYR	2.0
3	N	58	PRO	2.0
3	O	140	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	3	GLN	2.0
3	N	49	LEU	2.0
3	N	164	THR	2.0
1	A	312	SER	2.0
1	D	294	PHE	2.0
1	C	155	THR	2.0
2	I	96	CYS	2.0
1	B	291	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

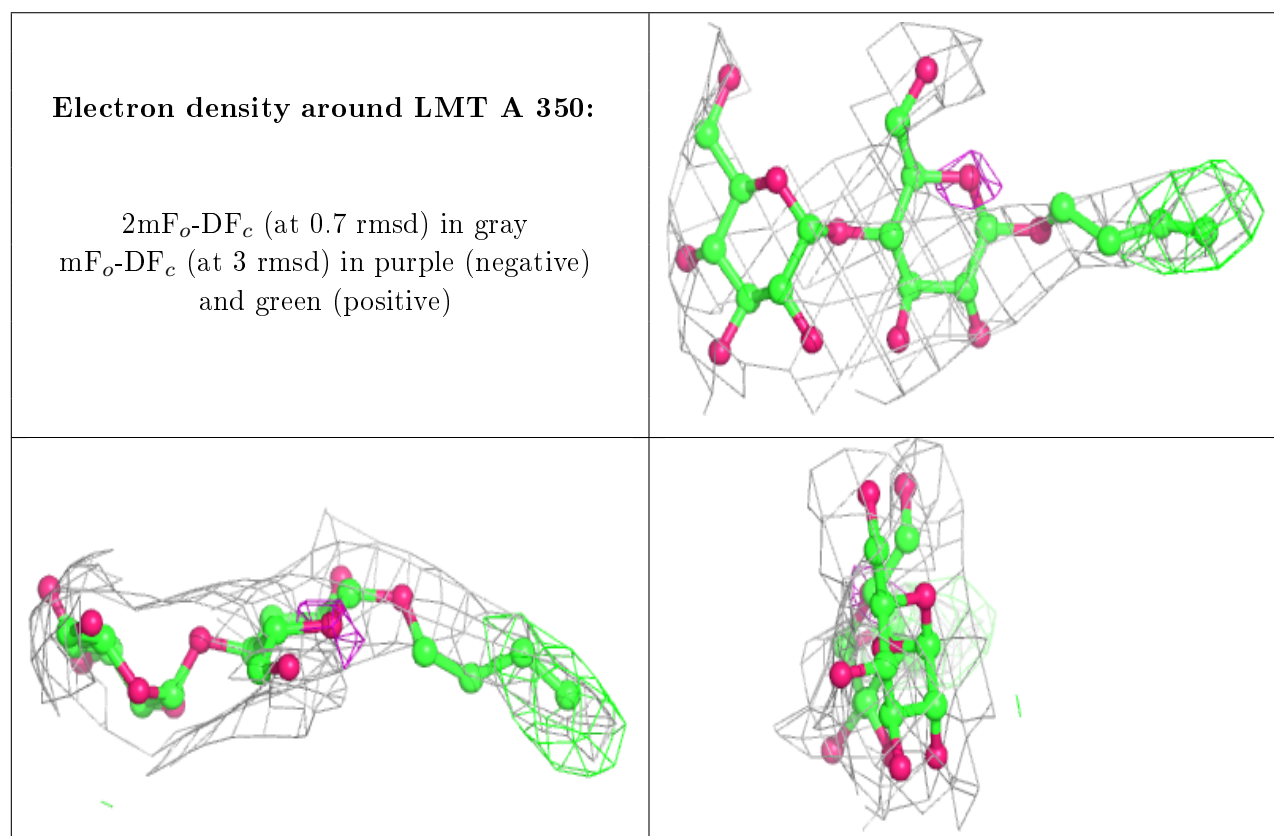
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	LMT	A	350	27/35	0.56	0.33	149,149,149,149	0
6	NAG	E	400	14/15	0.70	0.41	162,166,169,171	0
6	NAG	C	400	14/15	0.72	0.44	119,123,126,128	0
8	UND	B	352	11/11	0.72	0.25	63,63,63,63	0
5	LMT	B	350	26/35	0.73	0.35	166,166,166,166	0
6	NAG	B	400	14/15	0.79	0.38	132,137,140,142	0
7	OCT	D	350	8/8	0.82	0.39	61,61,61,61	0
7	OCT	E	348	8/8	0.82	0.44	74,74,74,74	0
5	LMT	A	349	26/35	0.85	0.31	110,110,110,110	0
7	OCT	B	351	8/8	0.86	0.56	68,68,68,68	0
4	IVM	D	348	62/62	0.93	0.35	57,75,99,115	0
4	IVM	D	349	62/62	0.93	0.33	52,68,94,111	0
4	IVM	B	348	62/62	0.94	0.34	47,63,89,106	0
4	IVM	A	348	62/62	0.94	0.32	56,70,97,114	0
4	IVM	B	349	62/62	0.94	0.36	55,70,97,114	0

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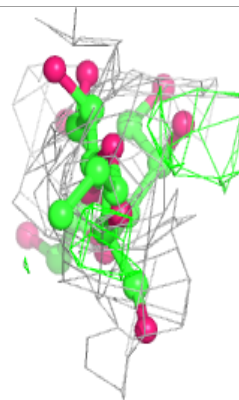
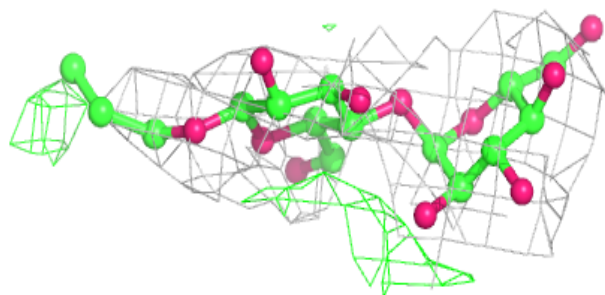
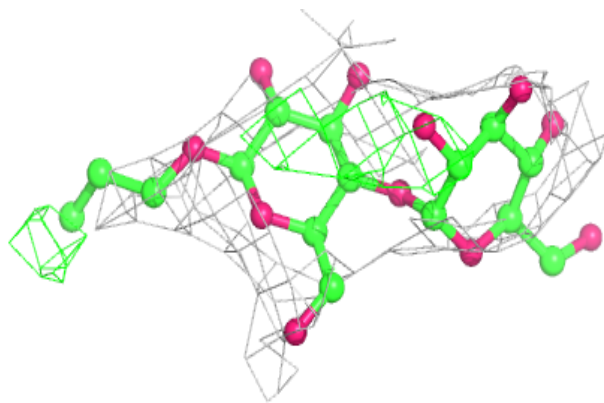
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CL	C	348	1/1	0.95	0.20	83,83,83,83	0

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.

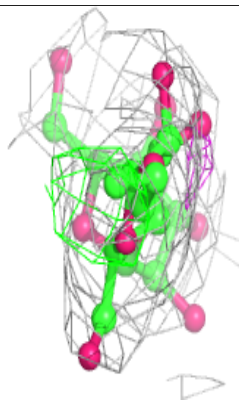
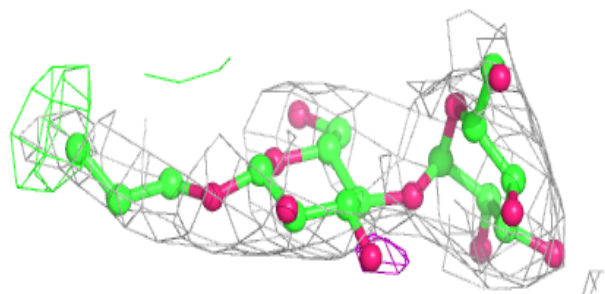
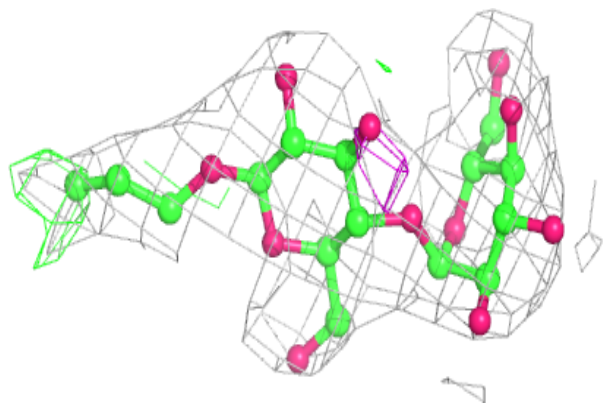


Electron density around LMT B 350:

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

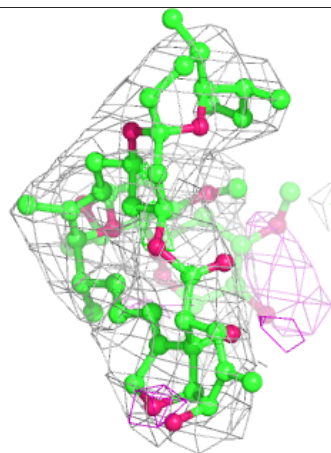
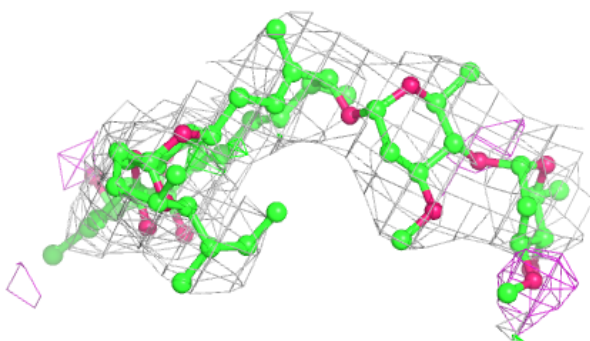
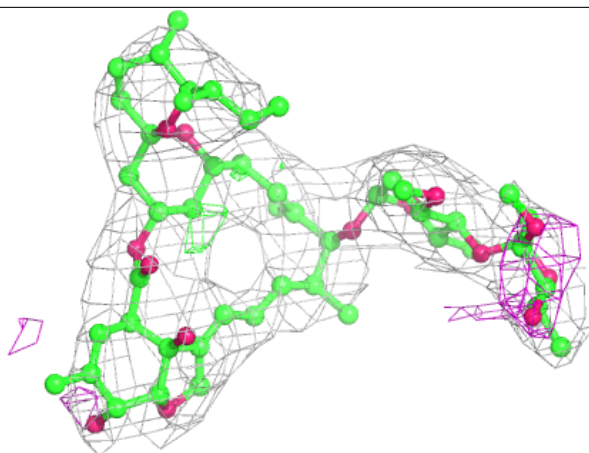
**Electron density around LMT A 349:**

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



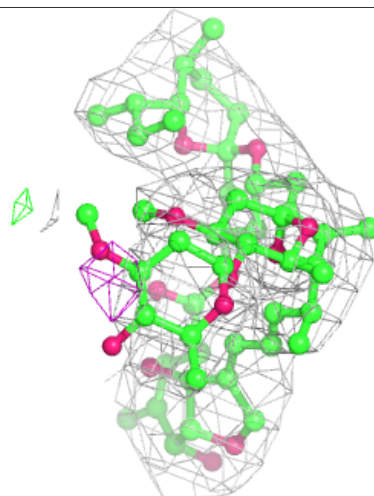
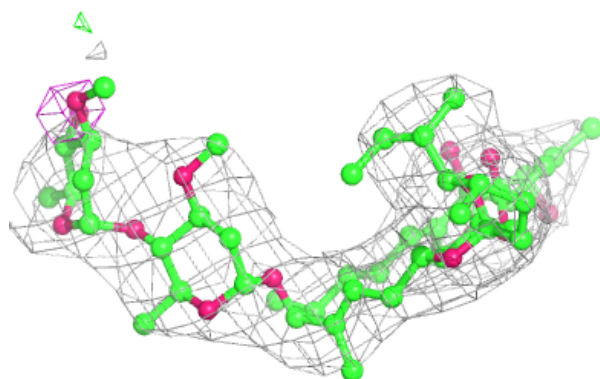
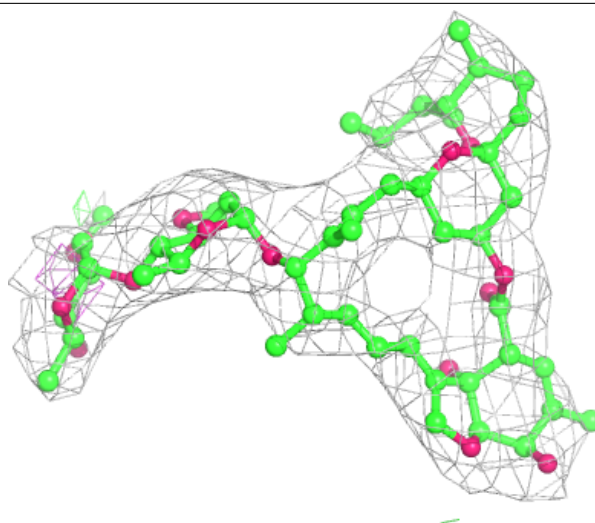
Electron density around IVM D 348:

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



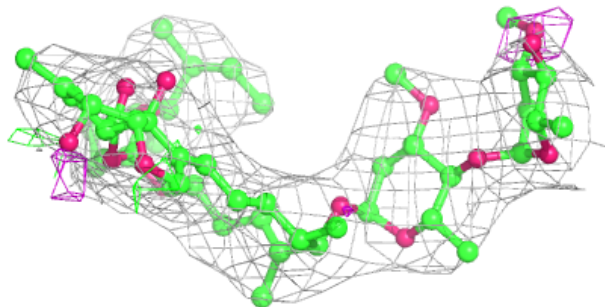
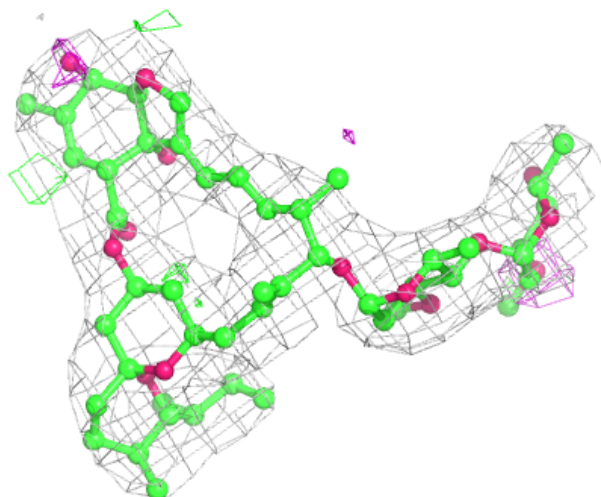
Electron density around IVM D 349:

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



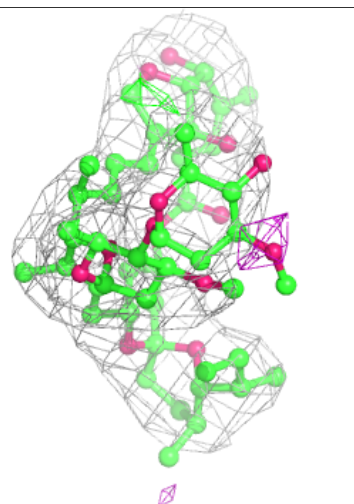
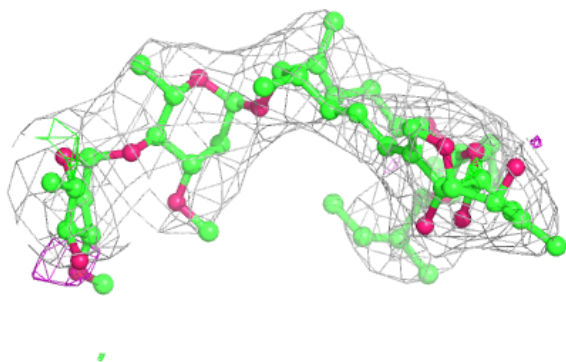
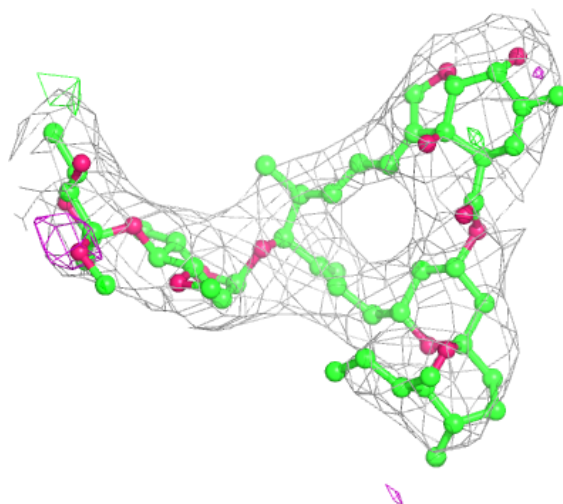
Electron density around IVM B 348:

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



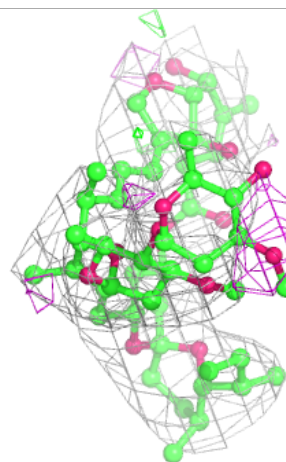
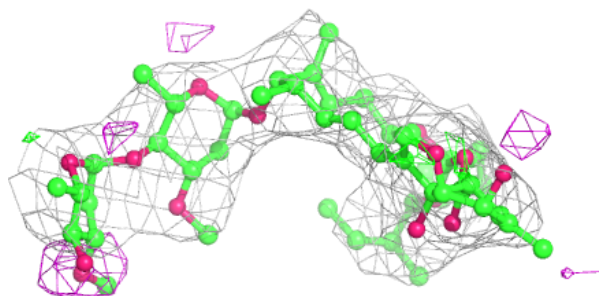
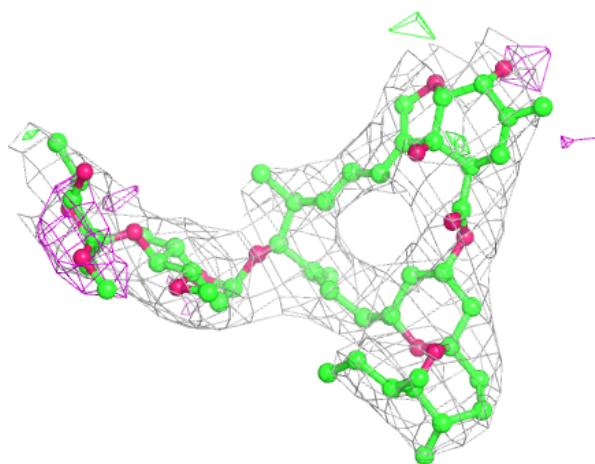
Electron density around IVM A 348:

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



Electron density around IVM B 349:

$2mF_o-DF_c$ (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.