



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:32 AM BST

PDB ID : 3RIF
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab, ivermectin and glutamate.
Authors : Hibbs, R.E.; Gouaux, E.
Deposited on : 2011-04-13
Resolution : 3.35 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

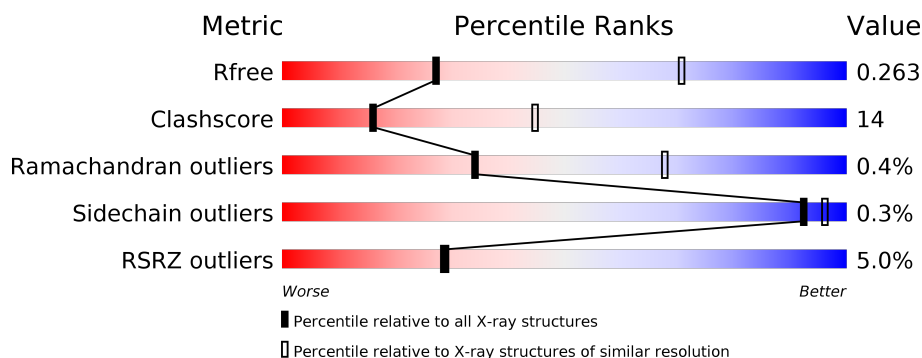
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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>%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div> </div>
1	B	347	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>31%</div> <div>.</div> </div> </div>
1	C	347	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>31%</div> <div>.</div> </div> </div>
1	D	347	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>30%</div> <div>.</div> </div> </div>
1	E	347	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>.</div> </div> </div>
2	F	221	<div> <div>9%</div> <div> <div></div> <div>59%</div> <div>18%</div> <div>23%</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
10	UND	B	406	-	-	-	X
6	LMT	A	405	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29020 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
			2720	1771	442	492	15			
1	B	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	C	339	Total	C	N	O	S	0	0	0
			2710	1765	439	491	15			
1	D	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2720	1771	442	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	171	Total	C	N	O	S	0	0	0
			1324	846	213	259	6			

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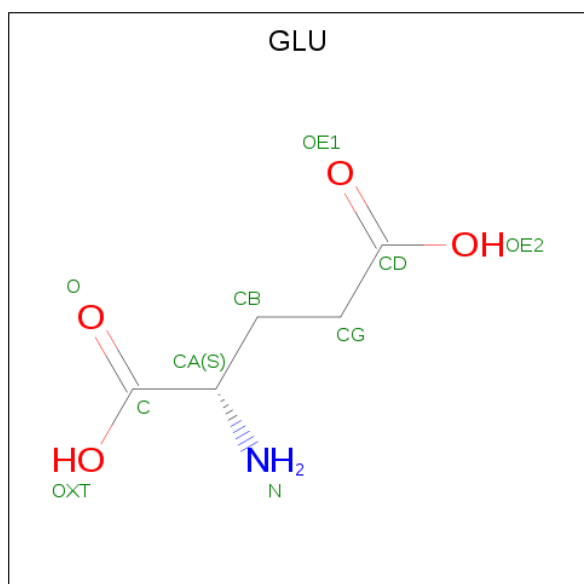
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	214	Total	C	N	O	S	0	0	0
			1631	1038	263	323	7			
2	H	221	Total	C	N	O	S	0	0	0
			1675	1061	271	335	8			
2	I	192	Total	C	N	O	S	0	0	0
			1466	932	238	288	8			
2	J	200	Total	C	N	O	S	0	0	0
			1526	971	247	301	7			

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

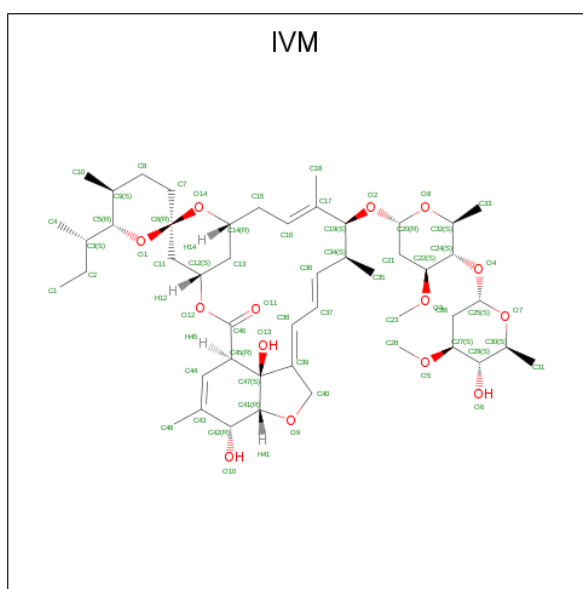
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	210	Total	C	N	O	S	0	0	0
			1579	993	260	320	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1576	991	262	317	6			
3	N	148	Total	C	N	O	S	0	0	0
			1075	678	180	214	3			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	243	294	6			

- Molecule 4 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



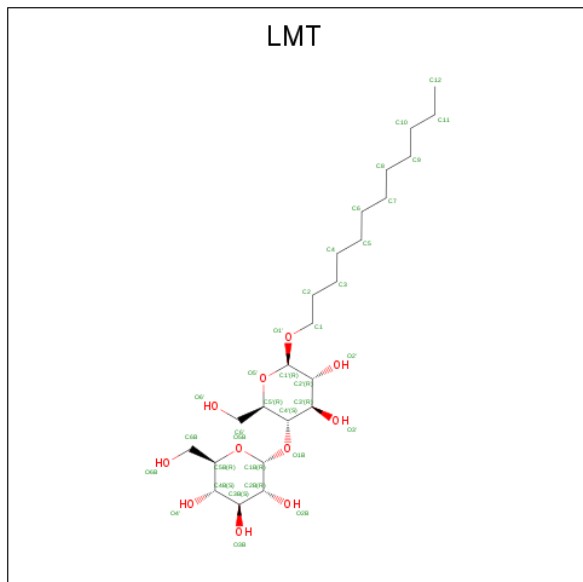
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	1	4		
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	C	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		
4	E	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 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]benzodioxacyclooctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl- α -L-arabino-hexopyranosyl)-3-O-methyl- α -L-arabino-hexopyranoside (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄).



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

- Molecule 6 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

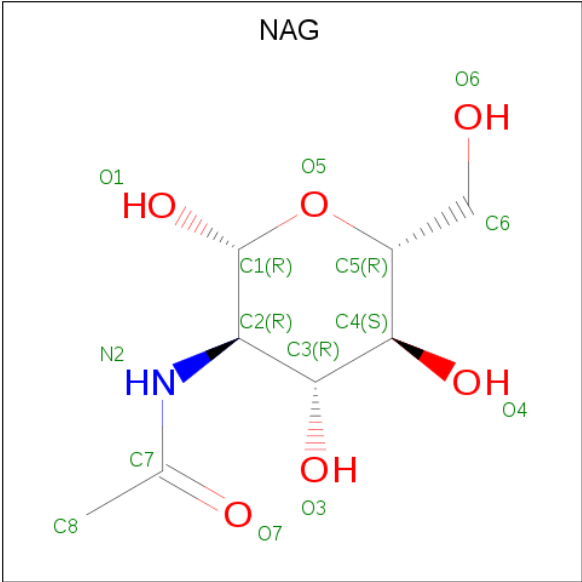


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			26	15	11		
6	A	1	Total	C	O	0	0
			27	16	11		
6	B	1	Total	C	O	0	0
			26	15	11		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

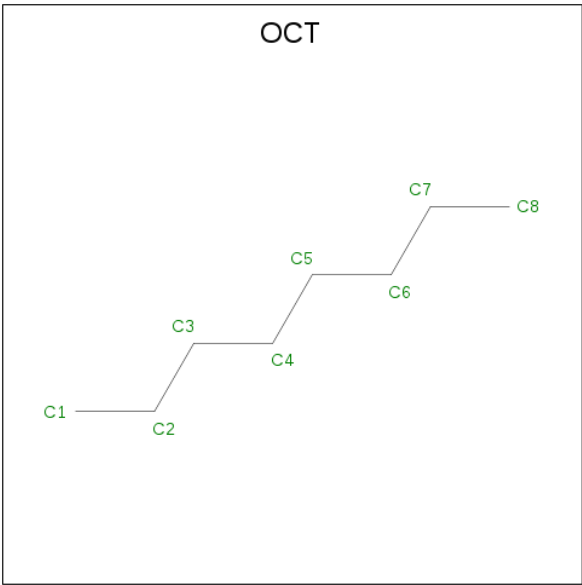
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



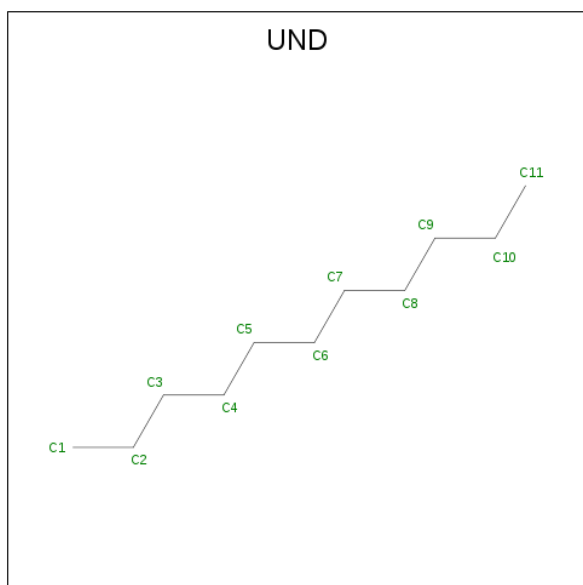
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			8	8		

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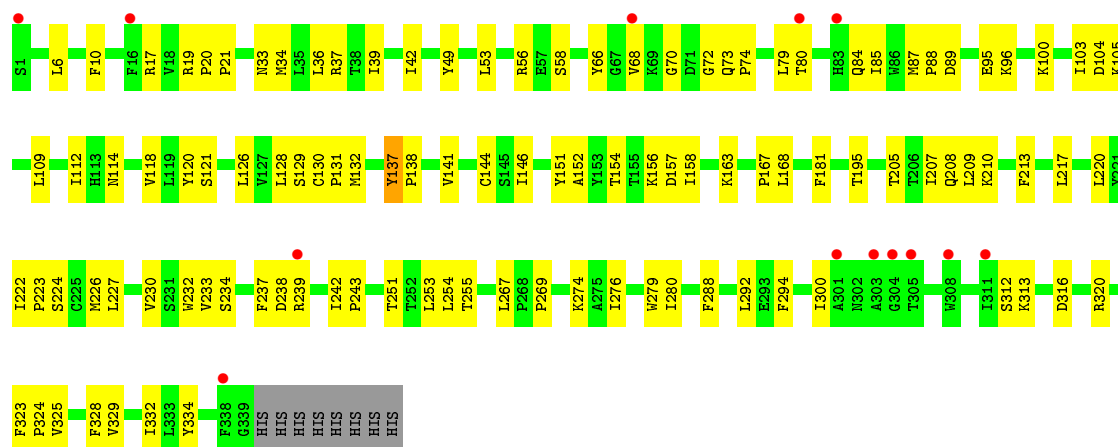
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C 8 8	0	0
9	E	1	Total C 8 8	0	0

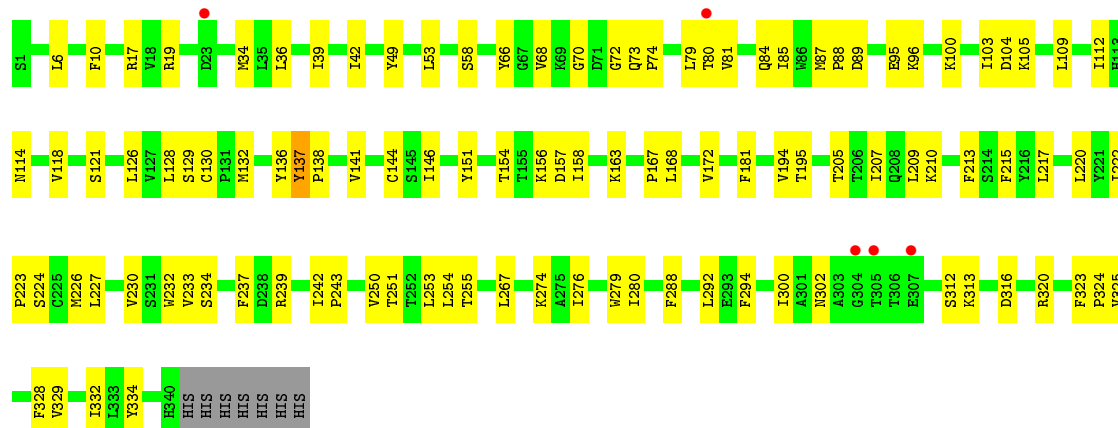
- Molecule 10 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).



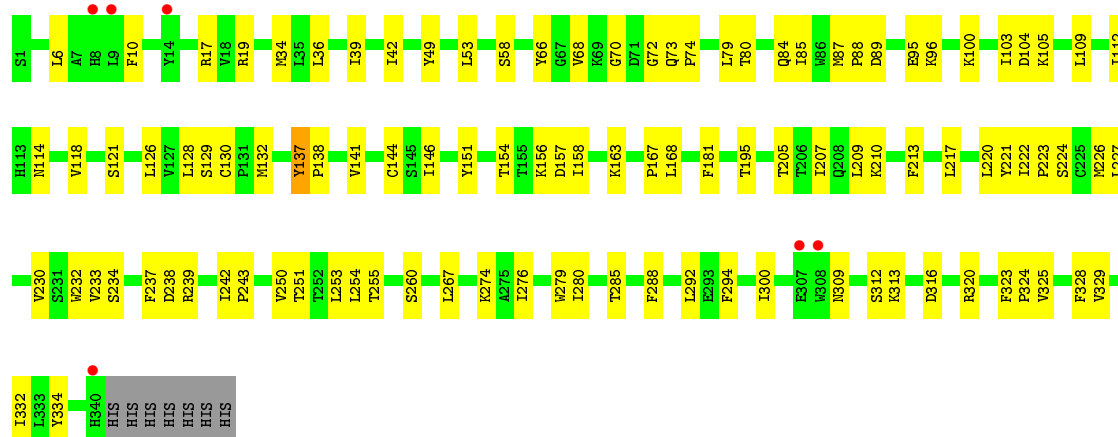
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 11 11	0	0



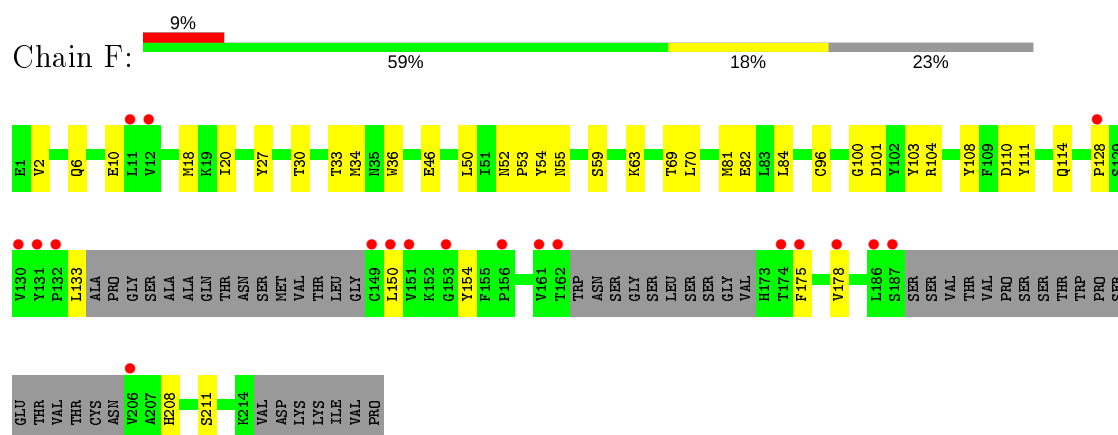
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



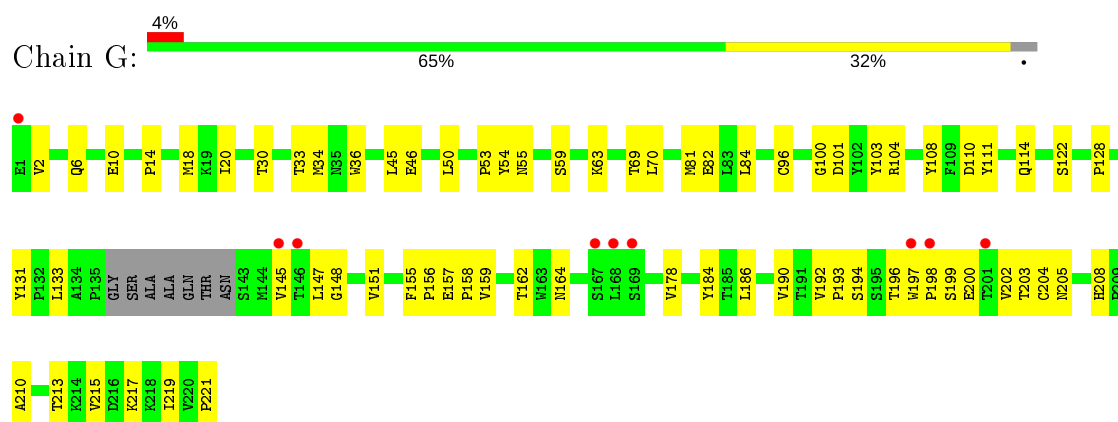
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



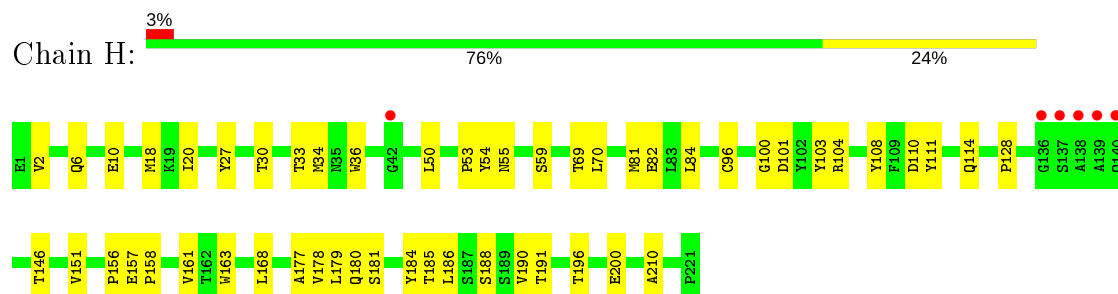
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



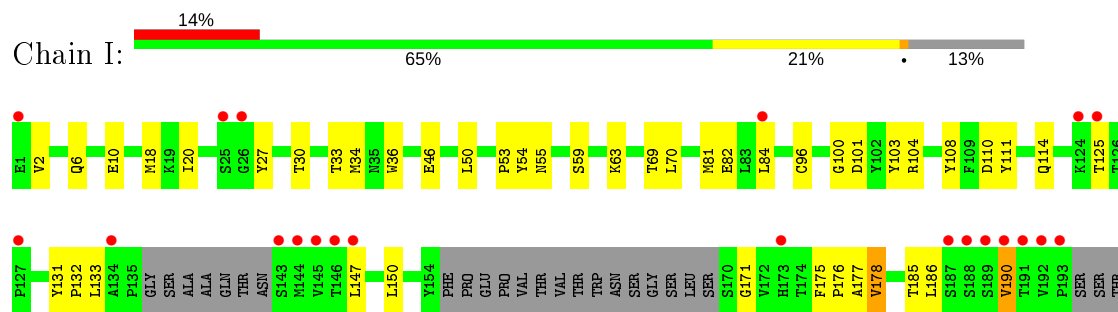
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

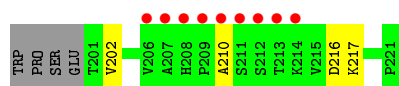


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

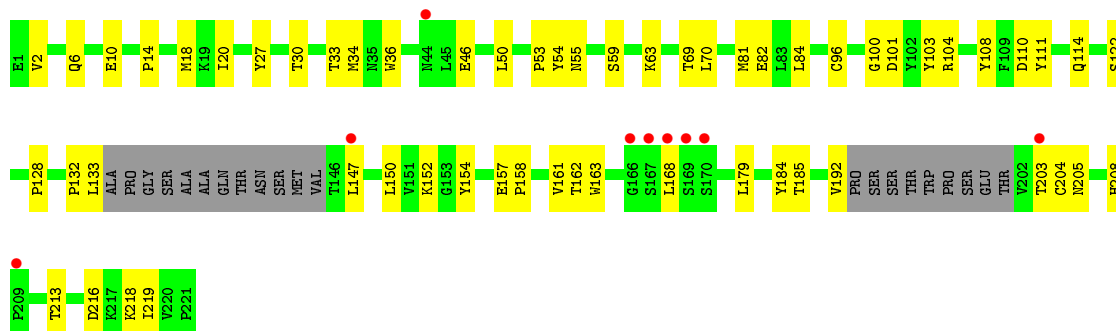


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

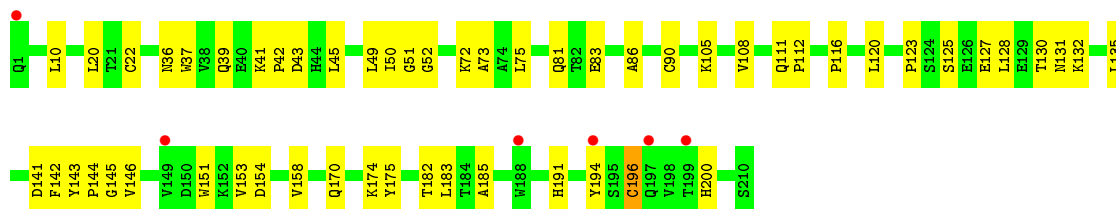
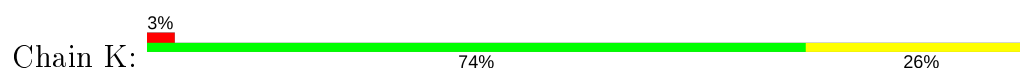




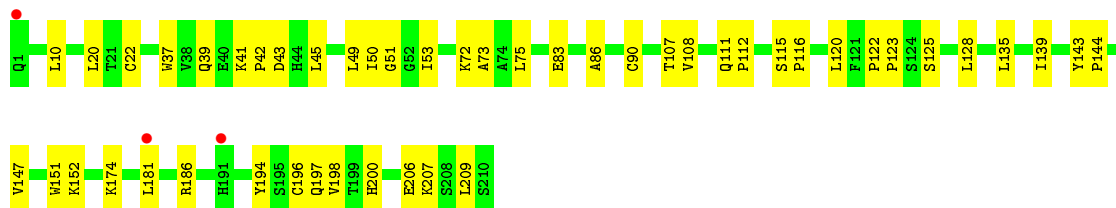
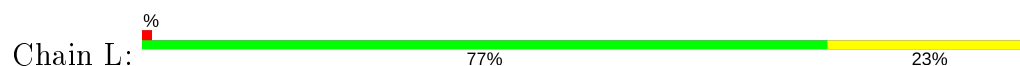
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



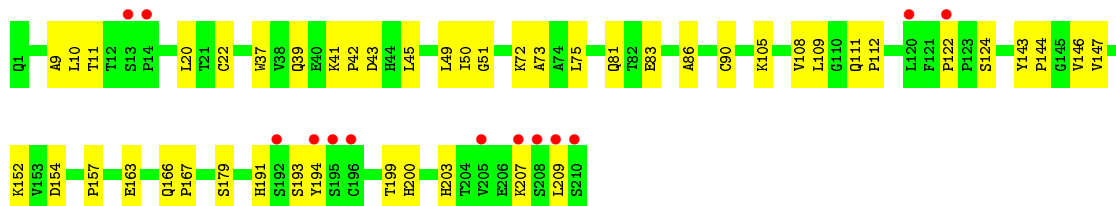
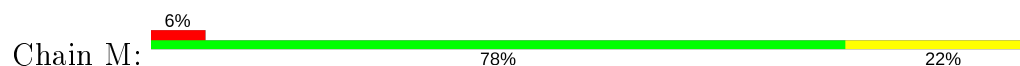
- Molecule 3: Mouse monoclonal Fab fragment, light chain



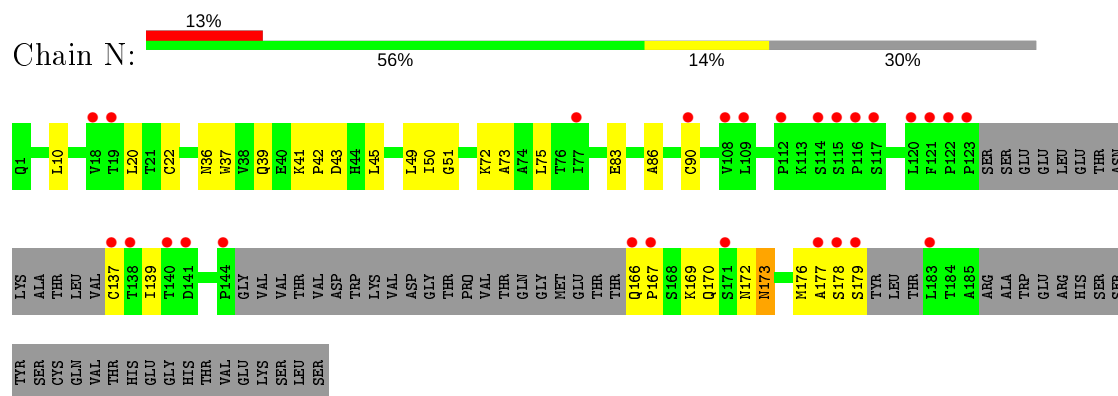
- Molecule 3: Mouse monoclonal Fab fragment, light chain



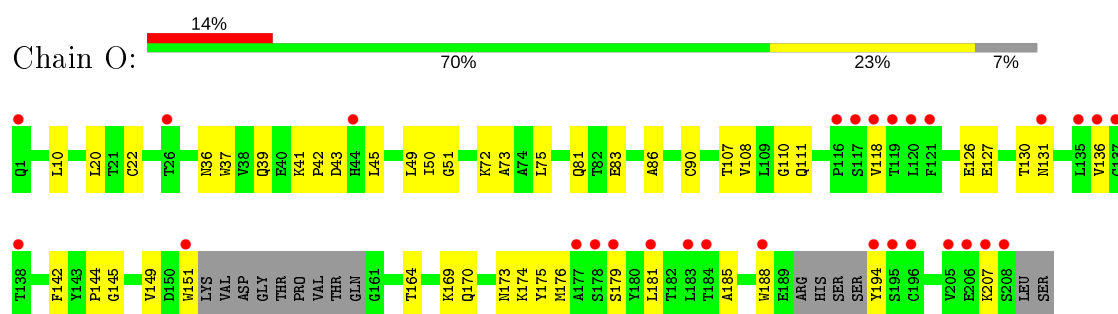
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- 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	155.44Å 155.44Å 575.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 3.35 39.73 – 3.34	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.73-3.35) 99.4 (39.73-3.34)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.248 , 0.271 0.243 , 0.263	Depositor DCC
R_{free} test set	5136 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29020	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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

5.1 Standard geometry

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	0.25	0/2793	0.39	0/3813
1	B	0.25	0/2793	0.39	0/3813
1	C	0.25	0/2782	0.39	0/3798
1	D	0.25	0/2793	0.39	0/3813
1	E	0.26	0/2793	0.39	0/3813
2	F	0.26	0/1359	0.41	0/1849
2	G	0.26	0/1676	0.44	0/2290
2	H	0.25	0/1721	0.42	0/2352
2	I	0.25	0/1501	0.41	0/2040
2	J	0.25	0/1565	0.41	0/2133
3	K	0.26	0/1617	0.43	0/2212
3	L	0.24	0/1629	0.43	0/2226
3	M	0.25	0/1614	0.42	0/2210
3	N	0.27	0/1098	0.42	0/1503
3	O	0.25	0/1504	0.42	0/2056
All	All	0.25	0/29238	0.41	0/39921

There are no bond length outliers.

There are no bond angle outliers.

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	2720	0	2720	105	0
1	B	2720	0	2719	110	0
1	C	2710	0	2712	111	0
1	D	2720	0	2720	105	0
1	E	2720	0	2719	103	0
2	F	1324	0	1265	31	0
2	G	1631	0	1574	58	0
2	H	1675	0	1610	42	0
2	I	1466	0	1428	37	0
2	J	1526	0	1468	41	0
3	K	1579	0	1520	41	0
3	L	1591	0	1542	36	0
3	M	1576	0	1518	33	0
3	N	1075	0	1026	25	0
3	O	1470	0	1412	35	0
4	A	10	0	5	0	0
4	B	10	0	5	2	0
4	C	10	0	5	1	0
4	D	10	0	5	1	0
4	E	10	0	5	1	0
5	A	124	0	148	11	0
5	B	62	0	74	5	0
5	D	62	0	74	3	0
5	E	62	0	74	3	0
6	A	53	0	52	13	0
6	B	26	0	25	7	0
7	B	1	0	0	0	0
8	B	14	0	13	1	0
8	C	14	0	13	1	0
8	E	14	0	13	0	0
9	B	8	0	18	0	0
9	D	8	0	18	0	0
9	E	8	0	18	3	0
10	B	11	0	24	0	0
All	All	29020	0	28542	831	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 14.

All (831) 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:299:HIS:CD2	6:A:404:LMT:H12	1.75	1.21
1:A:299:HIS:HD2	6:A:404:LMT:H12	1.25	0.97
1:B:100:LYS:HE2	1:C:104:ASP:H	1.27	0.96
1:D:89:ASP:HA	1:E:105:LYS:HG3	1.49	0.95
1:C:100:LYS:HE2	1:D:104:ASP:H	1.31	0.93
1:C:17:ARG:HB3	1:D:80:THR:HB	1.50	0.92
1:A:89:ASP:HA	1:B:105:LYS:HG3	1.57	0.87
1:A:104:ASP:H	1:E:100:LYS:HE2	1.39	0.87
3:L:107:THR:HG21	3:L:144:PRO:HB3	1.58	0.86
1:B:17:ARG:HB3	1:C:80:THR:HB	1.58	0.86
1:D:100:LYS:HE2	1:E:104:ASP:H	1.40	0.83
3:K:131:ASN:HA	3:K:185:ALA:HB2	1.61	0.83
1:B:195:THR:HA	2:F:55:ASN:HD21	1.43	0.82
1:A:80:THR:HB	1:E:17:ARG:HB3	1.63	0.81
1:A:105:LYS:HG3	1:E:89:ASP:HA	1.62	0.81
3:K:131:ASN:C	3:K:185:ALA:HB2	2.02	0.80
3:K:131:ASN:CA	3:K:185:ALA:HB2	2.11	0.79
1:B:195:THR:HA	2:F:55:ASN:ND2	1.98	0.78
6:A:404:LMT:H11	6:B:404:LMT:H2'	1.67	0.77
2:G:157:GLU:HB3	2:G:158:PRO:HA	1.67	0.76
1:A:100:LYS:HE2	1:B:104:ASP:H	1.50	0.76
3:L:125:SER:HA	3:L:128:LEU:HD12	1.67	0.76
1:B:100:LYS:HE2	1:C:104:ASP:N	2.00	0.76
2:F:208:HIS:HD2	2:F:211:SER:H	1.34	0.75
1:C:100:LYS:HE2	1:D:104:ASP:N	2.01	0.75
1:E:195:THR:HA	2:J:55:ASN:ND2	2.01	0.74
3:L:152:LYS:HD3	3:L:197:GLN:NE2	2.01	0.74
2:G:164:ASN:HD21	2:G:202:VAL:HG22	1.53	0.74
3:L:206:GLU:O	3:L:207:LYS:HD2	1.86	0.74
1:E:226:MET:HG3	5:E:402:IVM:H11A	1.70	0.74
3:L:139:ILE:HD12	3:L:198:VAL:HG21	1.70	0.74
2:J:128:PRO:HB3	2:J:154:TYR:HB3	1.69	0.73
1:D:226:MET:HG3	5:D:402:IVM:H11A	1.71	0.72
3:O:149:VAL:HB	3:O:164:THR:HG21	1.70	0.72
3:O:118:VAL:O	3:O:207:LYS:HE3	1.89	0.72
1:B:302:ASN:ND2	1:C:238:ASP:HB3	2.05	0.72
6:A:404:LMT:H1'	6:B:404:LMT:O3'	1.89	0.71
1:B:89:ASP:HA	1:C:105:LYS:HG3	1.71	0.71
1:E:195:THR:HA	2:J:55:ASN:HD21	1.54	0.71
2:G:164:ASN:OD1	2:G:202:VAL:HG13	1.89	0.70
3:N:169:LYS:NZ	3:N:169:LYS:HB3	2.07	0.70
3:L:122:PRO:HB3	3:L:209:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ASP:HA	1:D:105:LYS:HG3	1.72	0.70
1:D:17:ARG:HB3	1:E:80:THR:HB	1.73	0.70
1:A:210:LYS:CE	6:A:405:LMT:O3B	2.40	0.69
1:A:195:THR:HA	2:H:55:ASN:ND2	2.08	0.68
1:A:195:THR:HA	2:H:55:ASN:HD21	1.58	0.68
1:D:195:THR:HA	2:I:55:ASN:ND2	2.08	0.68
1:D:195:THR:HA	2:I:55:ASN:HD21	1.58	0.68
1:D:224:SER:HB2	1:D:279:TRP:CH2	2.29	0.68
1:B:224:SER:HB2	1:B:279:TRP:CH2	2.29	0.67
1:B:250:VAL:CG1	1:C:251:THR:HG21	2.24	0.67
1:D:85:ILE:HD11	1:D:112:ILE:HD11	1.76	0.67
1:C:224:SER:HB2	1:C:279:TRP:CH2	2.29	0.67
3:L:120:LEU:HD12	3:L:196:CYS:HB3	1.77	0.67
1:B:151:TYR:O	4:B:401:GLU:HB2	1.93	0.67
1:D:151:TYR:O	4:D:401:GLU:HB2	1.95	0.67
3:O:39:GLN:HB2	3:O:49:LEU:HD21	1.76	0.67
1:E:224:SER:HB2	1:E:279:TRP:CH2	2.30	0.67
3:L:39:GLN:HB2	3:L:49:LEU:HD21	1.77	0.67
5:B:403:IVM:H11A	1:C:226:MET:HG3	1.75	0.66
3:K:39:GLN:HB2	3:K:49:LEU:HD21	1.77	0.66
3:K:132:LYS:NZ	3:K:182:THR:HG23	2.11	0.66
1:A:224:SER:HB2	1:A:279:TRP:CH2	2.30	0.66
3:M:39:GLN:HB2	3:M:49:LEU:HD21	1.76	0.66
1:A:42:ILE:HD13	1:A:209:LEU:HD13	1.76	0.66
1:C:100:LYS:CE	1:D:104:ASP:HA	2.26	0.66
3:N:39:GLN:HB2	3:N:49:LEU:HD21	1.76	0.66
1:D:42:ILE:HD13	1:D:209:LEU:HD13	1.77	0.66
1:D:79:LEU:HD22	1:D:85:ILE:HD12	1.78	0.66
1:D:288:PHE:CE2	1:D:292:LEU:HD11	2.31	0.65
3:N:139:ILE:HB	3:N:177:ALA:HB3	1.77	0.65
1:A:137:TYR:HB3	1:A:138:PRO:HD3	1.77	0.65
1:E:42:ILE:HD13	1:E:209:LEU:HD13	1.77	0.65
1:A:104:ASP:N	1:E:100:LYS:HE2	2.10	0.65
3:L:122:PRO:HB3	3:L:209:LEU:CD1	2.26	0.65
1:A:299:HIS:NE2	6:A:404:LMT:H12	2.09	0.65
1:B:85:ILE:HD11	1:B:112:ILE:HD11	1.78	0.65
1:B:42:ILE:HD13	1:B:209:LEU:HD13	1.78	0.65
1:E:288:PHE:CE2	1:E:292:LEU:HD11	2.32	0.65
3:O:170:GLN:OE1	3:O:176:MET:HB3	1.96	0.65
1:A:85:ILE:HD11	1:A:112:ILE:HD11	1.78	0.65
1:A:288:PHE:CE2	1:A:292:LEU:HD11	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ILE:HD13	1:C:209:LEU:HD13	1.77	0.65
1:D:100:LYS:HE2	1:E:104:ASP:N	2.12	0.65
1:E:85:ILE:HD11	1:E:112:ILE:HD11	1.78	0.65
1:C:85:ILE:HD11	1:C:112:ILE:HD11	1.79	0.64
1:A:210:LYS:NZ	6:A:405:LMT:O3B	2.31	0.64
1:C:288:PHE:CE2	1:C:292:LEU:HD11	2.33	0.64
5:B:403:IVM:H4B	1:C:226:MET:HB2	1.79	0.64
1:C:195:THR:HA	2:G:55:ASN:ND2	2.13	0.64
3:K:170:GLN:HG2	3:K:174:LYS:O	1.99	0.63
1:A:79:LEU:HD22	1:A:85:ILE:HD12	1.81	0.63
1:B:288:PHE:CE2	1:B:292:LEU:HD11	2.33	0.63
2:J:147:LEU:HD22	2:J:219:ILE:HG21	1.79	0.63
6:A:404:LMT:H6'2	6:B:404:LMT:O4'	1.98	0.63
1:E:79:LEU:HD22	1:E:85:ILE:HD12	1.81	0.63
1:C:79:LEU:HD22	1:C:85:ILE:HD12	1.81	0.63
2:H:6:GLN:H	2:H:114:GLN:HE22	1.47	0.63
3:L:135:LEU:HB2	3:L:181:LEU:HB3	1.80	0.62
1:A:226:MET:HB2	5:A:403:IVM:H4B	1.81	0.62
1:B:100:LYS:CE	1:C:104:ASP:HA	2.29	0.62
1:B:79:LEU:HD22	1:B:85:ILE:HD12	1.81	0.62
3:N:167:PRO:HA	3:N:176:MET:O	1.99	0.62
3:K:111:GLN:HG3	3:K:112:PRO:HD2	1.81	0.62
2:G:6:GLN:H	2:G:114:GLN:HE22	1.48	0.62
3:O:41:LYS:HE2	3:O:83:GLU:O	2.00	0.62
1:A:210:LYS:HE2	6:A:405:LMT:O3B	2.00	0.61
6:A:404:LMT:C6'	6:A:404:LMT:H1B	2.29	0.61
1:B:250:VAL:HG13	1:C:251:THR:HG21	1.83	0.61
1:E:137:TYR:HB3	1:E:138:PRO:HD3	1.83	0.61
3:M:41:LYS:HE2	3:M:83:GLU:O	2.01	0.61
3:N:41:LYS:HE2	3:N:83:GLU:O	2.00	0.61
1:D:137:TYR:HB3	1:D:138:PRO:HD3	1.82	0.61
1:A:17:ARG:HB3	1:B:80:THR:HB	1.83	0.60
2:J:6:GLN:H	2:J:114:GLN:HE22	1.48	0.60
1:A:19:ARG:HH11	1:A:157:ASP:HA	1.66	0.60
1:C:137:TYR:HB3	1:C:138:PRO:HD3	1.83	0.60
2:I:6:GLN:H	2:I:114:GLN:HE22	1.49	0.60
3:L:41:LYS:HE2	3:L:83:GLU:O	2.00	0.60
1:D:19:ARG:HH11	1:D:157:ASP:HA	1.66	0.60
2:F:208:HIS:CD2	2:F:211:SER:H	2.16	0.60
2:H:157:GLU:HG3	2:H:184:TYR:CD2	2.37	0.60
3:K:41:LYS:HE2	3:K:83:GLU:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ILE:HD11	1:D:294:PHE:HB3	1.82	0.60
1:A:104:ASP:HA	1:E:100:LYS:CE	2.31	0.60
1:E:19:ARG:HH11	1:E:157:ASP:HA	1.66	0.60
1:B:19:ARG:HH11	1:B:157:ASP:HA	1.67	0.60
1:B:302:ASN:HD22	1:C:238:ASP:HB3	1.65	0.60
1:E:242:ILE:HD11	1:E:294:PHE:HB3	1.83	0.60
2:G:162:THR:OG1	2:G:205:ASN:HB2	2.02	0.60
1:D:87:MET:O	1:E:105:LYS:NZ	2.35	0.59
1:B:137:TYR:HB3	1:B:138:PRO:HD3	1.82	0.59
1:A:242:ILE:HD11	1:A:294:PHE:HB3	1.84	0.59
1:B:88:PRO:HB3	1:B:158:ILE:HD11	1.85	0.59
1:B:17:ARG:HB3	1:C:80:THR:CB	2.31	0.59
1:C:19:ARG:HH11	1:C:157:ASP:HA	1.66	0.59
1:B:242:ILE:HD11	1:B:294:PHE:HB3	1.84	0.59
1:C:17:ARG:HB3	1:D:80:THR:CB	2.28	0.59
1:C:88:PRO:HB3	1:C:158:ILE:HD11	1.85	0.59
2:H:179:LEU:HD13	2:H:184:TYR:CE1	2.36	0.59
1:C:151:TYR:O	4:C:401:GLU:HB2	2.03	0.59
1:D:88:PRO:HB3	1:D:158:ILE:HD11	1.85	0.58
1:C:195:THR:HA	2:G:55:ASN:HD21	1.68	0.58
2:J:203:THR:HA	2:J:218:LYS:HA	1.85	0.58
2:H:156:PRO:HD2	2:H:210:ALA:CB	2.33	0.58
1:A:253:LEU:HD11	1:B:226:MET:CE	2.34	0.58
2:F:6:GLN:H	2:F:114:GLN:HE22	1.50	0.58
1:C:242:ILE:HD11	1:C:294:PHE:HB3	1.85	0.58
3:M:147:VAL:HG12	3:M:200:HIS:HB2	1.84	0.58
1:E:224:SER:HB2	1:E:279:TRP:HH2	1.69	0.58
1:E:234:SER:HA	1:E:237:PHE:HD2	1.69	0.58
1:B:234:SER:HA	1:B:237:PHE:HD2	1.69	0.58
1:D:234:SER:HA	1:D:237:PHE:HD2	1.68	0.58
1:D:36:LEU:HD23	1:D:39:ILE:HD11	1.86	0.58
2:G:131:TYR:CD1	3:K:127:GLU:HB3	2.39	0.58
1:D:224:SER:HB2	1:D:279:TRP:HH2	1.68	0.57
1:B:73:GLN:HB3	1:B:74:PRO:HD2	1.86	0.57
1:A:224:SER:HB2	1:A:279:TRP:HH2	1.69	0.57
1:B:320:ARG:NH1	6:B:404:LMT:H6D	2.19	0.57
1:C:234:SER:HA	1:C:237:PHE:HD2	1.70	0.57
3:K:131:ASN:HA	3:K:185:ALA:CB	2.34	0.57
3:O:169:LYS:HA	3:O:175:TYR:HA	1.86	0.57
1:A:88:PRO:HB3	1:A:158:ILE:HD11	1.86	0.57
1:A:234:SER:HA	1:A:237:PHE:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:PRO:HB3	1:E:158:ILE:HD11	1.85	0.57
3:K:50:ILE:HG22	3:K:51:GLY:H	1.69	0.57
1:B:224:SER:HB2	1:B:279:TRP:HH2	1.68	0.57
1:E:36:LEU:HD23	1:E:39:ILE:HD11	1.87	0.57
3:M:22:CYS:CB	3:M:90:CYS:SG	2.93	0.57
1:B:36:LEU:HD23	1:B:39:ILE:HD11	1.86	0.57
3:M:50:ILE:HG22	3:M:51:GLY:H	1.69	0.57
5:A:403:IVM:C18	9:E:403:OCT:H61	2.35	0.56
2:J:50:LEU:CD2	2:J:59:SER:HB3	2.35	0.56
3:N:50:ILE:HG22	3:N:51:GLY:H	1.70	0.56
3:O:50:ILE:HG22	3:O:51:GLY:H	1.70	0.56
1:A:325:VAL:O	1:A:329:VAL:HG23	2.05	0.56
6:A:404:LMT:H6E	6:A:404:LMT:H1B	1.87	0.56
2:I:50:LEU:CD2	2:I:59:SER:HB3	2.34	0.56
1:C:325:VAL:O	1:C:329:VAL:HG23	2.05	0.56
3:M:199:THR:HG23	3:M:203:HIS:O	2.06	0.56
1:C:73:GLN:HB3	1:C:74:PRO:HD2	1.85	0.56
1:A:36:LEU:HD23	1:A:39:ILE:HD11	1.87	0.56
1:C:36:LEU:HD23	1:C:39:ILE:HD11	1.87	0.56
2:H:50:LEU:CD2	2:H:59:SER:HB3	2.35	0.56
3:K:132:LYS:HZ1	3:K:182:THR:HG23	1.69	0.56
1:C:224:SER:HB2	1:C:279:TRP:HH2	1.68	0.56
2:G:50:LEU:CD2	2:G:59:SER:HB3	2.35	0.56
1:C:120:TYR:OH	1:D:104:ASP:OD1	2.19	0.56
1:E:325:VAL:O	1:E:329:VAL:HG23	2.05	0.56
2:G:197:TRP:HZ2	2:G:219:ILE:O	1.88	0.56
2:G:203:THR:HG23	2:G:217:LYS:C	2.26	0.56
2:J:110:ASP:HB3	2:J:111:TYR:CD2	2.41	0.56
3:L:50:ILE:HG22	3:L:51:GLY:H	1.71	0.56
2:J:132:PRO:O	3:M:124:SER:HB3	2.06	0.56
3:O:151:TRP:CE3	3:O:181:LEU:HD12	2.41	0.56
2:F:50:LEU:CD2	2:F:59:SER:HB3	2.35	0.56
3:L:108:VAL:O	3:L:143:TYR:OH	2.24	0.56
1:B:128:LEU:HD13	1:B:146:ILE:HG12	1.88	0.56
5:A:403:IVM:H18	9:E:403:OCT:H61	1.88	0.56
1:E:73:GLN:HB3	1:E:74:PRO:HD2	1.87	0.56
3:M:37:TRP:CE2	3:M:75:LEU:HB2	2.41	0.56
1:B:325:VAL:O	1:B:329:VAL:HG23	2.07	0.55
1:E:232:TRP:CH2	1:E:324:PRO:HA	2.41	0.55
1:B:232:TRP:CH2	1:B:324:PRO:HA	2.41	0.55
1:A:73:GLN:HB3	1:A:74:PRO:HD2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:VAL:O	1:D:329:VAL:HG23	2.06	0.55
3:K:153:VAL:HG22	3:K:194:TYR:HD2	1.71	0.55
3:L:37:TRP:CE2	3:L:75:LEU:HB2	2.41	0.55
3:N:37:TRP:CE2	3:N:75:LEU:HB2	2.41	0.55
1:C:230:VAL:O	1:C:233:VAL:HG22	2.07	0.55
1:B:194:VAL:HG13	2:F:52:ASN:HD22	1.71	0.55
1:C:232:TRP:CH2	1:C:324:PRO:HA	2.42	0.55
3:L:107:THR:HG21	3:L:144:PRO:CB	2.34	0.55
1:B:100:LYS:HZ1	1:C:104:ASP:HA	1.72	0.55
2:I:147:LEU:HD12	2:I:202:VAL:HG11	1.88	0.55
1:C:239:ARG:CZ	1:C:313:LYS:HG2	2.37	0.55
1:E:230:VAL:O	1:E:233:VAL:HG22	2.07	0.55
2:G:208:HIS:CE1	2:G:210:ALA:HB3	2.41	0.55
2:G:33:THR:HA	2:G:53:PRO:HD3	1.89	0.55
2:H:110:ASP:HB3	2:H:111:TYR:CD2	2.42	0.55
2:J:33:THR:HA	2:J:53:PRO:HD3	1.89	0.55
3:L:152:LYS:HD3	3:L:197:GLN:HE21	1.68	0.55
1:A:100:LYS:HE2	1:B:104:ASP:N	2.19	0.54
1:D:232:TRP:CH2	1:D:324:PRO:HA	2.42	0.54
1:D:73:GLN:HB3	1:D:74:PRO:HD2	1.88	0.54
2:G:110:ASP:HB3	2:G:111:TYR:CD2	2.42	0.54
2:G:192:VAL:HG23	2:G:193:PRO:O	2.05	0.54
1:A:220:LEU:HD11	1:A:280:ILE:HD11	1.89	0.54
6:A:404:LMT:H11	6:B:404:LMT:C2'	2.36	0.54
2:F:110:ASP:HB3	2:F:111:TYR:CD2	2.42	0.54
2:J:128:PRO:HD3	2:J:208:HIS:ND1	2.22	0.54
3:K:37:TRP:CE2	3:K:75:LEU:HB2	2.42	0.54
1:A:232:TRP:CH2	1:A:324:PRO:HA	2.41	0.54
1:A:239:ARG:CZ	1:A:313:LYS:HG2	2.37	0.54
2:I:33:THR:HA	2:I:53:PRO:HD3	1.90	0.54
2:H:33:THR:HA	2:H:53:PRO:HD3	1.90	0.54
2:J:133:LEU:HD21	2:J:150:LEU:HB2	1.90	0.54
1:C:79:LEU:HD13	1:C:112:ILE:HD11	1.90	0.54
1:C:220:LEU:HD11	1:C:280:ILE:HD11	1.90	0.54
2:H:50:LEU:HD21	2:H:59:SER:HB3	1.90	0.54
2:J:14:PRO:HD2	2:J:122:SER:HB3	1.90	0.54
3:O:107:THR:HG21	3:O:144:PRO:HB3	1.90	0.54
1:B:253:LEU:HD11	1:C:226:MET:CE	2.37	0.54
2:F:33:THR:HA	2:F:53:PRO:HD3	1.89	0.54
2:I:110:ASP:HB3	2:I:111:TYR:CD2	2.42	0.54
1:D:220:LEU:HD11	1:D:280:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:PRO:HD2	2:H:210:ALA:HB1	1.90	0.54
2:I:50:LEU:HD21	2:I:59:SER:HB3	1.90	0.54
3:M:122:PRO:HG3	3:M:209:LEU:HD11	1.90	0.54
1:B:239:ARG:CZ	1:B:313:LYS:HG2	2.38	0.54
1:E:128:LEU:HD13	1:E:146:ILE:HG12	1.89	0.54
3:O:37:TRP:CE2	3:O:75:LEU:HB2	2.42	0.54
1:A:230:VAL:O	1:A:233:VAL:HG22	2.08	0.53
1:A:288:PHE:CD2	5:A:402:IVM:H8A	2.42	0.53
1:D:254:LEU:HD12	1:E:251:THR:HG23	1.90	0.53
2:F:175:PHE:CD1	3:N:178:SER:HB3	2.43	0.53
2:G:147:LEU:O	2:G:190:VAL:HG12	2.08	0.53
2:G:213:THR:HG22	2:G:215:VAL:HG23	1.89	0.53
1:B:320:ARG:HH11	6:B:404:LMT:H6D	1.73	0.53
1:D:128:LEU:HD13	1:D:146:ILE:HG12	1.89	0.53
1:B:100:LYS:NZ	1:C:104:ASP:HA	2.23	0.53
2:I:177:ALA:HB2	2:I:186:LEU:HD23	1.90	0.53
1:B:220:LEU:HD11	1:B:280:ILE:HD11	1.90	0.53
1:A:128:LEU:HD13	1:A:146:ILE:HG12	1.89	0.53
1:B:242:ILE:N	1:B:243:PRO:CD	2.72	0.53
1:E:79:LEU:HD13	1:E:112:ILE:HD11	1.91	0.53
1:E:220:LEU:HD11	1:E:280:ILE:HD11	1.90	0.53
2:J:162:THR:OG1	2:J:205:ASN:HB2	2.08	0.53
2:J:69:THR:HB	2:J:82:GLU:HB2	1.90	0.53
1:B:66:TYR:CE2	1:B:114:ASN:HA	2.44	0.53
1:C:128:LEU:HD13	1:C:146:ILE:HG12	1.88	0.53
2:I:69:THR:HB	2:I:82:GLU:HB2	1.91	0.53
1:B:230:VAL:O	1:B:233:VAL:HG22	2.09	0.53
1:B:254:LEU:HD12	1:C:251:THR:HG23	1.91	0.53
1:D:239:ARG:CZ	1:D:313:LYS:HG2	2.39	0.53
1:E:239:ARG:CZ	1:E:313:LYS:HG2	2.38	0.53
1:E:242:ILE:N	1:E:243:PRO:CD	2.72	0.53
2:F:50:LEU:HD21	2:F:59:SER:HB3	1.90	0.53
1:A:79:LEU:HD13	1:A:112:ILE:HD11	1.91	0.53
1:B:126:LEU:HD13	1:B:128:LEU:HD21	1.91	0.53
2:J:179:LEU:HD13	2:J:184:TYR:CE1	2.44	0.53
1:D:230:VAL:O	1:D:233:VAL:HG22	2.09	0.53
1:D:100:LYS:CE	1:E:104:ASP:HA	2.38	0.53
2:H:186:LEU:C	2:H:186:LEU:HD12	2.29	0.53
1:C:87:MET:O	1:D:105:LYS:NZ	2.42	0.52
2:G:50:LEU:HD21	2:G:59:SER:HB3	1.91	0.52
2:G:69:THR:HB	2:G:82:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ILE:N	1:A:243:PRO:CD	2.72	0.52
1:A:100:LYS:CE	1:B:104:ASP:HA	2.39	0.52
1:B:79:LEU:HD13	1:B:112:ILE:HD11	1.91	0.52
1:C:163:LYS:O	1:C:167:PRO:HG3	2.09	0.52
3:M:22:CYS:O	3:M:72:LYS:HB2	2.09	0.52
1:A:163:LYS:O	1:A:167:PRO:HG3	2.10	0.52
1:D:79:LEU:HD13	1:D:112:ILE:HD11	1.92	0.52
2:I:131:TYR:CD2	3:O:127:GLU:HG2	2.45	0.52
1:D:250:VAL:CG1	1:E:251:THR:HG21	2.40	0.52
1:E:163:LYS:O	1:E:167:PRO:HG3	2.09	0.52
2:F:2:VAL:HG21	2:F:111:TYR:CD2	2.45	0.52
3:L:123:PRO:HD3	3:L:135:LEU:HD13	1.90	0.52
1:D:242:ILE:N	1:D:243:PRO:CD	2.73	0.52
2:J:2:VAL:HG21	2:J:111:TYR:CD2	2.45	0.52
1:C:66:TYR:CE2	1:C:114:ASN:HA	2.45	0.52
1:A:80:THR:CB	1:E:17:ARG:HB3	2.38	0.52
2:J:50:LEU:HD21	2:J:59:SER:HB3	1.91	0.52
3:N:172:ASN:O	3:N:173:ASN:HB2	2.10	0.52
1:D:126:LEU:HD13	1:D:128:LEU:HD21	1.92	0.52
2:H:2:VAL:HG21	2:H:111:TYR:CD2	2.45	0.52
1:C:126:LEU:HD13	1:C:128:LEU:HD21	1.92	0.52
1:D:234:SER:HA	1:D:237:PHE:CD2	2.45	0.52
1:A:105:LYS:NZ	1:E:87:MET:O	2.43	0.51
1:A:234:SER:HA	1:A:237:PHE:CD2	2.45	0.51
1:B:234:SER:HA	1:B:237:PHE:CD2	2.45	0.51
1:D:163:LYS:O	1:D:167:PRO:HG3	2.10	0.51
3:K:50:ILE:HG22	3:K:51:GLY:N	2.25	0.51
1:A:66:TYR:CE2	1:A:114:ASN:HA	2.45	0.51
3:L:22:CYS:O	3:L:72:LYS:HB2	2.10	0.51
3:O:42:PRO:O	3:O:43:ASP:HB2	2.10	0.51
2:F:133:LEU:HD11	2:F:150:LEU:HB2	1.93	0.51
2:F:69:THR:HB	2:F:82:GLU:HB2	1.90	0.51
2:I:2:VAL:HG21	2:I:111:TYR:CD2	2.45	0.51
3:O:142:PHE:HE1	3:O:145:GLY:HA2	1.74	0.51
2:H:69:THR:HB	2:H:82:GLU:HB2	1.92	0.51
3:L:111:GLN:HB2	3:L:112:PRO:HD2	1.93	0.51
3:O:22:CYS:O	3:O:72:LYS:HB2	2.11	0.51
1:C:242:ILE:N	1:C:243:PRO:CD	2.73	0.51
1:E:66:TYR:CE2	1:E:114:ASN:HA	2.45	0.51
2:J:168:LEU:HD21	2:J:192:VAL:HG12	1.91	0.51
3:K:22:CYS:O	3:K:72:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:50:ILE:HG22	3:M:51:GLY:N	2.25	0.51
3:N:169:LYS:HZ3	3:N:169:LYS:HB3	1.74	0.51
2:G:203:THR:HG23	2:G:217:LYS:O	2.11	0.51
1:B:163:LYS:O	1:B:167:PRO:HG3	2.11	0.51
1:C:100:LYS:HZ1	1:D:104:ASP:HA	1.75	0.51
1:E:234:SER:HA	1:E:237:PHE:CD2	2.46	0.51
1:D:66:TYR:CE2	1:D:114:ASN:HA	2.45	0.50
1:E:226:MET:HB2	5:E:402:IVM:H4B	1.93	0.50
1:E:126:LEU:HD13	1:E:128:LEU:HD21	1.92	0.50
3:M:111:GLN:HB2	3:M:112:PRO:HD2	1.92	0.50
1:A:104:ASP:HA	1:E:100:LYS:HZ1	1.77	0.50
1:B:96:LYS:HD2	1:B:129:SER:HB3	1.94	0.50
1:E:96:LYS:HD2	1:E:129:SER:HB3	1.94	0.50
5:A:403:IVM:H48B	1:E:260:SER:HB3	1.91	0.50
1:C:96:LYS:HD2	1:C:129:SER:HB3	1.93	0.50
1:C:234:SER:HA	1:C:237:PHE:CD2	2.46	0.50
2:G:196:THR:O	2:G:200:GLU:HB3	2.10	0.50
2:I:30:THR:HA	2:I:53:PRO:HB2	1.94	0.50
3:M:22:CYS:HB2	3:M:90:CYS:SG	2.52	0.50
1:A:126:LEU:HD13	1:A:128:LEU:HD21	1.92	0.50
1:A:39:ILE:HD13	1:A:207:ILE:CD1	2.42	0.50
3:M:42:PRO:O	3:M:43:ASP:HB2	2.12	0.50
2:G:197:TRP:CZ2	2:G:219:ILE:O	2.64	0.50
3:K:42:PRO:O	3:K:43:ASP:HB2	2.11	0.50
3:L:42:PRO:O	3:L:43:ASP:HB2	2.11	0.50
3:M:105:LYS:HD2	3:M:146:VAL:HG22	1.93	0.50
3:O:50:ILE:HG22	3:O:51:GLY:N	2.27	0.50
1:D:224:SER:HB2	1:D:279:TRP:CZ3	2.47	0.50
1:D:96:LYS:HD2	1:D:129:SER:HB3	1.94	0.49
2:G:178:VAL:O	2:G:184:TYR:HA	2.12	0.49
2:G:186:LEU:HD12	2:G:186:LEU:C	2.32	0.49
2:G:203:THR:HG22	2:G:204:CYS:N	2.26	0.49
1:B:128:LEU:CD1	1:B:146:ILE:HG12	2.42	0.49
1:B:39:ILE:HD13	1:B:207:ILE:CD1	2.42	0.49
1:E:39:ILE:HD13	1:E:207:ILE:CD1	2.42	0.49
3:N:22:CYS:O	3:N:72:LYS:HB2	2.11	0.49
2:G:2:VAL:HG21	2:G:111:TYR:CD2	2.47	0.49
3:K:125:SER:HA	3:K:128:LEU:HD12	1.94	0.49
3:L:50:ILE:HG22	3:L:51:GLY:N	2.27	0.49
3:N:50:ILE:HG22	3:N:51:GLY:N	2.26	0.49
1:C:128:LEU:CD1	1:C:146:ILE:HG12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:ARG:HD2	1:D:81:VAL:O	2.11	0.49
2:H:177:ALA:HA	2:H:186:LEU:HB3	1.93	0.49
1:A:130:CYS:O	1:A:132:MET:HG3	2.13	0.49
1:C:39:ILE:HD13	1:C:207:ILE:CD1	2.43	0.49
1:D:253:LEU:HD11	1:E:226:MET:CE	2.43	0.49
1:E:224:SER:HB2	1:E:279:TRP:CZ3	2.48	0.49
2:J:30:THR:HA	2:J:53:PRO:HB2	1.94	0.49
3:N:42:PRO:O	3:N:43:ASP:HB2	2.12	0.49
1:A:84:GLN:HE21	1:A:84:GLN:HA	1.78	0.49
1:A:250:VAL:CG1	1:B:251:THR:HG21	2.42	0.49
1:D:39:ILE:HD13	1:D:207:ILE:CD1	2.43	0.49
2:H:178:VAL:HG22	2:H:185:THR:O	2.12	0.49
2:J:157:GLU:HB3	2:J:158:PRO:HA	1.95	0.49
2:J:161:VAL:HA	2:J:205:ASN:O	2.13	0.49
3:O:169:LYS:CG	3:O:173:ASN:HA	2.42	0.49
3:O:131:ASN:OD1	3:O:185:ALA:HB3	2.12	0.49
1:A:234:SER:HG	1:A:294:PHE:HZ	1.60	0.49
1:A:137:TYR:CE1	1:A:267:LEU:HD21	2.48	0.49
1:A:224:SER:HB2	1:A:279:TRP:CZ3	2.48	0.49
1:B:224:SER:HB2	1:B:279:TRP:CZ3	2.48	0.49
2:F:30:THR:HA	2:F:53:PRO:HB2	1.94	0.49
2:G:157:GLU:HB3	2:G:158:PRO:CA	2.41	0.49
2:G:30:THR:HA	2:G:53:PRO:HB2	1.95	0.49
2:H:36:TRP:CD1	2:H:70:LEU:HD22	2.48	0.49
3:K:120:LEU:HD12	3:K:196:CYS:H	1.77	0.49
1:A:103:ILE:HG23	1:A:103:ILE:O	2.13	0.48
2:I:46:GLU:OE1	2:I:63:LYS:HE2	2.12	0.48
1:A:96:LYS:HD2	1:A:129:SER:HB3	1.95	0.48
1:A:253:LEU:HD11	1:B:226:MET:HE1	1.94	0.48
1:C:100:LYS:NZ	1:D:104:ASP:HA	2.27	0.48
2:F:46:GLU:OE1	2:F:63:LYS:HE2	2.13	0.48
1:B:87:MET:O	1:C:105:LYS:NZ	2.47	0.48
1:C:208:GLN:HB2	8:C:400:NAG:H82	1.95	0.48
1:C:224:SER:HB2	1:C:279:TRP:CZ3	2.48	0.48
1:E:130:CYS:O	1:E:132:MET:HG3	2.13	0.48
2:I:36:TRP:CD1	2:I:70:LEU:HD22	2.49	0.48
3:L:120:LEU:HD23	3:L:120:LEU:C	2.34	0.48
3:M:152:LYS:HG2	3:M:157:PRO:HA	1.95	0.48
2:H:168:LEU:HD23	2:H:190:VAL:HG21	1.94	0.48
3:N:10:LEU:HD12	3:N:20:LEU:CD2	2.44	0.48
1:A:128:LEU:CD1	1:A:146:ILE:HG12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:CYS:O	1:B:132:MET:HG3	2.13	0.48
1:D:84:GLN:HE21	1:D:84:GLN:HA	1.79	0.48
1:E:70:GLY:C	1:E:72:GLY:H	2.17	0.48
2:G:156:PRO:HD2	2:G:210:ALA:CB	2.43	0.48
1:B:187:SER:HB3	8:B:400:NAG:O7	2.13	0.48
1:D:128:LEU:CD1	1:D:146:ILE:HG12	2.44	0.48
1:D:172:VAL:HA	2:G:54:TYR:OH	2.13	0.48
1:E:288:PHE:HE2	1:E:292:LEU:HD11	1.77	0.48
3:O:151:TRP:CD2	3:O:181:LEU:HD12	2.48	0.48
1:B:253:LEU:HD11	1:C:226:MET:HE1	1.95	0.48
1:D:137:TYR:CE1	1:D:267:LEU:HD21	2.49	0.48
1:D:130:CYS:O	1:D:132:MET:HG3	2.13	0.48
2:H:157:GLU:HB3	2:H:158:PRO:HA	1.96	0.48
3:K:10:LEU:HD12	3:K:20:LEU:CD2	2.44	0.48
3:L:10:LEU:HD12	3:L:20:LEU:CD2	2.44	0.48
2:G:133:LEU:HB2	2:G:148:GLY:O	2.14	0.47
2:G:46:GLU:OE1	2:G:63:LYS:HE2	2.14	0.47
2:J:208:HIS:HB3	2:J:213:THR:HB	1.96	0.47
1:A:70:GLY:C	1:A:72:GLY:H	2.17	0.47
1:A:104:ASP:HA	1:E:100:LYS:NZ	2.29	0.47
2:F:84:LEU:N	2:F:84:LEU:HD12	2.30	0.47
2:G:145:VAL:HG13	2:G:192:VAL:HG22	1.96	0.47
2:I:100:GLY:HA3	2:I:108:TYR:CZ	2.49	0.47
2:J:163:TRP:CZ3	2:J:204:CYS:HB3	2.49	0.47
2:J:46:GLU:OE1	2:J:63:LYS:HE2	2.14	0.47
3:L:151:TRP:CZ3	3:L:196:CYS:HB2	2.49	0.47
1:A:226:MET:CE	1:E:253:LEU:HD11	2.44	0.47
2:J:203:THR:CG2	2:J:216:ASP:HB3	2.44	0.47
1:C:137:TYR:CE1	1:C:267:LEU:HD21	2.50	0.47
2:F:36:TRP:CD1	2:F:70:LEU:HD22	2.48	0.47
2:I:6:GLN:N	2:I:114:GLN:HE22	2.12	0.47
2:J:36:TRP:CD1	2:J:70:LEU:HD22	2.50	0.47
3:M:143:TYR:HA	3:M:144:PRO:C	2.35	0.47
1:A:254:LEU:HD12	1:B:251:THR:HG23	1.95	0.47
1:B:70:GLY:C	1:B:72:GLY:H	2.17	0.47
1:B:84:GLN:HA	1:B:84:GLN:HE21	1.80	0.47
1:E:128:LEU:CD1	1:E:146:ILE:HG12	2.44	0.47
2:H:100:GLY:HA3	2:H:108:TYR:CZ	2.50	0.47
2:H:30:THR:HA	2:H:53:PRO:HB2	1.94	0.47
2:H:84:LEU:HD12	2:H:84:LEU:N	2.30	0.47
1:E:84:GLN:HA	1:E:84:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:6:GLN:N	2:G:114:GLN:HE22	2.11	0.47
2:H:6:GLN:N	2:H:114:GLN:HE22	2.11	0.47
3:K:130:THR:HG22	3:K:130:THR:O	2.14	0.47
1:C:253:LEU:HD11	1:D:226:MET:CE	2.45	0.47
2:G:36:TRP:CD1	2:G:70:LEU:HD22	2.49	0.47
2:I:101:ASP:HB3	2:I:104:ARG:HG3	1.97	0.47
2:J:101:ASP:HB3	2:J:104:ARG:HG3	1.96	0.47
2:J:84:LEU:HD12	2:J:84:LEU:N	2.30	0.47
1:C:154:THR:HG23	1:C:156:LYS:H	1.80	0.47
2:H:110:ASP:HB3	2:H:111:TYR:HD2	1.80	0.47
2:J:100:GLY:HA3	2:J:108:TYR:CZ	2.50	0.47
1:A:288:PHE:HE2	1:A:292:LEU:HD11	1.78	0.47
1:B:34:MET:SD	1:B:205:THR:HG21	2.55	0.47
1:B:137:TYR:CE1	1:B:267:LEU:HD21	2.50	0.47
1:E:137:TYR:CE1	1:E:267:LEU:HD21	2.50	0.47
1:C:242:ILE:HG22	1:C:243:PRO:HD3	1.95	0.47
1:C:34:MET:SD	1:C:205:THR:HG21	2.55	0.47
2:G:147:LEU:HD22	2:G:219:ILE:HG21	1.97	0.47
3:M:10:LEU:HD12	3:M:20:LEU:CD2	2.45	0.47
1:C:130:CYS:O	1:C:132:MET:HG3	2.15	0.47
1:C:234:SER:HG	1:C:294:PHE:HZ	1.62	0.47
2:F:6:GLN:N	2:F:114:GLN:HE22	2.13	0.47
3:K:116:PRO:HA	3:K:142:PHE:HB3	1.96	0.47
1:D:288:PHE:HE2	1:D:292:LEU:HD11	1.77	0.46
1:E:103:ILE:HG23	1:E:103:ILE:O	2.15	0.46
1:E:154:THR:HG23	1:E:156:LYS:H	1.80	0.46
1:B:242:ILE:HG22	1:B:243:PRO:HD3	1.98	0.46
1:C:288:PHE:HE2	1:C:292:LEU:HD11	1.79	0.46
1:C:70:GLY:C	1:C:72:GLY:H	2.17	0.46
1:D:103:ILE:HG23	1:D:103:ILE:O	2.15	0.46
2:F:100:GLY:HA3	2:F:108:TYR:CZ	2.49	0.46
2:G:84:LEU:N	2:G:84:LEU:HD12	2.30	0.46
2:H:146:THR:HG22	2:H:191:THR:HB	1.97	0.46
1:B:236:TRP:CH2	6:B:404:LMT:H12	2.50	0.46
1:C:84:GLN:HE21	1:C:84:GLN:HA	1.80	0.46
1:D:70:GLY:C	1:D:72:GLY:H	2.18	0.46
1:E:242:ILE:HG22	1:E:243:PRO:HD3	1.97	0.46
1:A:87:MET:O	1:B:105:LYS:NZ	2.49	0.46
1:C:103:ILE:HG23	1:C:103:ILE:O	2.15	0.46
1:D:141:VAL:HG12	1:D:210:LYS:HA	1.96	0.46
1:D:242:ILE:HG22	1:D:243:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:VAL:HG12	1:E:210:LYS:HA	1.97	0.46
3:M:11:THR:HG23	3:M:109:LEU:HD13	1.98	0.46
1:A:242:ILE:HG22	1:A:243:PRO:HD3	1.98	0.46
1:A:84:GLN:NE2	1:A:84:GLN:HA	2.31	0.46
2:H:101:ASP:HB3	2:H:104:ARG:HG3	1.97	0.46
2:I:216:ASP:O	2:I:217:LYS:HD2	2.15	0.46
1:C:222:ILE:N	1:C:223:PRO:HD2	2.31	0.46
2:F:110:ASP:HB3	2:F:111:TYR:HD2	1.80	0.46
3:K:37:TRP:CZ3	3:K:90:CYS:HB3	2.50	0.46
3:O:37:TRP:CZ3	3:O:90:CYS:HB3	2.51	0.46
1:A:251:THR:HG21	1:E:250:VAL:CG1	2.45	0.46
2:G:100:GLY:HA3	2:G:108:TYR:CZ	2.50	0.46
2:G:110:ASP:HB3	2:G:111:TYR:HD2	1.80	0.46
2:I:84:LEU:N	2:I:84:LEU:HD12	2.31	0.46
2:J:179:LEU:HD13	2:J:184:TYR:CZ	2.50	0.46
3:N:41:LYS:HB2	3:N:45:LEU:HB2	1.98	0.46
1:E:34:MET:SD	1:E:205:THR:HG21	2.56	0.46
3:M:22:CYS:HG	3:M:90:CYS:HG	0.46	0.46
1:C:141:VAL:HG12	1:C:210:LYS:HA	1.97	0.46
2:F:101:ASP:HB3	2:F:104:ARG:HG3	1.97	0.46
2:F:30:THR:HG23	2:F:103:TYR:OH	2.16	0.46
2:J:30:THR:HG23	2:J:103:TYR:OH	2.16	0.46
3:K:41:LYS:HD3	3:K:86:ALA:HB2	1.98	0.46
1:D:328:PHE:CE2	1:D:332:ILE:HD11	2.51	0.46
2:H:30:THR:HG23	2:H:103:TYR:OH	2.16	0.46
2:I:132:PRO:HD3	2:I:217:LYS:HE2	1.98	0.46
3:O:164:THR:HG22	3:O:179:SER:OG	2.15	0.46
1:B:141:VAL:HG12	1:B:210:LYS:HA	1.97	0.45
2:G:101:ASP:HB3	2:G:104:ARG:HG3	1.97	0.45
2:J:30:THR:O	2:J:54:TYR:HB2	2.17	0.45
3:L:37:TRP:CZ3	3:L:90:CYS:HB3	2.51	0.45
3:O:10:LEU:HD12	3:O:20:LEU:CD2	2.45	0.45
1:D:84:GLN:NE2	1:D:84:GLN:HA	2.32	0.45
1:E:323:PHE:HB2	1:E:324:PRO:HD3	1.99	0.45
2:J:6:GLN:N	2:J:114:GLN:HE22	2.12	0.45
3:O:41:LYS:HB2	3:O:45:LEU:HB2	1.98	0.45
1:A:222:ILE:N	1:A:223:PRO:HD2	2.32	0.45
3:M:41:LYS:HB3	3:M:42:PRO:HD2	1.98	0.45
1:A:103:ILE:C	1:A:105:LYS:H	2.20	0.45
1:B:154:THR:HG23	1:B:156:LYS:H	1.81	0.45
1:D:154:THR:HG23	1:D:156:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:196:THR:HB	2:G:200:GLU:OE2	2.16	0.45
3:O:131:ASN:HA	3:O:185:ALA:HB2	1.99	0.45
1:B:288:PHE:CD2	5:B:403:IVM:H8A	2.52	0.45
1:C:323:PHE:HB2	1:C:324:PRO:HD3	1.99	0.45
1:E:36:LEU:HD13	1:E:168:LEU:HD11	1.98	0.45
2:I:110:ASP:HB3	2:I:111:TYR:HD2	1.80	0.45
3:O:41:LYS:HD3	3:O:86:ALA:HB2	1.98	0.45
1:B:36:LEU:HD13	1:B:168:LEU:HD11	1.99	0.45
2:H:20:ILE:HD11	2:H:81:MET:HE1	1.98	0.45
3:K:145:GLY:HA3	3:K:175:TYR:CG	2.51	0.45
3:N:37:TRP:CZ3	3:N:90:CYS:HB3	2.51	0.45
1:B:224:SER:CB	1:B:279:TRP:CZ3	3.00	0.45
1:B:234:SER:HG	1:B:294:PHE:HZ	1.64	0.45
1:B:323:PHE:HB2	1:B:324:PRO:HD3	1.99	0.45
3:K:41:LYS:HB2	3:K:45:LEU:HB2	1.99	0.45
3:M:154:ASP:OD2	3:M:191:HIS:ND1	2.44	0.45
1:B:103:ILE:HG23	1:B:103:ILE:O	2.15	0.45
1:C:254:LEU:HD12	1:D:251:THR:HG23	1.99	0.45
1:D:222:ILE:N	1:D:223:PRO:HD2	2.32	0.45
1:E:316:ASP:O	1:E:320:ARG:HG3	2.17	0.45
2:G:159:VAL:CG2	2:G:186:LEU:HD21	2.47	0.45
2:G:30:THR:HG23	2:G:103:TYR:OH	2.16	0.45
1:A:141:VAL:HG12	1:A:210:LYS:HA	1.98	0.45
1:D:302:ASN:ND2	1:E:238:ASP:HB3	2.32	0.45
1:E:279:TRP:HB2	1:E:334:TYR:CE1	2.52	0.45
2:H:128:PRO:HB3	2:H:151:VAL:HG12	1.99	0.45
2:J:110:ASP:HB3	2:J:111:TYR:HD2	1.79	0.45
3:O:142:PHE:CE1	3:O:145:GLY:HA2	2.51	0.45
1:A:154:THR:HG23	1:A:156:LYS:H	1.80	0.45
1:C:279:TRP:HB2	1:C:334:TYR:CE1	2.52	0.45
1:C:152:ALA:HB1	1:D:109:LEU:HD13	1.99	0.45
1:E:222:ILE:N	1:E:223:PRO:HD2	2.32	0.45
2:G:14:PRO:HD2	2:G:122:SER:HB3	1.99	0.45
3:K:182:THR:O	3:K:183:LEU:HD23	2.17	0.45
3:N:41:LYS:HB3	3:N:42:PRO:HD2	1.99	0.45
3:N:41:LYS:HD3	3:N:86:ALA:HB2	1.98	0.44
3:O:41:LYS:HB3	3:O:42:PRO:HD2	1.99	0.44
1:A:34:MET:CG	1:A:53:LEU:HD12	2.47	0.44
1:C:34:MET:HG3	1:C:53:LEU:HD12	1.99	0.44
1:D:224:SER:CB	1:D:279:TRP:CZ3	3.00	0.44
1:D:36:LEU:HD13	1:D:168:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:LEU:HB3	1:E:121:SER:HB3	1.99	0.44
2:G:30:THR:O	2:G:54:TYR:HB2	2.16	0.44
2:I:20:ILE:HD11	2:I:81:MET:HE1	1.99	0.44
3:M:166:GLN:HG3	3:M:167:PRO:HD2	1.99	0.44
1:B:288:PHE:HE2	1:B:292:LEU:HD11	1.79	0.44
1:C:100:LYS:CE	1:D:104:ASP:CA	2.95	0.44
1:C:17:ARG:CD	1:D:81:VAL:O	2.66	0.44
1:D:34:MET:SD	1:D:205:THR:HG21	2.57	0.44
1:D:323:PHE:HB2	1:D:324:PRO:HD3	1.99	0.44
1:E:213:PHE:CE2	1:E:217:LEU:HB2	2.52	0.44
2:J:20:ILE:HD11	2:J:81:MET:HE1	1.99	0.44
3:M:41:LYS:HD3	3:M:86:ALA:HB2	1.99	0.44
1:B:84:GLN:NE2	1:B:84:GLN:HA	2.33	0.44
1:C:36:LEU:HD13	1:C:168:LEU:HD11	1.98	0.44
1:C:213:PHE:CE2	1:C:217:LEU:HB2	2.52	0.44
1:C:84:GLN:NE2	1:C:84:GLN:HA	2.33	0.44
2:I:30:THR:HG23	2:I:103:TYR:OH	2.16	0.44
3:L:41:LYS:HB3	3:L:42:PRO:HD2	1.99	0.44
1:A:213:PHE:CE2	1:A:217:LEU:HB2	2.53	0.44
1:C:328:PHE:CE2	1:C:332:ILE:HD11	2.53	0.44
2:H:34:MET:CE	2:H:96:CYS:HB2	2.48	0.44
2:I:125:THR:HG21	2:I:210:ALA:O	2.17	0.44
3:K:41:LYS:HB3	3:K:42:PRO:HD2	1.99	0.44
1:A:58:SER:HA	1:A:118:VAL:O	2.17	0.44
1:A:34:MET:SD	1:A:205:THR:HG21	2.57	0.44
1:C:224:SER:CB	1:C:279:TRP:CZ3	3.00	0.44
2:F:128:PRO:HB3	2:F:154:TYR:HB3	2.00	0.44
2:I:30:THR:O	2:I:54:TYR:HB2	2.17	0.44
3:L:111:GLN:HE22	3:L:174:LYS:HG3	1.83	0.44
1:A:224:SER:CB	1:A:279:TRP:CZ3	3.01	0.44
1:C:100:LYS:HE2	1:D:104:ASP:CA	2.48	0.44
1:D:267:LEU:HD13	1:D:274:LYS:HE3	1.99	0.44
1:D:58:SER:HA	1:D:118:VAL:O	2.18	0.44
3:L:115:SER:HB3	3:L:116:PRO:HD2	1.99	0.44
1:B:213:PHE:CE2	1:B:217:LEU:HB2	2.53	0.44
1:B:222:ILE:N	1:B:223:PRO:HD2	2.33	0.44
1:B:279:TRP:HB2	1:B:334:TYR:CE1	2.53	0.44
1:B:39:ILE:HD13	1:B:207:ILE:HD13	2.00	0.44
1:C:58:SER:HA	1:C:118:VAL:O	2.18	0.44
1:E:84:GLN:HA	1:E:84:GLN:NE2	2.32	0.44
1:B:109:LEU:HB3	1:B:121:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ILE:C	1:C:105:LYS:H	2.21	0.44
1:E:151:TYR:O	4:E:401:GLU:HB2	2.17	0.44
3:K:143:TYR:HA	3:K:144:PRO:C	2.38	0.44
3:M:37:TRP:CZ3	3:M:90:CYS:HB3	2.52	0.44
1:A:227:LEU:HD21	1:A:255:THR:CG2	2.48	0.43
1:B:34:MET:HG3	1:B:53:LEU:HD12	2.00	0.43
1:C:34:MET:CG	1:C:53:LEU:HD12	2.47	0.43
1:E:267:LEU:HD13	1:E:274:LYS:HE3	1.99	0.43
3:N:22:CYS:HB3	3:N:73:ALA:HB3	2.00	0.43
1:A:103:ILE:O	1:A:103:ILE:CG2	2.65	0.43
1:A:109:LEU:HB3	1:A:121:SER:HB3	2.00	0.43
1:A:323:PHE:HB2	1:A:324:PRO:HD3	1.99	0.43
1:A:279:TRP:HB2	1:A:334:TYR:CE1	2.52	0.43
1:C:109:LEU:HB3	1:C:121:SER:HB3	2.00	0.43
1:D:279:TRP:HB2	1:D:334:TYR:CE1	2.53	0.43
1:A:34:MET:HG3	1:A:53:LEU:HD12	2.00	0.43
1:E:224:SER:CB	1:E:279:TRP:CZ3	3.01	0.43
1:A:251:THR:HG23	1:E:254:LEU:HD12	2.00	0.43
1:E:58:SER:HA	1:E:118:VAL:O	2.18	0.43
2:F:30:THR:O	2:F:54:TYR:HB2	2.17	0.43
3:N:10:LEU:HD12	3:N:20:LEU:HD23	2.01	0.43
1:A:328:PHE:CE2	1:A:332:ILE:HD11	2.53	0.43
5:A:402:IVM:H14	5:A:402:IVM:H1B	2.00	0.43
5:B:403:IVM:H14	5:B:403:IVM:H1B	2.00	0.43
2:F:20:ILE:HD11	2:F:81:MET:HE1	2.01	0.43
3:L:41:LYS:HD3	3:L:86:ALA:HB2	1.99	0.43
3:M:41:LYS:HB2	3:M:45:LEU:HB2	2.00	0.43
1:B:58:SER:HA	1:B:118:VAL:O	2.18	0.43
1:C:267:LEU:HD13	1:C:274:LYS:HE3	1.99	0.43
1:D:213:PHE:CE2	1:D:217:LEU:HB2	2.53	0.43
5:E:402:IVM:H14	5:E:402:IVM:H1B	2.00	0.43
2:F:10:GLU:HG3	2:F:18:MET:CE	2.49	0.43
2:G:198:PRO:HG3	2:G:221:PRO:HG3	2.00	0.43
1:A:6:LEU:O	1:A:10:PHE:HD2	2.01	0.43
2:I:10:GLU:HG3	2:I:18:MET:CE	2.49	0.43
2:I:34:MET:CE	2:I:96:CYS:HB2	2.49	0.43
3:M:22:CYS:HB3	3:M:73:ALA:HB3	2.01	0.43
1:A:36:LEU:HD13	1:A:168:LEU:HD11	1.99	0.43
1:A:222:ILE:HG23	5:A:403:IVM:H2A	2.00	0.43
1:E:34:MET:CG	1:E:53:LEU:HD12	2.48	0.43
1:E:39:ILE:HD13	1:E:207:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:LEU:O	1:E:10:PHE:HD2	2.02	0.43
2:H:30:THR:O	2:H:54:TYR:HB2	2.18	0.43
3:K:142:PHE:HB2	3:K:200:HIS:CE1	2.54	0.43
3:K:153:VAL:HG22	3:K:194:TYR:CD2	2.54	0.43
1:B:267:LEU:HD13	1:B:274:LYS:HE3	2.01	0.43
1:D:34:MET:CG	1:D:53:LEU:HD12	2.48	0.43
2:G:157:GLU:CB	2:G:158:PRO:HA	2.35	0.43
2:H:180:GLN:O	2:H:181:SER:HB2	2.17	0.43
2:J:2:VAL:HG21	2:J:111:TYR:CE2	2.54	0.43
1:A:39:ILE:HD13	1:A:207:ILE:HD13	2.00	0.43
1:B:34:MET:CG	1:B:53:LEU:HD12	2.48	0.43
1:B:6:LEU:O	1:B:10:PHE:HD2	2.02	0.43
1:D:103:ILE:C	1:D:105:LYS:H	2.21	0.43
1:D:6:LEU:O	1:D:10:PHE:HD2	2.02	0.43
1:D:300:ILE:HG13	1:D:312:SER:HB2	2.01	0.43
3:L:41:LYS:HB2	3:L:45:LEU:HB2	2.00	0.43
2:I:131:TYR:CD1	3:O:126:GLU:HB3	2.54	0.43
1:B:103:ILE:C	1:B:105:LYS:H	2.22	0.43
1:B:227:LEU:HD21	1:B:255:THR:CG2	2.49	0.43
1:C:42:ILE:HD12	1:C:181:PHE:CD2	2.54	0.43
3:L:22:CYS:HB3	3:L:73:ALA:HB3	2.01	0.43
1:A:20:PRO:HA	1:A:21:PRO:HD3	1.86	0.42
1:D:109:LEU:HB3	1:D:121:SER:HB3	2.00	0.42
3:O:188:TRP:HA	3:O:194:TYR:OH	2.19	0.42
5:A:402:IVM:H11A	1:B:226:MET:HG3	2.00	0.42
1:D:276:ILE:O	1:D:280:ILE:HG12	2.19	0.42
2:I:171:GLY:O	2:I:190:VAL:HA	2.19	0.42
3:K:154:ASP:OD2	3:K:191:HIS:ND1	2.50	0.42
3:N:36:ASN:O	3:N:90:CYS:HA	2.19	0.42
3:O:130:THR:HG22	3:O:130:THR:O	2.19	0.42
1:A:267:LEU:HD13	1:A:274:LYS:HE3	2.01	0.42
1:C:227:LEU:HD21	1:C:255:THR:CG2	2.49	0.42
2:G:203:THR:CG2	2:G:204:CYS:N	2.82	0.42
2:J:34:MET:CE	2:J:96:CYS:HB2	2.48	0.42
3:K:22:CYS:HB3	3:K:73:ALA:HB3	2.00	0.42
3:N:166:GLN:HA	3:N:167:PRO:HD3	1.95	0.42
1:B:100:LYS:HE2	1:C:104:ASP:CA	2.49	0.42
1:C:39:ILE:HD13	1:C:207:ILE:HD13	2.00	0.42
1:E:103:ILE:CG2	1:E:103:ILE:O	2.67	0.42
1:E:227:LEU:HD21	1:E:255:THR:CG2	2.50	0.42
1:C:316:ASP:O	1:C:320:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:MET:CE	2:F:96:CYS:HB2	2.49	0.42
2:H:10:GLU:HG3	2:H:18:MET:CE	2.50	0.42
3:O:22:CYS:HB3	3:O:73:ALA:HB3	2.02	0.42
1:A:276:ILE:O	1:A:280:ILE:HG12	2.19	0.42
5:D:402:IVM:H1B	5:D:402:IVM:H14	2.00	0.42
1:D:34:MET:HG3	1:D:53:LEU:HD12	2.01	0.42
1:E:328:PHE:CE2	1:E:332:ILE:HD11	2.55	0.42
2:G:155:PHE:CD2	2:G:156:PRO:HA	2.55	0.42
2:G:156:PRO:HD2	2:G:210:ALA:HB1	2.01	0.42
2:G:20:ILE:HD11	2:G:81:MET:HE1	2.00	0.42
3:K:123:PRO:HD3	3:K:135:LEU:HG	2.02	0.42
3:O:151:TRP:CE2	3:O:181:LEU:HB2	2.54	0.42
1:C:146:ILE:HB	1:C:205:THR:CG2	2.50	0.42
1:D:194:VAL:HG11	2:I:33:THR:HG21	2.00	0.42
2:G:157:GLU:HG3	2:G:184:TYR:CD2	2.55	0.42
2:H:163:TRP:HZ2	2:H:188:SER:O	2.01	0.42
3:N:137:CYS:HB3	3:N:179:SER:HB3	2.00	0.42
1:D:227:LEU:HD21	1:D:255:THR:CG2	2.50	0.42
1:E:146:ILE:HB	1:E:205:THR:CG2	2.50	0.42
1:D:253:LEU:HD11	1:E:226:MET:HE1	2.02	0.42
2:G:155:PHE:CG	2:G:156:PRO:HA	2.55	0.42
2:H:2:VAL:HG21	2:H:111:TYR:CE2	2.55	0.42
2:H:161:VAL:HG11	2:H:188:SER:HB3	2.02	0.42
1:A:42:ILE:CD1	1:A:209:LEU:HD13	2.49	0.42
1:A:227:LEU:HD21	1:A:255:THR:HG22	2.02	0.42
1:D:89:ASP:HA	1:E:105:LYS:CG	2.35	0.42
2:I:2:VAL:HG12	2:I:27:TYR:HB3	2.02	0.42
2:I:2:VAL:HG21	2:I:111:TYR:CE2	2.55	0.42
2:J:10:GLU:HG3	2:J:18:MET:CE	2.50	0.42
1:A:146:ILE:HB	1:A:205:THR:CG2	2.49	0.42
5:A:402:IVM:H4B	1:B:226:MET:HB2	2.01	0.42
1:B:316:ASP:O	1:B:320:ARG:HG3	2.20	0.42
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.85	0.42
1:D:103:ILE:CG2	1:D:103:ILE:O	2.68	0.42
2:F:10:GLU:HG3	2:F:18:MET:HE1	2.02	0.42
2:G:128:PRO:HB2	2:G:151:VAL:HG13	2.01	0.42
2:H:10:GLU:HG3	2:H:18:MET:HE1	2.01	0.42
3:K:146:VAL:O	3:K:146:VAL:HG23	2.20	0.42
3:L:194:TYR:HB2	3:L:209:LEU:HD21	2.02	0.42
3:M:193:SER:O	3:M:194:TYR:CG	2.73	0.42
1:C:49:TYR:CE2	1:C:144:CYS:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:O	1:C:10:PHE:HD2	2.02	0.41
1:D:234:SER:HG	1:D:294:PHE:HZ	1.62	0.41
1:D:39:ILE:HD13	1:D:207:ILE:HD13	2.01	0.41
2:F:2:VAL:HG21	2:F:111:TYR:CE2	2.55	0.41
3:K:105:LYS:HD2	3:K:146:VAL:HG13	2.02	0.41
3:M:10:LEU:HD12	3:M:20:LEU:HD23	2.02	0.41
1:B:273:ILE:HD11	5:B:403:IVM:H30	2.02	0.41
1:C:276:ILE:O	1:C:280:ILE:HG12	2.20	0.41
1:C:269:PRO:HB3	1:D:215:PHE:CG	2.55	0.41
2:G:34:MET:CE	2:G:96:CYS:HB2	2.50	0.41
2:H:157:GLU:HG3	2:H:184:TYR:CE2	2.54	0.41
2:I:150:LEU:HD13	3:O:136:VAL:HG21	2.02	0.41
3:K:151:TRP:HB2	3:K:158:VAL:HB	2.02	0.41
3:L:10:LEU:HD12	3:L:20:LEU:HD23	2.02	0.41
1:A:303:ALA:CB	6:A:404:LMT:H6D	2.50	0.41
1:B:146:ILE:HB	1:B:205:THR:CG2	2.50	0.41
1:B:42:ILE:CD1	1:B:209:LEU:HD13	2.50	0.41
1:B:328:PHE:CE2	1:B:332:ILE:HD11	2.55	0.41
1:D:146:ILE:HB	1:D:205:THR:CG2	2.50	0.41
1:D:42:ILE:HD12	1:D:181:PHE:CD2	2.55	0.41
1:E:103:ILE:C	1:E:105:LYS:H	2.23	0.41
1:A:81:VAL:O	1:E:17:ARG:HD2	2.20	0.41
3:M:81:GLN:O	3:M:108:VAL:HG21	2.20	0.41
1:A:137:TYR:CB	1:A:138:PRO:HD3	2.46	0.41
5:A:403:IVM:H1B	5:A:403:IVM:H14	2.01	0.41
1:B:49:TYR:CE2	1:B:144:CYS:HB3	2.55	0.41
1:C:33:ASN:OD1	1:C:56:ARG:HD2	2.21	0.41
1:D:226:MET:HB2	5:D:402:IVM:H4B	2.01	0.41
1:E:103:ILE:HD12	1:E:103:ILE:HA	1.98	0.41
2:J:2:VAL:HG12	2:J:27:TYR:HB3	2.02	0.41
3:O:81:GLN:O	3:O:108:VAL:HG21	2.21	0.41
1:A:300:ILE:HG13	1:A:312:SER:HB2	2.01	0.41
1:D:316:ASP:O	1:D:320:ARG:HG3	2.20	0.41
1:E:234:SER:HG	1:E:294:PHE:HZ	1.63	0.41
2:J:152:LYS:HA	2:J:185:THR:HG23	2.01	0.41
3:M:207:LYS:HA	3:M:207:LYS:HD3	1.94	0.41
1:A:42:ILE:HD12	1:A:181:PHE:CD2	2.56	0.41
1:B:276:ILE:O	1:B:280:ILE:HG12	2.19	0.41
1:C:103:ILE:CG2	1:C:103:ILE:O	2.68	0.41
1:E:227:LEU:HD12	1:E:227:LEU:HA	1.91	0.41
1:E:309:ASN:O	1:E:312:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:MET:HG3	1:E:53:LEU:HD12	2.01	0.41
2:I:175:PHE:HB3	2:I:176:PRO:HD2	2.03	0.41
3:K:10:LEU:HD12	3:K:20:LEU:HD23	2.01	0.41
3:N:170:GLN:CB	3:N:172:ASN:OD1	2.68	0.41
1:A:49:TYR:CE2	1:A:144:CYS:HB3	2.56	0.41
2:G:147:LEU:HD22	2:G:219:ILE:CG2	2.50	0.41
3:K:36:ASN:O	3:K:90:CYS:HA	2.21	0.41
3:L:186:ARG:H	3:L:186:ARG:HG2	1.74	0.41
1:B:103:ILE:CG2	1:B:103:ILE:O	2.68	0.41
1:A:302:ASN:HD22	1:B:238:ASP:HB3	1.85	0.41
1:D:302:ASN:HD22	1:E:238:ASP:HB3	1.86	0.41
2:F:2:VAL:HG12	2:F:27:TYR:HB3	2.02	0.41
2:H:128:PRO:HB3	2:H:151:VAL:CG1	2.50	0.41
3:L:53:ILE:HD13	3:L:53:ILE:HA	1.93	0.41
3:M:9:ALA:HB2	3:M:146:VAL:HG21	2.03	0.41
3:N:169:LYS:NZ	3:N:169:LYS:CB	2.80	0.41
1:A:302:ASN:ND2	1:B:238:ASP:HB3	2.36	0.41
1:E:49:TYR:CE2	1:E:144:CYS:HB3	2.55	0.41
2:G:10:GLU:HG3	2:G:18:MET:CE	2.50	0.41
2:H:157:GLU:CB	2:H:158:PRO:HA	2.50	0.41
2:I:133:LEU:HD11	2:I:150:LEU:HB2	2.03	0.41
3:M:163:GLU:O	3:M:179:SER:HA	2.20	0.41
1:B:100:LYS:CE	1:C:104:ASP:CA	2.96	0.41
3:O:111:GLN:HE22	3:O:174:LYS:HE3	1.86	0.41
1:B:220:LEU:HD23	1:B:221:TYR:CE2	2.56	0.40
1:B:227:LEU:HD21	1:B:255:THR:HG22	2.03	0.40
1:B:300:ILE:HG13	1:B:312:SER:HB2	2.02	0.40
1:C:130:CYS:HA	1:C:131:PRO:HD2	1.95	0.40
1:E:220:LEU:HD23	1:E:221:TYR:CE2	2.56	0.40
1:B:137:TYR:CB	1:B:138:PRO:HD3	2.51	0.40
1:B:42:ILE:HD12	1:B:181:PHE:CD2	2.56	0.40
1:C:300:ILE:HG13	1:C:312:SER:HB2	2.02	0.40
3:L:147:VAL:HG12	3:L:200:HIS:HB2	2.03	0.40
3:O:36:ASN:O	3:O:90:CYS:HA	2.21	0.40
4:B:401:GLU:OXT	1:C:37:ARG:NH2	2.54	0.40
1:C:73:GLN:CB	1:C:74:PRO:HD2	2.51	0.40
1:D:49:TYR:CE2	1:D:144:CYS:HB3	2.56	0.40
1:E:300:ILE:HG13	1:E:312:SER:HB2	2.02	0.40
1:E:285:THR:HG21	9:E:403:OCT:H21	2.01	0.40
1:E:42:ILE:HD12	1:E:181:PHE:CD2	2.56	0.40
1:E:73:GLN:CB	1:E:74:PRO:HD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:VAL:HG22	2:I:185:THR:O	2.22	0.40
3:K:81:GLN:O	3:K:108:VAL:HG21	2.21	0.40
1:A:226:MET:HG3	5:A:403:IVM:H11A	2.04	0.40
1:D:42:ILE:CD1	1:D:209:LEU:HD13	2.49	0.40
1:D:250:VAL:HG13	1:E:251:THR:HG21	2.02	0.40
1:D:136:TYR:O	1:D:137:TYR:C	2.59	0.40
1:E:276:ILE:O	1:E:280:ILE:HG12	2.20	0.40
2:H:196:THR:O	2:H:200:GLU:HB2	2.21	0.40
2:H:2:VAL:HG12	2:H:27:TYR:HB3	2.02	0.40
2:G:108:TYR:HB3	3:K:52:GLY:N	2.37	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%)	317 (94%)	19 (6%)	2 (1%)	25	60
1	B	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	60
1	C	337/347 (97%)	316 (94%)	19 (6%)	2 (1%)	25	60
1	D	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	60
1	E	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	60
2	F	163/221 (74%)	150 (92%)	12 (7%)	1 (1%)	25	60
2	G	210/221 (95%)	196 (93%)	13 (6%)	1 (0%)	29	63
2	H	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
2	I	184/221 (83%)	172 (94%)	10 (5%)	2 (1%)	14	47
2	J	194/221 (88%)	180 (93%)	14 (7%)	0	100	100
3	K	208/210 (99%)	189 (91%)	19 (9%)	0	100	100
3	L	208/210 (99%)	195 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	208/210 (99%)	194 (93%)	14 (7%)	0	100	100
3	N	140/210 (67%)	128 (91%)	11 (8%)	1 (1%)	22	57
3	O	189/210 (90%)	168 (89%)	20 (11%)	1 (0%)	29	63
All	All	3612/3890 (93%)	3362 (93%)	234 (6%)	16 (0%)	34	68

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	TYR
1	B	137	TYR
1	C	137	TYR
1	D	137	TYR
1	E	137	TYR
2	I	190	VAL
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
2	G	199	SER
3	N	173	ASN
2	I	178	VAL
3	O	110	GLY
2	F	178	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	308/316 (98%)	307 (100%)	1 (0%)	92	96
1	B	308/316 (98%)	307 (100%)	1 (0%)	92	96
1	C	307/316 (97%)	306 (100%)	1 (0%)	92	96
1	D	308/316 (98%)	307 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	308/316 (98%)	307 (100%)	1 (0%)	92	96
2	F	145/190 (76%)	145 (100%)	0	100	100
2	G	184/190 (97%)	182 (99%)	2 (1%)	73	86
2	H	188/190 (99%)	188 (100%)	0	100	100
2	I	164/190 (86%)	164 (100%)	0	100	100
2	J	170/190 (90%)	170 (100%)	0	100	100
3	K	176/178 (99%)	174 (99%)	2 (1%)	73	86
3	L	178/178 (100%)	178 (100%)	0	100	100
3	M	175/178 (98%)	175 (100%)	0	100	100
3	N	115/178 (65%)	115 (100%)	0	100	100
3	O	162/178 (91%)	162 (100%)	0	100	100
All	All	3196/3420 (94%)	3187 (100%)	9 (0%)	92	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	B	95	GLU
1	C	95	GLU
1	D	95	GLU
1	E	95	GLU
2	G	45	LEU
2	G	194	SER
3	K	141	ASP
3	K	196	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	84	GLN
1	A	101	HIS
1	A	169	GLN
1	A	264	ASN
1	B	46	ASN
1	B	84	GLN
1	B	101	HIS

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Mol	Chain	Res	Type
1	B	169	GLN
1	B	264	ASN
1	C	46	ASN
1	C	84	GLN
1	C	101	HIS
1	C	169	GLN
1	C	264	ASN
1	D	46	ASN
1	D	84	GLN
1	D	101	HIS
1	D	169	GLN
1	D	264	ASN
1	E	46	ASN
1	E	84	GLN
1	E	101	HIS
1	E	169	GLN
1	E	264	ASN
2	F	5	GLN
2	F	55	ASN
2	F	62	GLN
2	F	180	GLN
2	F	208	HIS
2	G	5	GLN
2	G	62	GLN
2	H	5	GLN
2	H	62	GLN
2	H	180	GLN
2	I	5	GLN
2	I	55	ASN
2	I	62	GLN
2	I	180	GLN
2	J	5	GLN
2	J	62	GLN
3	L	111	GLN
3	L	197	GLN
3	M	160	GLN
3	N	166	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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$
8	NAG	B	400	1	14,14,15	0.58	0	17,19,21	0.88	1 (5%)
6	LMT	A	405	-	28,28,36	1.43	5 (17%)	39,39,47	1.39	5 (12%)
9	OCT	E	403	-	7,7,7	0.25	0	6,6,6	0.48	0
8	NAG	C	400	1	14,14,15	0.48	0	17,19,21	1.67	2 (11%)
8	NAG	E	400	1	14,14,15	0.46	0	17,19,21	1.20	2 (11%)
6	LMT	A	404	-	27,27,36	1.48	4 (14%)	37,38,47	1.76	11 (29%)
9	OCT	B	405	-	7,7,7	0.25	0	6,6,6	0.42	0
5	IVM	A	403	-	65,68,68	0.81	1 (1%)	82,102,102	1.65	16 (19%)
5	IVM	E	402	-	65,68,68	0.80	1 (1%)	82,102,102	1.65	16 (19%)
5	IVM	D	402	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
10	UND	B	406	-	10,10,10	0.26	0	9,9,9	0.46	0
6	LMT	B	404	-	27,27,36	1.45	4 (14%)	37,38,47	1.45	7 (18%)
5	IVM	A	402	-	65,68,68	0.80	1 (1%)	82,102,102	1.65	16 (19%)
9	OCT	D	403	-	7,7,7	0.25	0	6,6,6	0.42	0
5	IVM	B	403	-	65,68,68	0.80	1 (1%)	82,102,102	1.63	16 (19%)

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
8	NAG	B	400	1	-	0/6/23/26	0/1/1/1
6	LMT	A	405	-	-	5/13/53/61	0/2/2/2
9	OCT	E	403	-	-	0/5/5/5	-
8	NAG	C	400	1	-	0/6/23/26	0/1/1/1
8	NAG	E	400	1	-	4/6/23/26	0/1/1/1
6	LMT	A	404	-	-	9/12/52/61	0/2/2/2
9	OCT	B	405	-	-	0/5/5/5	-
5	IVM	A	403	-	-	6/45/141/141	0/6/7/7
5	IVM	E	402	-	-	6/45/141/141	0/6/7/7
5	IVM	D	402	-	-	7/45/141/141	0/6/7/7
10	UND	B	406	-	-	0/8/8/8	-
6	LMT	B	404	-	-	5/12/52/61	0/2/2/2
5	IVM	A	402	-	-	7/45/141/141	0/6/7/7
9	OCT	D	403	-	-	0/5/5/5	-
5	IVM	B	403	-	-	7/45/141/141	0/6/7/7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	402	IVM	O12-C46	4.84	1.45	1.34
5	B	403	IVM	O12-C46	4.83	1.45	1.34
5	A	402	IVM	O12-C46	4.83	1.45	1.34
5	A	403	IVM	O12-C46	4.81	1.45	1.34
5	D	402	IVM	O12-C46	4.77	1.45	1.34
6	B	404	LMT	C3'-C4'	-3.92	1.41	1.52
6	A	404	LMT	C3'-C4'	-3.89	1.41	1.52
6	A	405	LMT	C3'-C4'	-3.67	1.42	1.52
6	A	405	LMT	C4B-C3B	-3.49	1.43	1.52
6	B	404	LMT	C4B-C3B	-3.49	1.43	1.52
6	A	404	LMT	C4B-C3B	-3.44	1.43	1.52
6	A	405	LMT	C3B-C2B	-2.78	1.45	1.52
6	A	404	LMT	C3B-C2B	-2.52	1.45	1.52
6	B	404	LMT	C3B-C2B	-2.45	1.46	1.52
6	A	404	LMT	O2'-C2'	-2.32	1.37	1.43
6	A	405	LMT	O5'-C5'	2.11	1.49	1.44
6	B	404	LMT	O2'-C2'	-2.10	1.38	1.43
6	A	405	LMT	O2'-C2'	-2.07	1.38	1.43

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	IVM	O12-C46-C45	6.80	120.81	110.97
5	E	402	IVM	O12-C46-C45	6.76	120.75	110.97
5	A	402	IVM	O12-C46-C45	6.68	120.64	110.97
5	B	403	IVM	O12-C46-C45	6.63	120.56	110.97
5	D	402	IVM	O12-C46-C45	6.62	120.56	110.97
8	C	400	NAG	C1-O5-C5	5.60	119.78	112.19
5	E	402	IVM	C13-C14-C15	-4.87	106.68	113.21
5	A	402	IVM	C13-C14-C15	-4.83	106.74	113.21
5	D	402	IVM	C13-C14-C15	-4.81	106.76	113.21
5	B	403	IVM	C13-C14-C15	-4.71	106.89	113.21
5	A	403	IVM	C13-C14-C15	-4.53	107.14	113.21
6	A	404	LMT	C1B-O5B-C5B	-3.99	105.85	113.69
5	D	402	IVM	O9-C40-C39	-3.79	102.24	105.73
5	B	403	IVM	O9-C40-C39	-3.69	102.32	105.73
5	A	403	IVM	O9-C40-C39	-3.67	102.34	105.73
5	A	402	IVM	O9-C40-C39	-3.67	102.35	105.73
6	B	404	LMT	C1-O1'-C1'	3.62	119.84	113.84
5	E	402	IVM	O9-C40-C39	-3.59	102.42	105.73
6	A	405	LMT	C1-O1'-C1'	3.33	119.36	113.84
5	A	403	IVM	C12-O12-C46	-3.16	112.50	117.69
6	A	404	LMT	C1-O1'-C1'	3.14	119.05	113.84
5	E	402	IVM	C12-O12-C46	-3.11	112.60	117.69
5	B	403	IVM	C12-O12-C46	-3.05	112.70	117.69
5	A	402	IVM	C12-O12-C46	-3.00	112.77	117.69
5	D	402	IVM	C12-O12-C46	-2.95	112.86	117.69
6	A	405	LMT	O3'-C3'-C2'	-2.91	103.62	110.35
6	A	404	LMT	O1B-C1B-C2B	2.88	115.56	108.10
6	A	404	LMT	C2'-C3'-C4'	2.85	116.19	109.68
6	B	404	LMT	O3'-C3'-C2'	-2.84	103.79	110.35
5	A	402	IVM	C15-C16-C17	-2.81	120.58	127.56
5	E	402	IVM	O12-C46-O11	-2.81	118.68	123.94
8	E	400	NAG	C1-O5-C5	2.79	115.97	112.19
5	B	403	IVM	C15-C16-C17	-2.78	120.67	127.56
5	E	402	IVM	C15-C16-C17	-2.77	120.68	127.56
5	D	402	IVM	C38-C37-C36	-2.77	117.81	124.53
5	A	403	IVM	C15-C16-C17	-2.77	120.69	127.56
5	A	403	IVM	O11-C46-C45	-2.75	120.33	125.05
5	A	402	IVM	O12-C46-O11	-2.75	118.80	123.94
5	D	402	IVM	C15-C16-C17	-2.75	120.73	127.56
5	A	403	IVM	O12-C46-O11	-2.74	118.81	123.94
5	B	403	IVM	O12-C46-O11	-2.74	118.82	123.94
5	A	403	IVM	C3-C5-C9	-2.72	111.64	116.50
5	D	402	IVM	O12-C46-O11	-2.72	118.86	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	IVM	O14-C14-C15	2.72	108.44	105.82
5	E	402	IVM	C3-C5-C9	-2.69	111.69	116.50
5	A	403	IVM	C38-C37-C36	-2.69	118.00	124.53
6	A	405	LMT	O1'-C1-C2	2.67	118.92	109.56
5	A	402	IVM	C38-C37-C36	-2.65	118.10	124.53
5	E	402	IVM	C38-C37-C36	-2.65	118.11	124.53
5	A	402	IVM	O11-C46-C45	-2.64	120.52	125.05
5	E	402	IVM	O11-C46-C45	-2.64	120.53	125.05
5	D	402	IVM	O11-C46-C45	-2.63	120.54	125.05
5	A	402	IVM	O14-C14-C15	2.61	108.34	105.82
5	B	403	IVM	O11-C46-C45	-2.61	120.58	125.05
5	D	402	IVM	C3-C5-C9	-2.61	111.84	116.50
6	A	404	LMT	O3'-C3'-C2'	-2.61	104.33	110.35
5	B	403	IVM	C3-C5-C9	-2.60	111.85	116.50
8	C	400	NAG	O5-C1-C2	2.60	115.39	111.29
5	A	402	IVM	C34-C19-C17	-2.58	108.74	113.89
5	A	402	IVM	C3-C5-C9	-2.58	111.89	116.50
5	E	402	IVM	O14-C14-C15	2.57	108.30	105.82
5	E	402	IVM	C34-C19-C17	-2.57	108.76	113.89
5	B	403	IVM	C38-C37-C36	-2.57	118.30	124.53
6	B	404	LMT	O1B-C1B-C2B	2.54	114.69	108.10
5	D	402	IVM	C34-C19-C17	-2.54	108.84	113.89
6	A	404	LMT	O1B-C1B-O5B	-2.51	103.66	110.67
5	D	402	IVM	O14-C14-C15	2.50	108.23	105.82
5	A	403	IVM	O14-C14-C15	2.50	108.23	105.82
6	A	404	LMT	C3B-C4B-C5B	2.48	114.67	110.24
5	A	403	IVM	C34-C19-C17	-2.47	108.97	113.89
6	B	404	LMT	C1B-O1B-C4'	-2.45	111.90	117.96
5	B	403	IVM	C34-C19-C17	-2.45	109.01	113.89
5	B	403	IVM	O1-C5-C3	2.44	109.84	106.12
5	A	403	IVM	O1-C5-C3	2.39	109.77	106.12
6	A	405	LMT	C1B-O1B-C4'	-2.33	112.20	117.96
5	A	402	IVM	C18-C17-C19	2.32	119.70	115.68
5	A	403	IVM	C37-C38-C39	-2.31	122.77	130.07
5	E	402	IVM	C37-C38-C39	-2.30	122.78	130.07
5	D	402	IVM	C37-C38-C39	-2.30	122.81	130.07
5	D	402	IVM	O1-C5-C3	2.29	109.62	106.12
5	E	402	IVM	O1-C5-C3	2.29	109.62	106.12
5	D	402	IVM	O14-C14-C13	2.29	113.25	108.94
6	A	404	LMT	O3B-C3B-C4B	-2.28	105.08	110.35
5	B	403	IVM	C37-C38-C39	-2.26	122.93	130.07
8	E	400	NAG	C1-C2-N2	2.25	114.33	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	402	IVM	O1-C5-C3	2.25	109.55	106.12
5	A	402	IVM	O14-C14-C13	2.23	113.13	108.94
5	A	402	IVM	C37-C38-C39	-2.22	123.05	130.07
5	A	403	IVM	C18-C17-C19	2.22	119.51	115.68
5	E	402	IVM	O14-C14-C13	2.20	113.07	108.94
5	A	403	IVM	O14-C14-C13	2.20	113.07	108.94
6	B	404	LMT	O3B-C3B-C4B	-2.20	105.27	110.35
5	B	403	IVM	C18-C17-C19	2.19	119.46	115.68
6	A	405	LMT	O6'-C6'-C5'	2.18	118.78	111.29
5	D	402	IVM	C18-C17-C19	2.17	119.44	115.68
5	B	403	IVM	O14-C14-C13	2.17	113.01	108.94
5	D	402	IVM	C8-C9-C5	2.15	111.66	108.41
5	E	402	IVM	C18-C17-C19	2.15	119.39	115.68
5	B	403	IVM	C8-C9-C5	2.13	111.62	108.41
5	A	402	IVM	C8-C9-C5	2.12	111.61	108.41
6	A	404	LMT	O5B-C5B-C6B	2.11	111.69	106.44
6	B	404	LMT	O6B-C6B-C5B	2.11	118.53	111.29
5	A	403	IVM	C8-C9-C5	2.10	111.58	108.41
8	B	400	NAG	O5-C1-C2	2.08	114.57	111.29
6	B	404	LMT	O6'-C6'-C5'	2.06	118.36	111.29
6	A	404	LMT	O1B-C4'-C3'	-2.05	101.82	107.28
5	E	402	IVM	C8-C9-C5	2.01	111.45	108.41
6	A	404	LMT	O2'-C2'-C3'	-2.00	105.72	110.35

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	405	LMT	C2'-C1'-O1'-C1
6	A	405	LMT	O5'-C1'-O1'-C1
5	A	403	IVM	O7-C25-O4-C24
5	A	403	IVM	C26-C25-O4-C24
5	E	402	IVM	O7-C25-O4-C24
5	E	402	IVM	C26-C25-O4-C24
5	A	402	IVM	O7-C25-O4-C24
5	A	402	IVM	C26-C25-O4-C24
8	E	400	NAG	C8-C7-N2-C2
8	E	400	NAG	O7-C7-N2-C2
5	D	402	IVM	O7-C25-O4-C24
5	D	402	IVM	C26-C25-O4-C24
5	B	403	IVM	O7-C25-O4-C24
5	B	403	IVM	C26-C25-O4-C24

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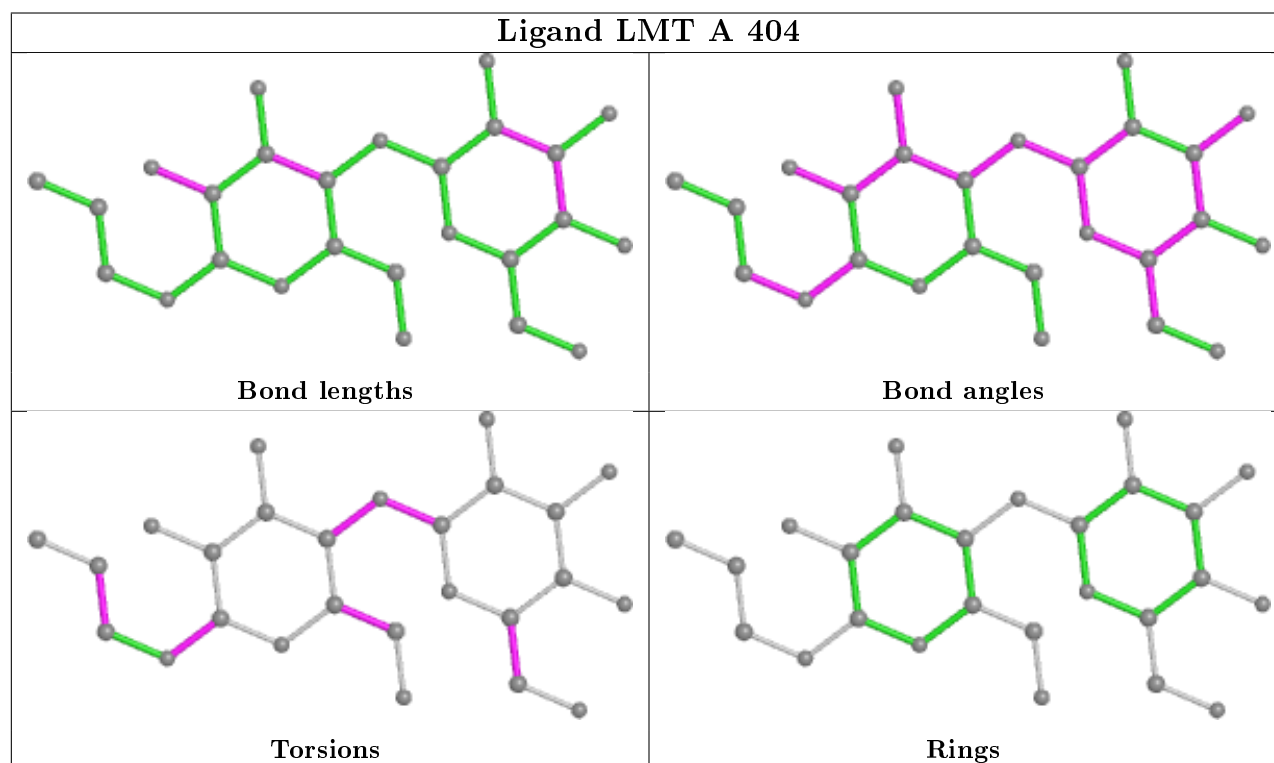
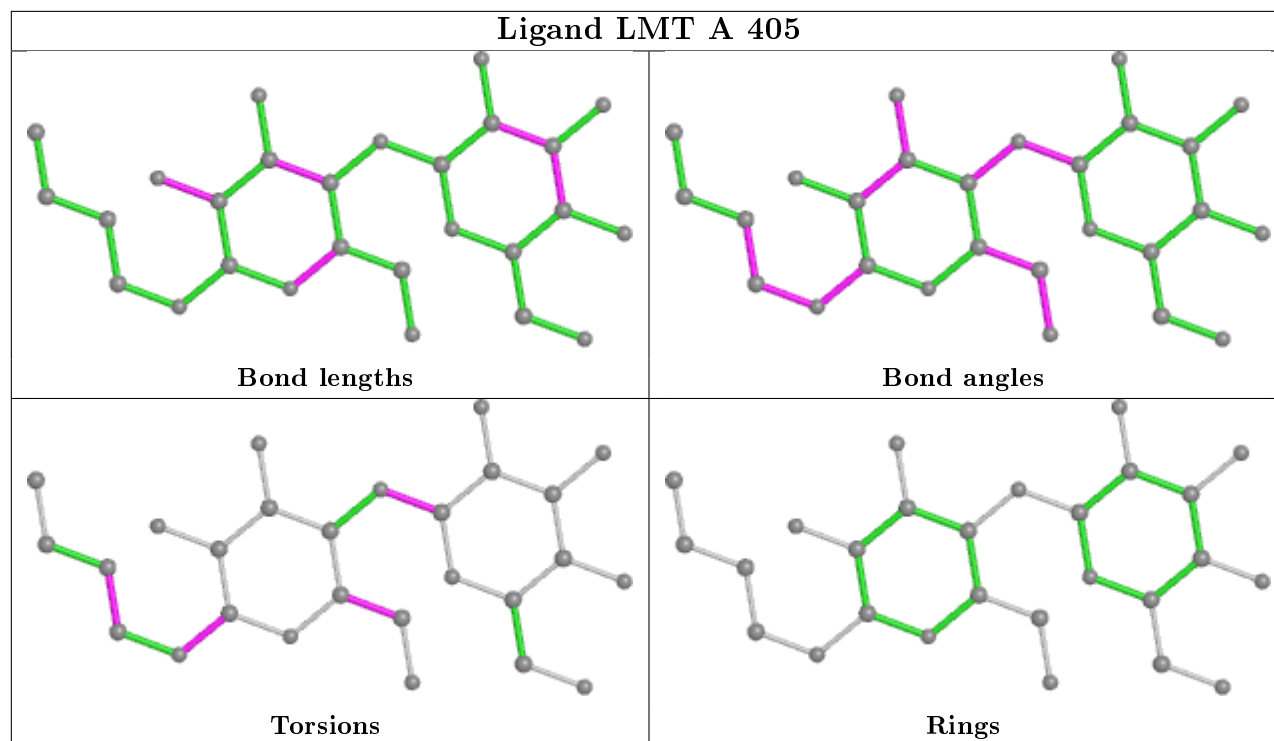
Mol	Chain	Res	Type	Atoms
6	A	404	LMT	O5B-C1B-O1B-C4'
6	A	404	LMT	C2B-C1B-O1B-C4'
6	B	404	LMT	C2B-C1B-O1B-C4'
8	E	400	NAG	C1-C2-N2-C7
6	A	404	LMT	O5'-C5'-C6'-O6'
6	B	404	LMT	O5'-C5'-C6'-O6'
6	B	404	LMT	O5B-C1B-O1B-C4'
6	A	405	LMT	O1'-C1-C2-C3
6	A	405	LMT	O5'-C5'-C6'-O6'
6	A	404	LMT	O5B-C5B-C6B-O6B
6	A	404	LMT	C3'-C4'-O1B-C1B
5	A	403	IVM	C45-C46-O12-C12
5	A	402	IVM	C45-C46-O12-C12
5	D	402	IVM	C45-C46-O12-C12
6	A	404	LMT	C5'-C4'-O1B-C1B
8	E	400	NAG	O5-C5-C6-O6
5	E	402	IVM	C45-C46-O12-C12
5	B	403	IVM	C45-C46-O12-C12
6	B	404	LMT	O5B-C5B-C6B-O6B
6	A	404	LMT	O1'-C1-C2-C3
6	A	404	LMT	C4'-C5'-C6'-O6'
5	A	402	IVM	O11-C46-O12-C12
5	A	403	IVM	O11-C46-O12-C12
6	B	404	LMT	C4'-C5'-C6'-O6'
5	E	402	IVM	O11-C46-O12-C12
5	D	402	IVM	O11-C46-O12-C12
5	B	403	IVM	O11-C46-O12-C12
5	D	402	IVM	C19-C34-C36-C37
5	A	403	IVM	C19-C34-C36-C37
5	E	402	IVM	C19-C34-C36-C37
5	A	402	IVM	C19-C34-C36-C37
5	B	403	IVM	C19-C34-C36-C37
6	A	404	LMT	C2'-C1'-O1'-C1
5	A	403	IVM	C26-C27-O5-C28
5	D	402	IVM	C26-C27-O5-C28
5	A	402	IVM	C26-C27-O5-C28
5	B	403	IVM	C26-C27-O5-C28
5	E	402	IVM	C26-C27-O5-C28
5	A	402	IVM	C14-C15-C16-C17
5	D	402	IVM	C14-C15-C16-C17
5	B	403	IVM	C14-C15-C16-C17
6	A	405	LMT	C2B-C1B-O1B-C4'

There are no ring outliers.

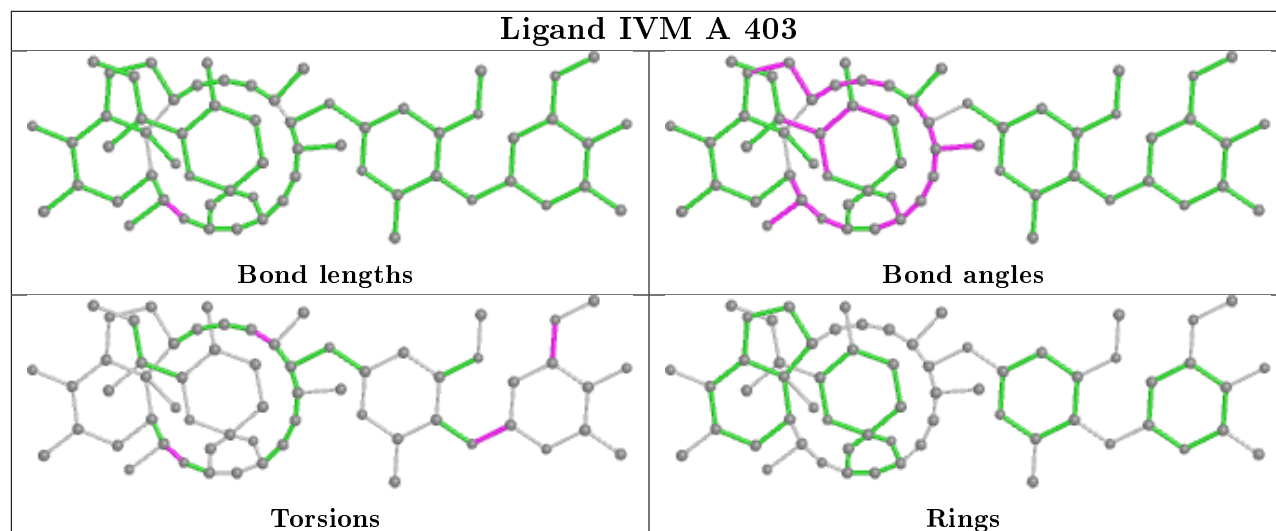
11 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	400	NAG	1	0
6	A	405	LMT	3	0
9	E	403	OCT	3	0
8	C	400	NAG	1	0
6	A	404	LMT	10	0
5	A	403	IVM	7	0
5	E	402	IVM	3	0
5	D	402	IVM	3	0
6	B	404	LMT	7	0
5	A	402	IVM	4	0
5	B	403	IVM	5	0

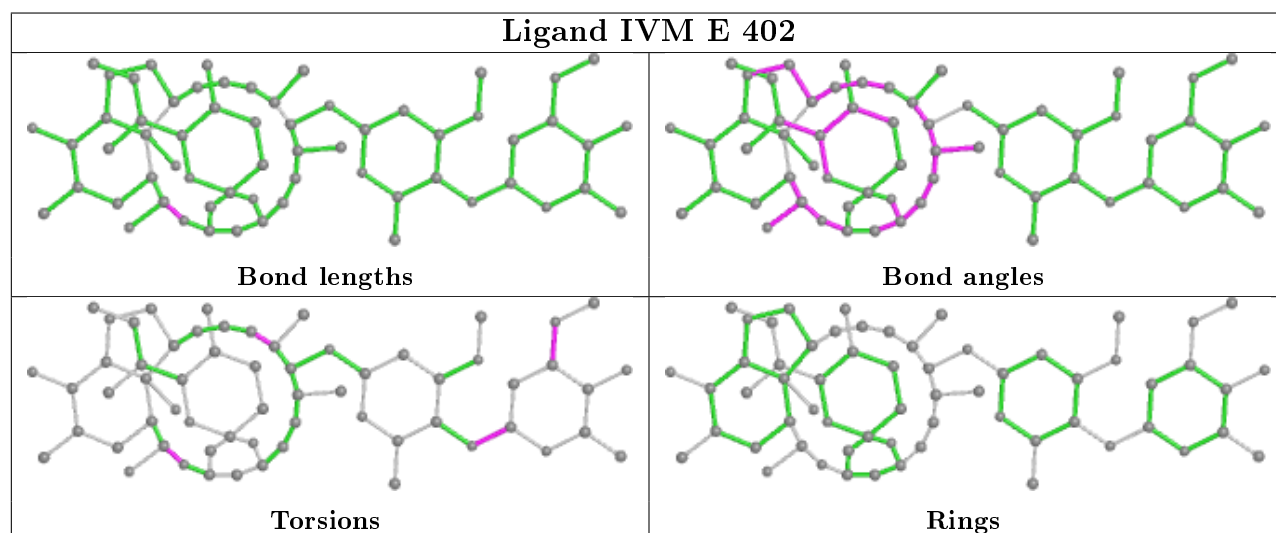
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



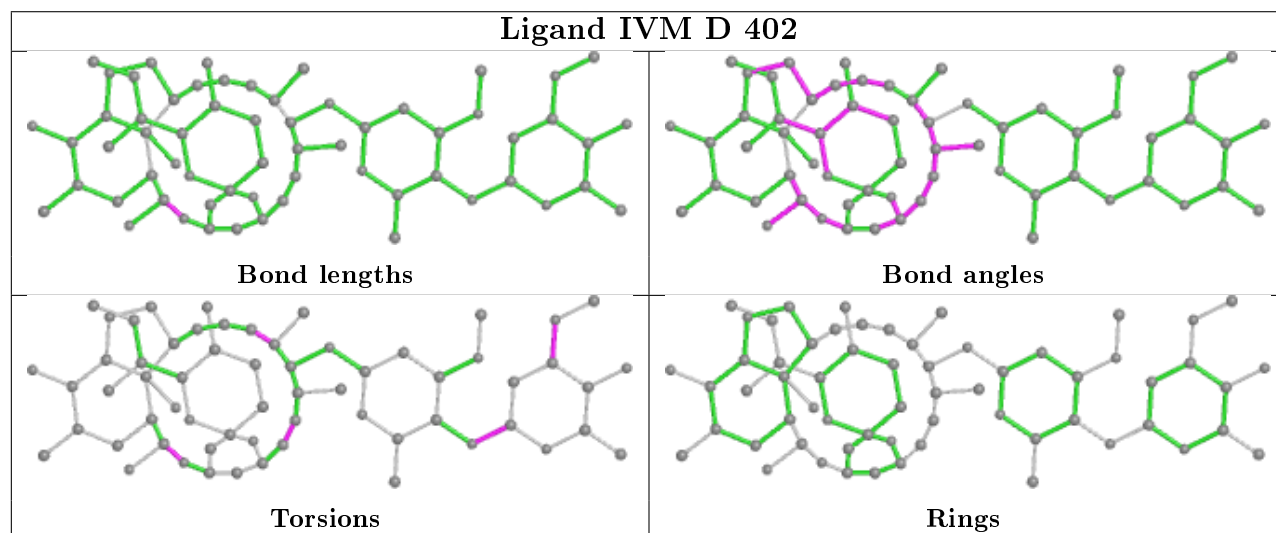
Ligand IVM A 403

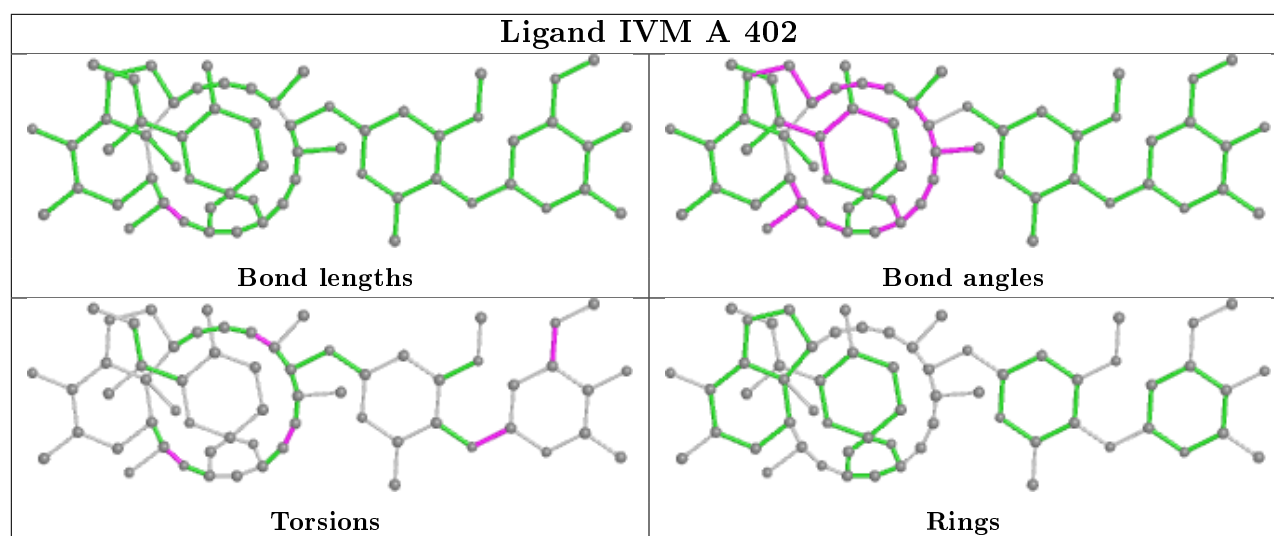
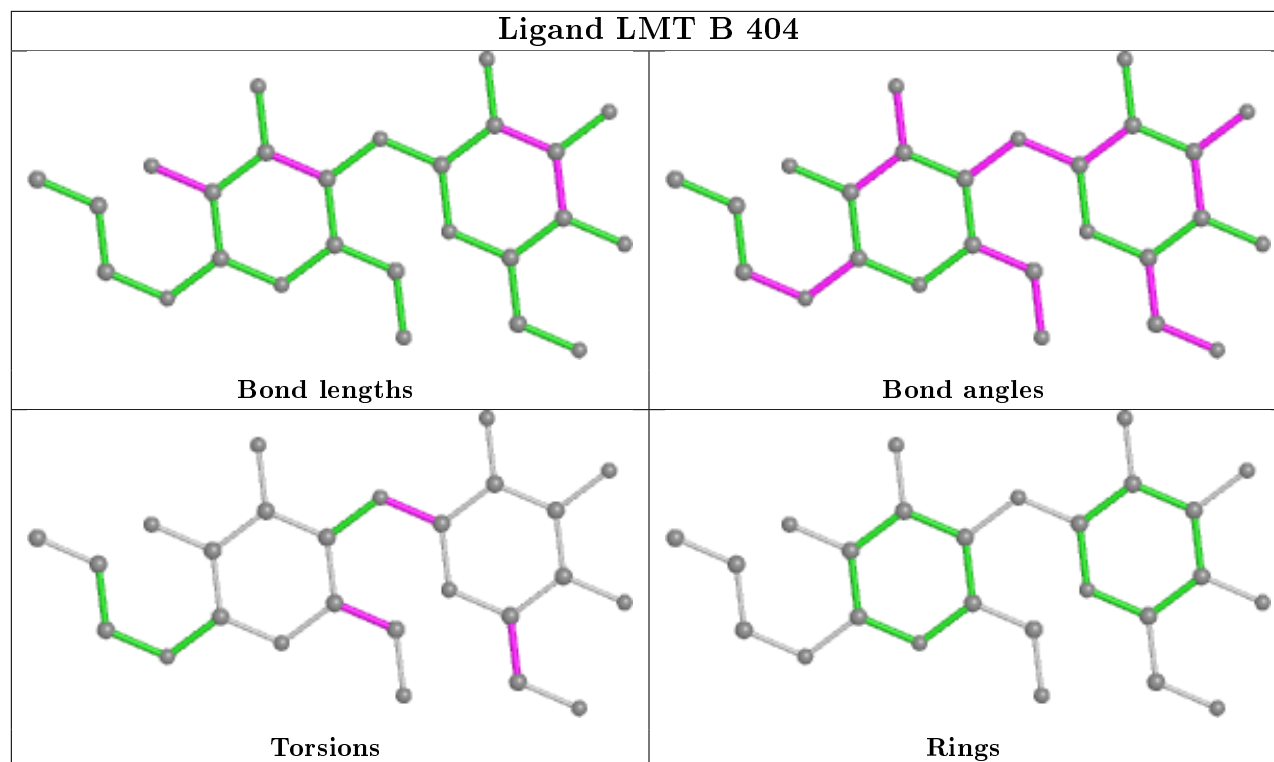


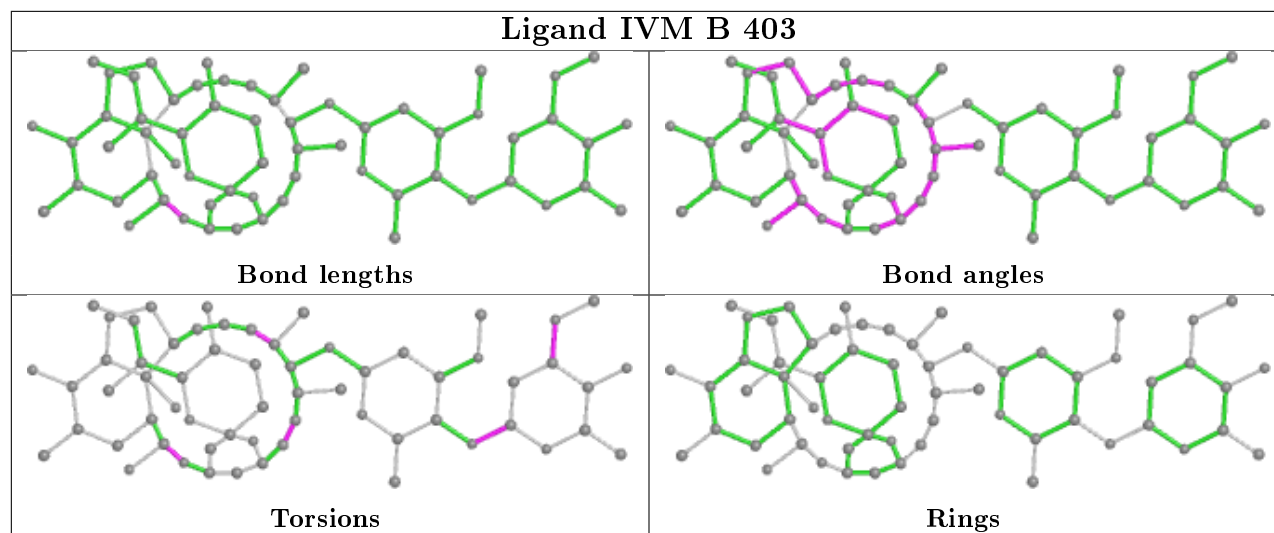
Ligand IVM E 402



Ligand IVM D 402







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%)	0.04	3 (0%) 84 85	32, 66, 123, 196	0
1	B	340/347 (97%)	-0.09	5 (1%) 73 72	38, 68, 125, 199	0
1	C	339/347 (97%)	0.08	13 (3%) 40 39	41, 71, 153, 279	0
1	D	340/347 (97%)	-0.12	5 (1%) 73 72	39, 72, 159, 243	0
1	E	340/347 (97%)	-0.00	6 (1%) 68 67	36, 69, 142, 210	0
2	F	171/221 (77%)	0.56	19 (11%) 5 5	58, 106, 163, 192	0
2	G	214/221 (96%)	0.29	9 (4%) 36 36	40, 89, 142, 182	0
2	H	221/221 (100%)	-0.10	6 (2%) 54 53	42, 76, 131, 201	0
2	I	192/221 (86%)	0.75	30 (15%) 2 1	57, 110, 171, 201	0
2	J	200/221 (90%)	0.09	9 (4%) 33 34	49, 90, 158, 182	0
3	K	210/210 (100%)	0.12	6 (2%) 51 51	50, 95, 139, 209	0
3	L	210/210 (100%)	0.00	3 (1%) 75 75	38, 73, 114, 159	0
3	M	210/210 (100%)	0.18	13 (6%) 20 21	49, 93, 143, 165	0
3	N	148/210 (70%)	0.85	27 (18%) 1 1	58, 119, 178, 202	0
3	O	195/210 (92%)	0.67	29 (14%) 2 2	63, 113, 167, 190	0
All	All	3670/3890 (94%)	0.16	183 (4%) 28 29	32, 82, 155, 279	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	208	SER	8.2
2	I	212	SER	7.3
2	I	188	SER	6.6
2	I	189	SER	6.5
2	I	213	THR	6.4
3	N	109	LEU	6.4
3	O	207	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	304	GLY	5.6
3	O	195	SER	5.5
3	O	1	GLN	5.3
2	F	187	SER	5.3
3	N	178	SER	5.0
1	C	303	ALA	4.9
1	E	340	HIS	4.9
1	C	305	THR	4.9
2	F	132	PRO	4.8
1	A	340	HIS	4.8
2	H	140	GLN	4.6
3	O	120	LEU	4.6
3	N	120	LEU	4.6
3	M	195	SER	4.4
2	I	173	HIS	4.4
3	K	188	TRP	4.4
2	I	146	THR	4.4
1	C	1	SER	4.4
2	H	137	SER	4.4
2	F	178	VAL	4.3
1	C	308	TRP	4.3
2	F	149	CYS	4.3
1	C	83	HIS	4.1
1	C	68	VAL	4.1
2	I	209	PRO	4.1
2	F	150	LEU	4.0
3	O	179	SER	3.9
3	O	183	LEU	3.9
2	I	192	VAL	3.9
2	I	191	THR	3.8
1	D	80	THR	3.8
2	F	161	VAL	3.7
2	G	168	LEU	3.7
2	I	143	SER	3.7
3	N	138	THR	3.7
3	N	123	PRO	3.7
1	C	239	ARG	3.7
1	C	80	THR	3.6
2	F	131	TYR	3.6
3	O	117	SER	3.6
2	G	197	TRP	3.6
3	O	151	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
3	N	116	PRO	3.5
2	I	147	LEU	3.5
3	M	209	LEU	3.5
3	N	171	SER	3.5
3	N	179	SER	3.5
2	I	144	MET	3.4
2	I	214	LYS	3.4
3	N	140	THR	3.4
1	D	304	GLY	3.4
2	G	169	SER	3.4
3	N	19	THR	3.4
3	N	167	PRO	3.4
3	N	115	SER	3.4
3	O	121	PHE	3.3
2	I	125	THR	3.3
2	I	207	ALA	3.3
3	N	177	ALA	3.3
2	F	175	PHE	3.3
3	N	122	PRO	3.2
2	I	145	VAL	3.2
2	I	193	PRO	3.2
3	N	137	CYS	3.2
2	F	206	VAL	3.2
3	O	206	GLU	3.2
2	I	190	VAL	3.1
1	B	308	TRP	3.1
3	O	194	TYR	3.1
3	M	120	LEU	3.1
2	I	124	LYS	3.0
2	I	134	ALA	3.0
3	O	177	ALA	3.0
2	H	42	GLY	3.0
3	N	108	VAL	3.0
3	O	135	LEU	3.0
1	A	339	GLY	3.0
2	F	151	VAL	2.9
2	H	136	GLY	2.9
2	J	167	SER	2.9
3	L	1	GLN	2.9
2	F	12	VAL	2.9
3	N	90	CYS	2.9
2	F	174	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	O	119	THR	2.9
1	E	14	TYR	2.9
2	I	25	SER	2.8
2	G	201	THR	2.8
2	I	187	SER	2.8
2	I	206	VAL	2.8
2	J	170	SER	2.8
1	C	338	PHE	2.8
3	O	196	CYS	2.7
1	E	307	GLU	2.7
2	G	167	SER	2.7
2	J	168	LEU	2.7
3	M	14	PRO	2.7
1	C	311	ILE	2.7
3	N	141	ASP	2.6
3	O	178	SER	2.6
2	I	84	LEU	2.6
1	C	301	ALA	2.6
3	L	191	HIS	2.6
3	N	18	VAL	2.6
3	O	138	THR	2.6
3	O	118	VAL	2.5
2	F	11	LEU	2.5
2	I	26	GLY	2.5
2	I	1	GLU	2.5
3	M	208	SER	2.5
3	K	197	GLN	2.5
2	F	156	PRO	2.5
2	G	1	GLU	2.4
3	N	144	PRO	2.4
3	K	1	GLN	2.4
2	I	210	ALA	2.4
3	M	122	PRO	2.4
3	K	194	TYR	2.4
2	H	139	ALA	2.3
2	F	130	VAL	2.3
3	N	117	SER	2.3
3	O	136	VAL	2.3
2	I	211	SER	2.3
1	A	83	HIS	2.3
3	M	207	LYS	2.3
2	J	209	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	N	121	PHE	2.3
2	G	198	PRO	2.3
3	M	192	SER	2.3
3	N	112	PRO	2.3
3	O	184	THR	2.3
3	M	205	VAL	2.3
3	O	188	TRP	2.2
3	O	181	LEU	2.2
1	D	307	GLU	2.2
1	D	305	THR	2.2
2	H	138	ALA	2.2
1	C	16	PHE	2.2
2	I	127	PRO	2.2
3	M	13	SER	2.2
2	F	186	LEU	2.2
1	E	308	TRP	2.2
2	F	128	PRO	2.2
3	M	196	CYS	2.2
3	N	77	ILE	2.2
2	I	208	HIS	2.2
1	B	307	GLU	2.2
3	N	166	GLN	2.2
2	J	203	THR	2.2
3	K	199	THR	2.2
3	K	149	VAL	2.1
3	O	116	PRO	2.1
2	F	162	THR	2.1
2	J	44	ASN	2.1
3	O	26	THR	2.1
3	N	114	SER	2.1
3	O	131	ASN	2.1
3	M	194	TYR	2.1
2	J	169	SER	2.1
1	E	9	LEU	2.1
3	N	183	LEU	2.1
1	B	301	ALA	2.1
2	G	145	VAL	2.1
1	D	23	ASP	2.1
3	O	205	VAL	2.1
2	F	153	GLY	2.1
1	E	8	HIS	2.1
2	G	146	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	311	ILE	2.0
3	M	210	SER	2.0
3	O	44	HIS	2.0
2	J	166	GLY	2.0
1	B	340	HIS	2.0
2	J	147	LEU	2.0
3	L	181	LEU	2.0
3	O	137	CYS	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.

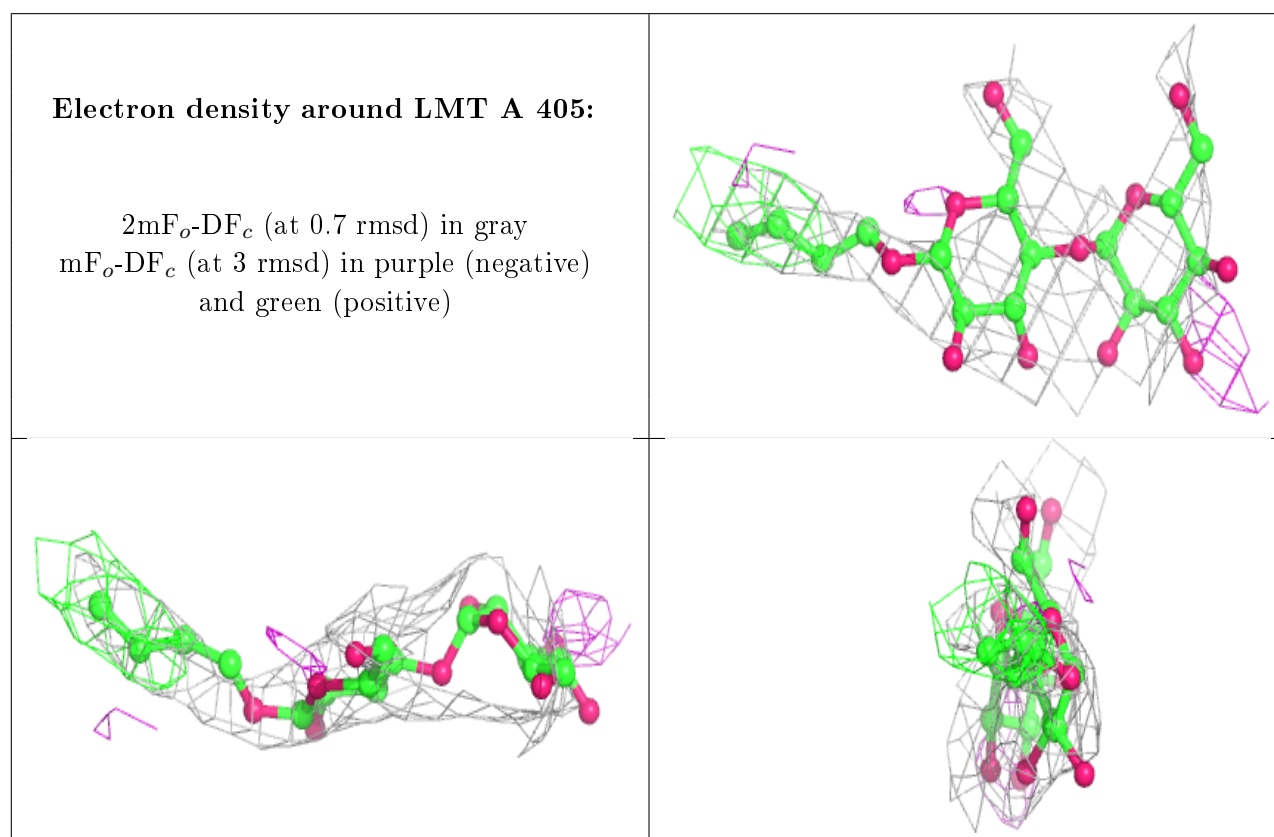
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	LMT	A	405	27/35	0.58	0.59	143,143,143,143	0
10	UND	B	406	11/11	0.59	0.49	60,60,60,60	0
9	OCT	E	403	8/8	0.73	0.39	79,79,79,79	0
8	NAG	C	400	14/15	0.76	0.37	128,132,137,137	0
6	LMT	B	404	26/35	0.76	0.38	145,145,145,145	0
8	NAG	E	400	14/15	0.82	0.35	172,176,179,180	0
9	OCT	D	403	8/8	0.82	0.60	59,59,59,59	0
7	CL	B	402	1/1	0.83	1.01	72,72,72,72	0
8	NAG	B	400	14/15	0.84	0.60	138,141,143,145	0
9	OCT	B	405	8/8	0.84	0.32	60,60,60,60	0
6	LMT	A	404	26/35	0.86	0.25	106,106,106,106	0
5	IVM	A	402	62/62	0.87	0.25	55,58,69,70	0
5	IVM	B	403	62/62	0.89	0.30	60,68,83,84	0
4	GLU	A	401	10/10	0.90	0.35	73,74,77,78	0
5	IVM	D	402	62/62	0.90	0.23	61,70,84,85	0

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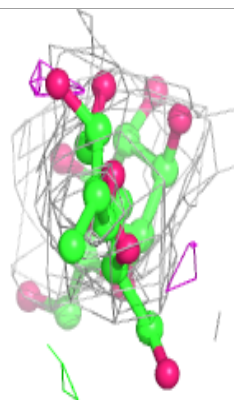
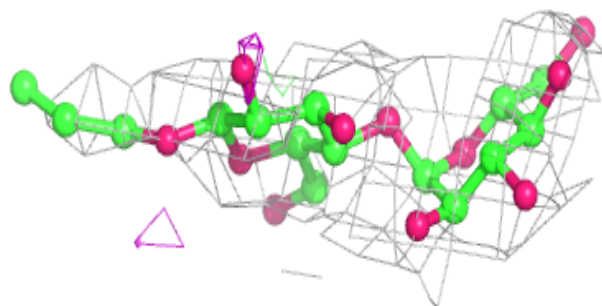
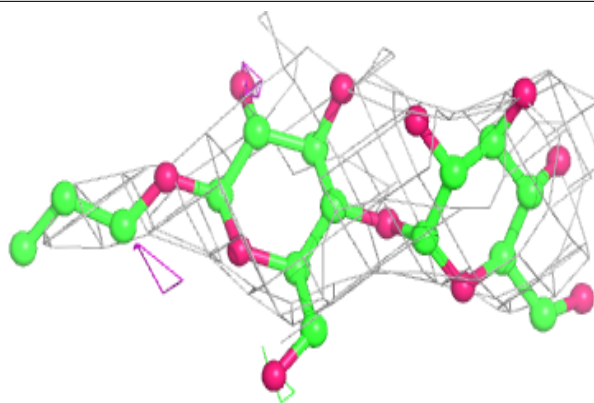
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IVM	A	403	62/62	0.90	0.24	70,73,80,81	0
4	GLU	B	401	10/10	0.90	0.27	67,68,71,71	0
5	IVM	E	402	62/62	0.91	0.30	65,69,73,75	0
4	GLU	D	401	10/10	0.92	0.33	66,67,69,69	0
4	GLU	C	401	10/10	0.92	0.23	74,76,79,80	0
4	GLU	E	401	10/10	0.95	0.20	66,67,69,70	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.

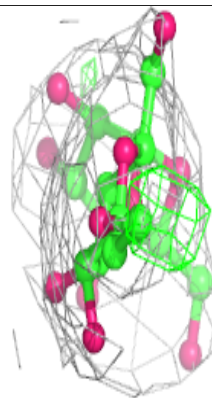
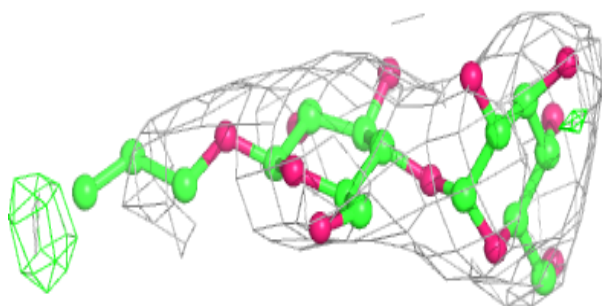
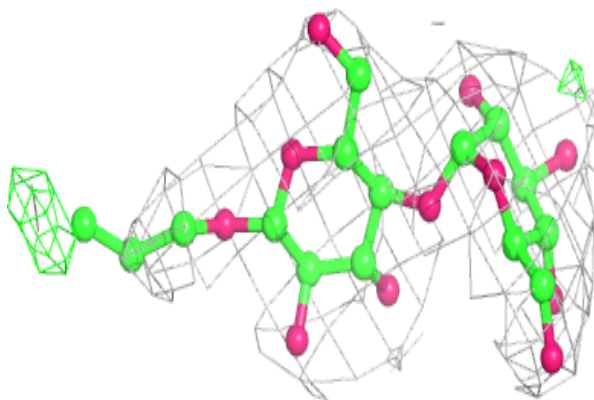


Electron density around LMT B 404:

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

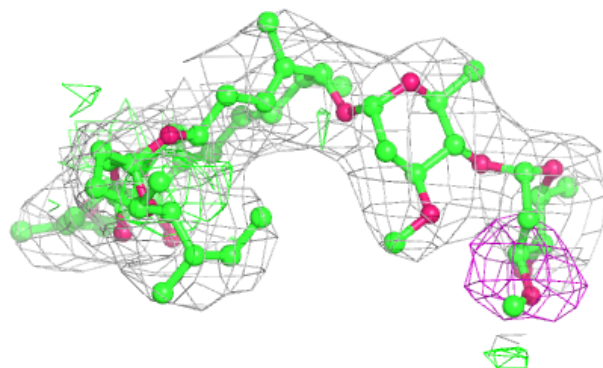
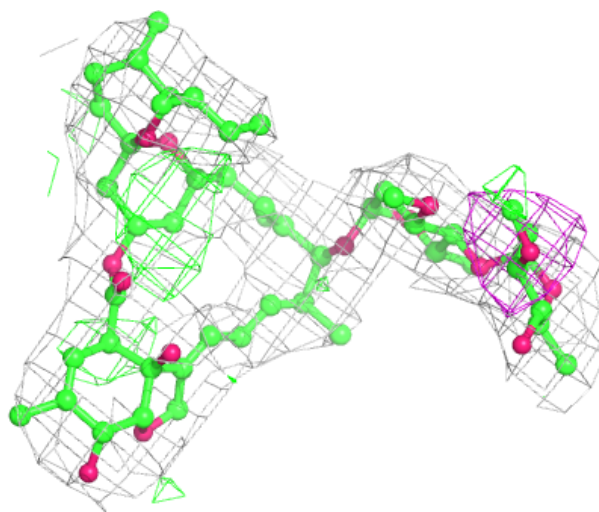
**Electron density around LMT A 404:**

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



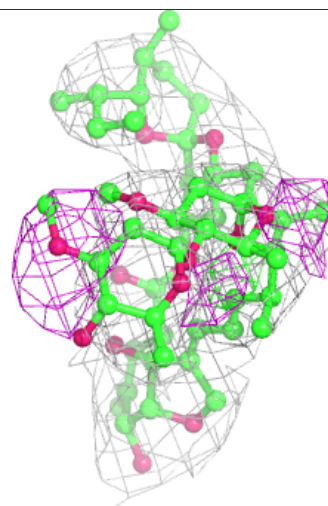
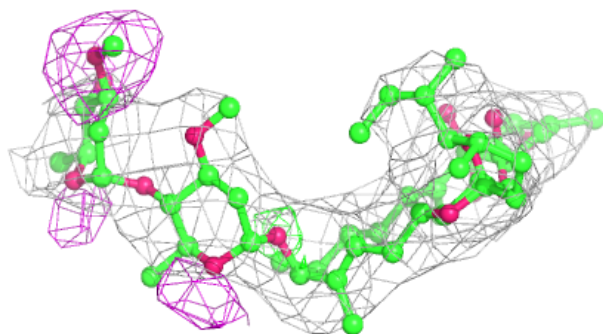
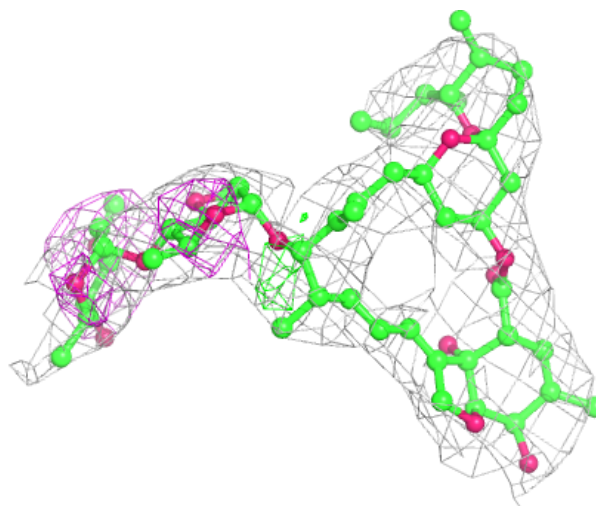
Electron density around IVM A 402:

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



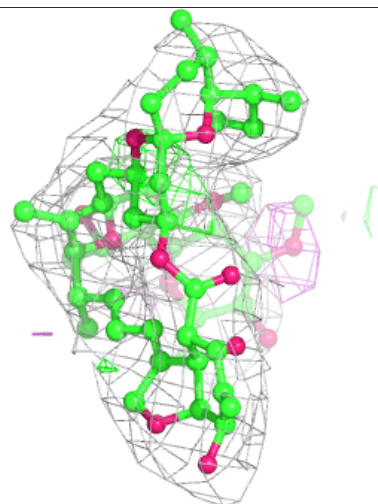
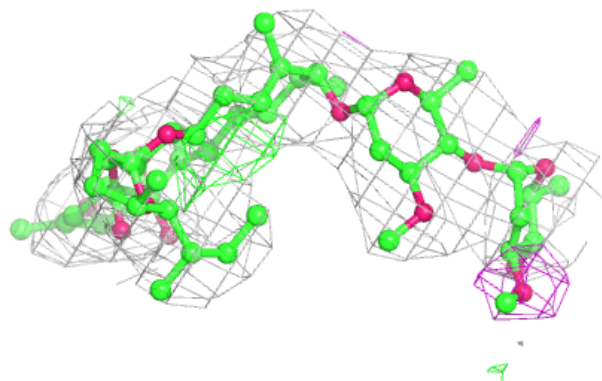
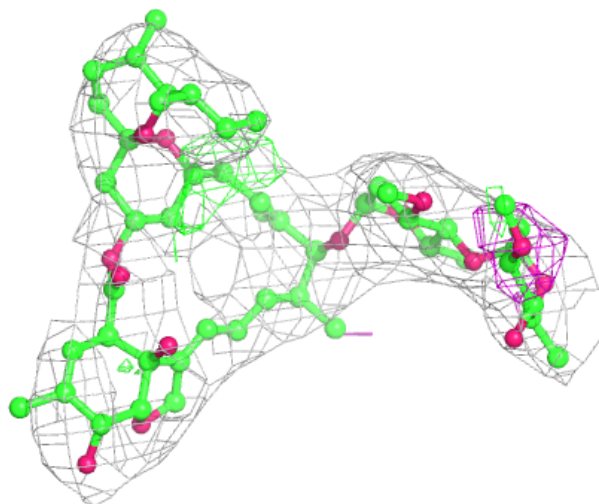
Electron density around IVM B 403:

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



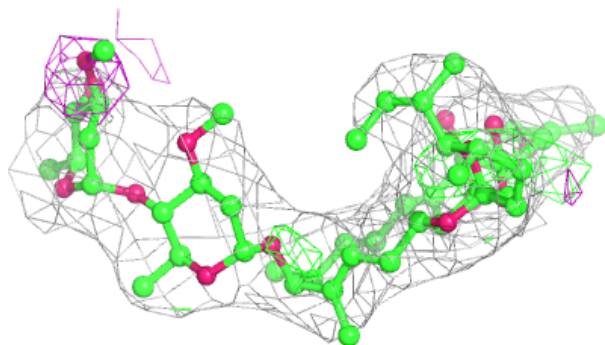
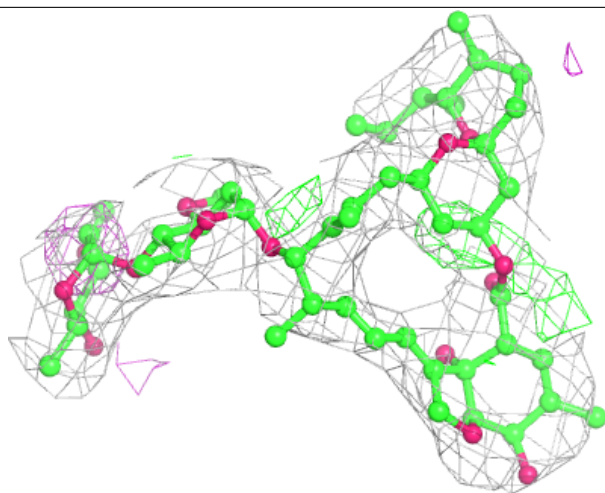
Electron density around IVM D 402:

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



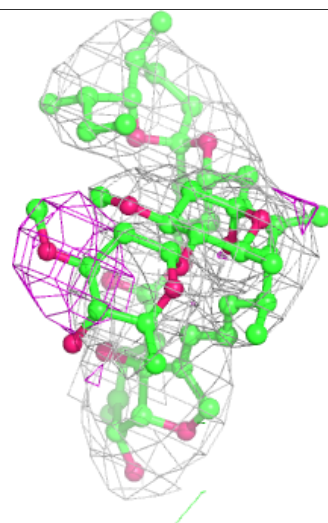
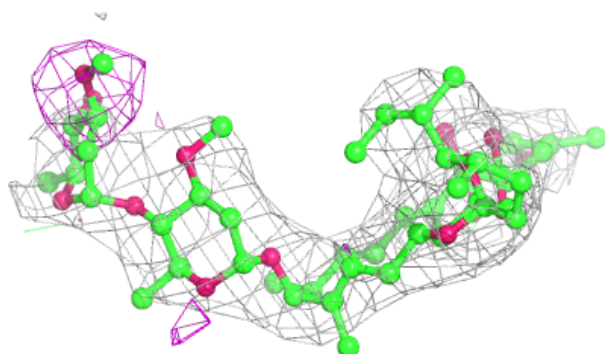
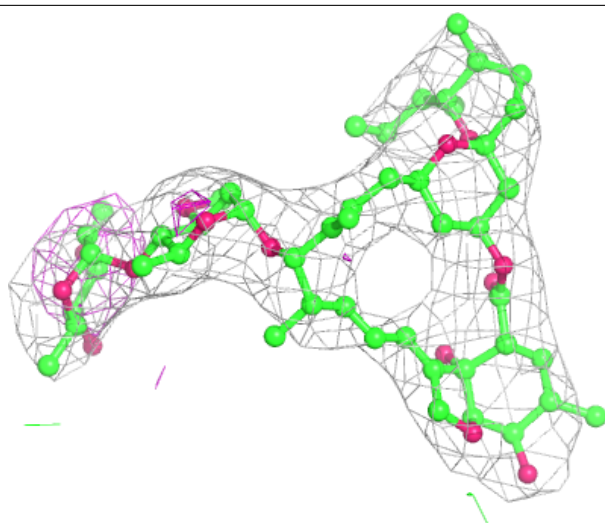
Electron density around IVM A 403:

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



Electron density around IVM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.