



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 2R56 / pdb_00002r56
Title : Crystal Structure of a Recombinant IgE Fab Fragment in Complex with Bovine Beta-Lactoglobulin Allergen
Authors : Niemi, M.; Kallio, J.M.; Hakulinen, N.; Rouvinen, J.
Deposited on : 2007-09-03
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

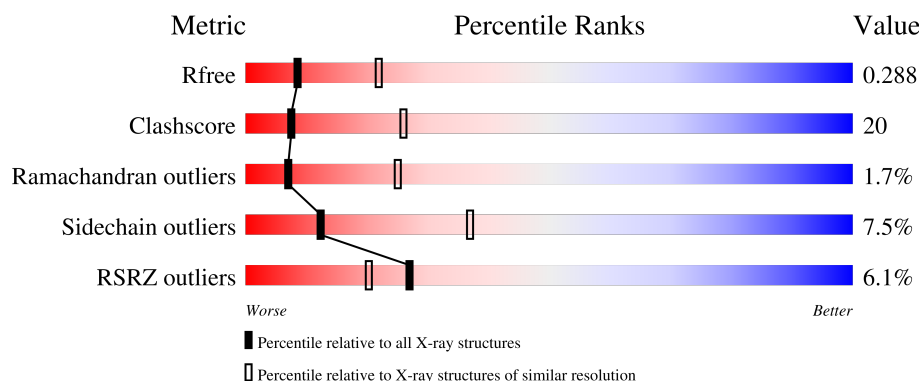
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	162	13% 51% 43% ..
1	B	162	12% 49% 46% ..
2	L	211	2% 63% 34% .
2	M	211	2% 59% 37% .
3	H	221	3% 63% 32% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	221	7% 61% 33% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9136 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 Beta-lactoglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1257	800	203	245	9			
1	B	159	Total	C	N	O	S	0	0	0
			1257	800	203	245	9			

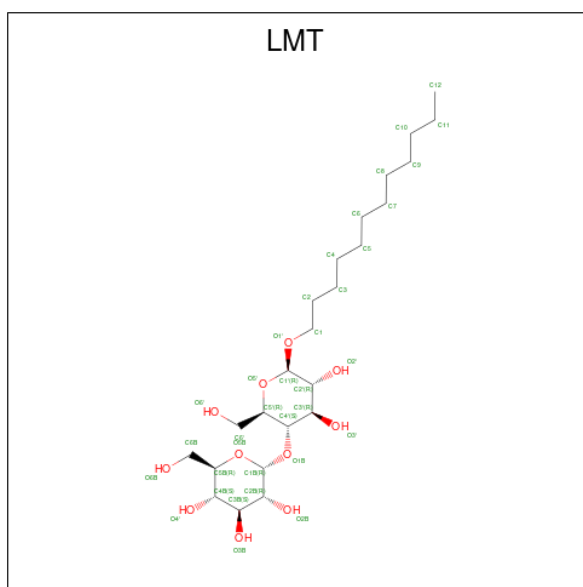
- Molecule 2 is a protein called IgE Fab Fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1627	1021	274	327	5			
2	M	211	Total	C	N	O	S	0	0	0
			1627	1021	274	327	5			

- Molecule 3 is a protein called IgE Fab Fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1649	1031	291	321	6			
3	I	221	Total	C	N	O	S	0	0	0
			1649	1031	291	321	6			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

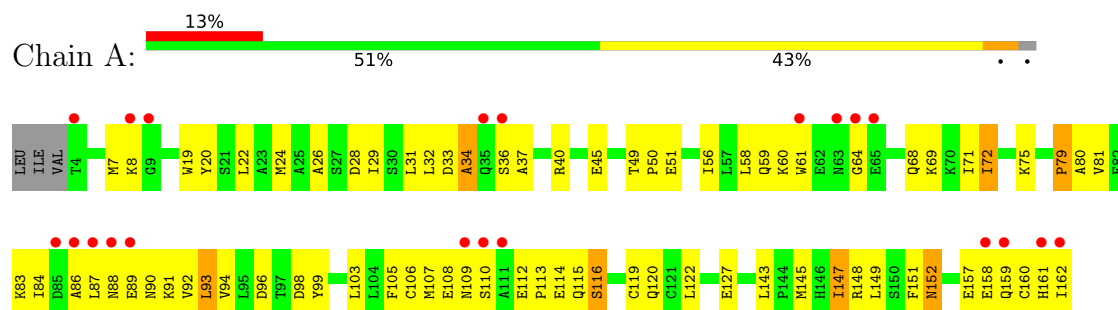


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0
4	B	1	Total C O 35 24 11	0	0

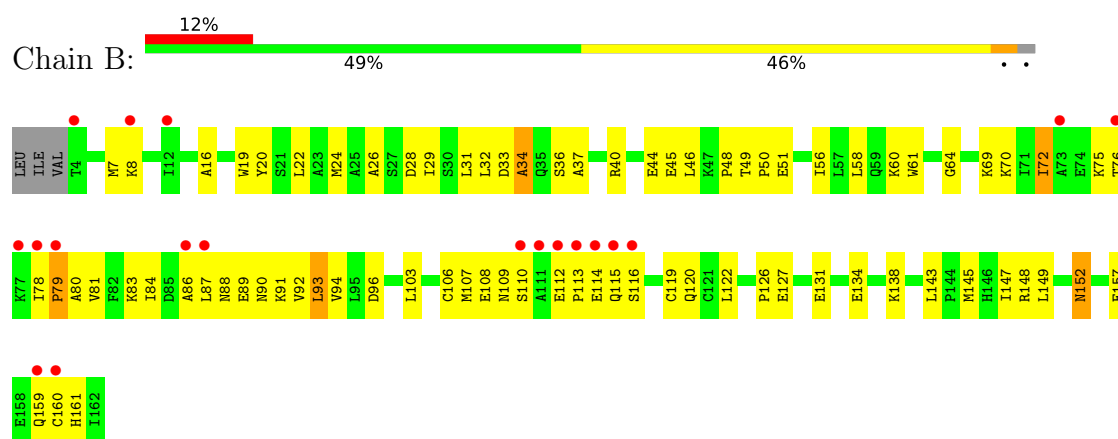
3 Residue-property plots [i](#)

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

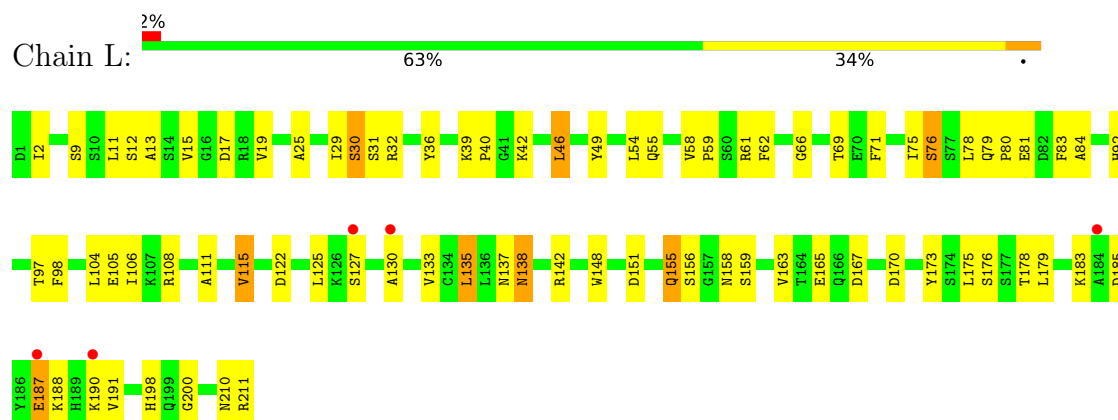
• Molecule 1: Beta-lactoglobulin



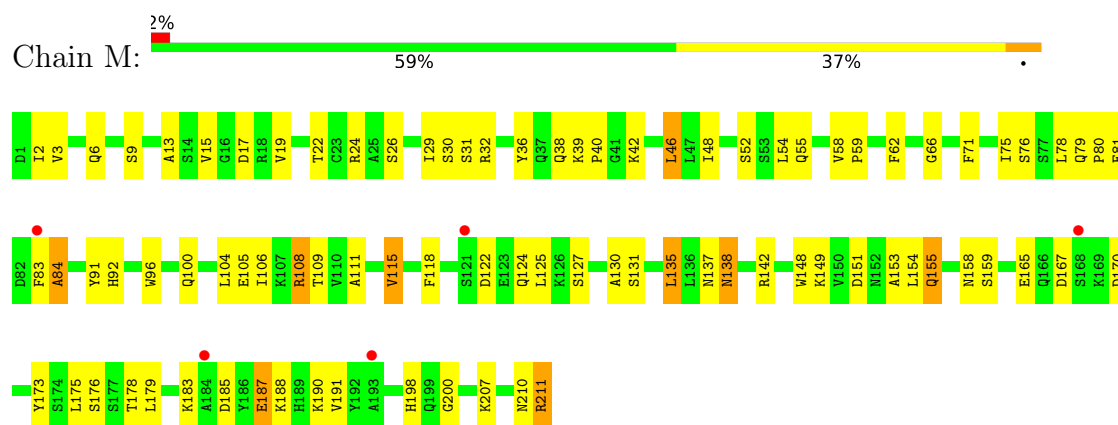
• Molecule 1: Beta-lactoglobulin



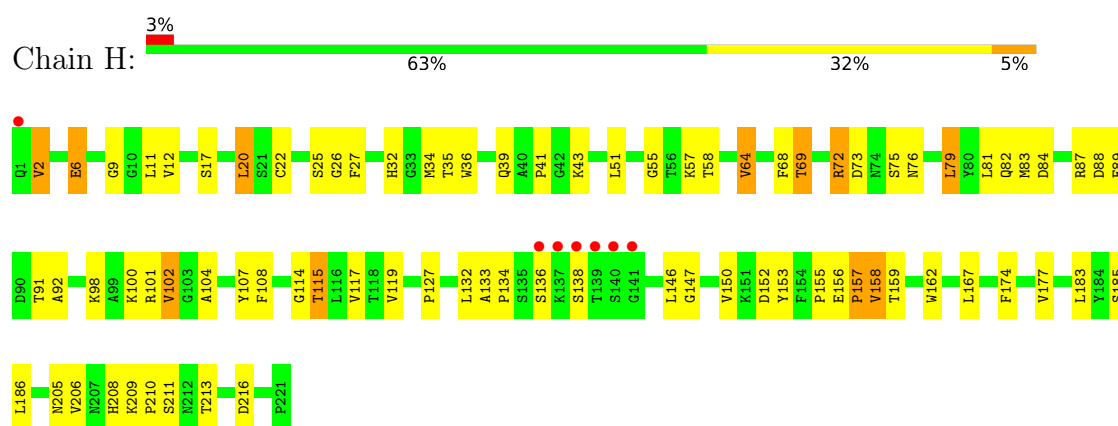
• Molecule 2: IgE Fab Fragment, light chain



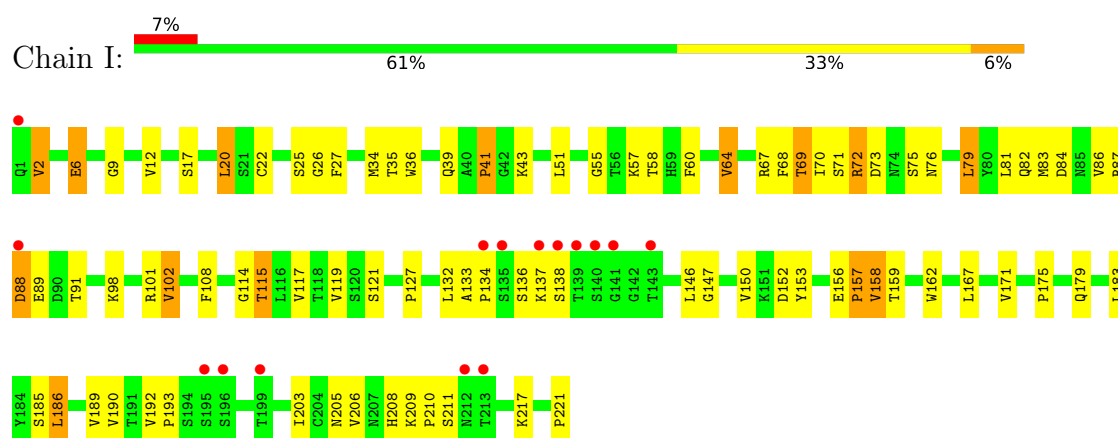
- Molecule 2: IgE Fab Fragment, light chain



- Molecule 3: IgE Fab Fragment, heavy chain



- Molecule 3: IgE Fab Fragment, heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.04Å 100.64Å 168.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.80) 99.6 (20.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.291 0.246 , 0.288	Depositor DCC
R_{free} test set	1434 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9136	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT

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	0.50	0/1278	0.82	0/1728
1	B	0.50	0/1278	0.81	0/1728
2	L	0.50	0/1664	0.89	4/2258 (0.2%)
2	M	0.50	0/1664	0.88	2/2258 (0.1%)
3	H	0.55	0/1687	0.94	1/2291 (0.0%)
3	I	0.54	0/1687	0.92	2/2291 (0.1%)
All	All	0.52	0/9258	0.88	9/12554 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	104	ALA	N-CA-C	-6.37	98.43	108.63
2	M	115	VAL	N-CA-C	5.93	117.27	109.21
3	I	86	VAL	N-CA-C	5.86	116.62	109.30
2	M	135	LEU	N-CA-C	5.53	117.91	108.90
3	I	121	SER	N-CA-C	-5.46	106.29	113.17
2	L	163	VAL	N-CA-C	5.19	116.06	108.53
2	L	135	LEU	N-CA-C	5.16	117.31	108.90
2	L	115	VAL	N-CA-C	5.15	116.21	109.21
2	L	30	SER	CB-CA-C	-5.10	110.72	116.63

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	1257	0	1270	72	0
1	B	1257	0	1270	60	0
2	L	1627	0	1587	65	0
2	M	1627	0	1587	68	0
3	H	1649	0	1624	65	0
3	I	1649	0	1624	70	0
4	A	35	0	46	3	0
4	B	35	0	46	2	0
All	All	9136	0	9054	370	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 20.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:69:THR:HG23	3:I:82:GLN:HB3	1.37	1.06
2:L:40:PRO:HG2	2:L:165:GLU:CG	1.92	0.97
2:L:40:PRO:HG2	2:L:165:GLU:HG2	1.01	0.97
3:H:69:THR:HG23	3:H:82:GLN:HB3	1.46	0.97
2:L:155:GLN:HG3	2:L:158:ASN:HD22	1.31	0.95
2:M:19:VAL:HG22	2:M:75:ILE:HB	1.55	0.88
2:L:40:PRO:CG	2:L:165:GLU:HG2	1.97	0.87
1:A:162:ILE:HD11	3:H:57:LYS:NZ	1.91	0.86
2:M:155:GLN:HG3	2:M:158:ASN:HD22	1.42	0.85
3:I:134:PRO:HG3	3:I:146:LEU:HB3	1.60	0.83
2:L:19:VAL:HG22	2:L:75:ILE:HB	1.60	0.83
3:H:134:PRO:HG3	3:H:146:LEU:HB3	1.60	0.82
3:H:208:HIS:CD2	3:H:210:PRO:HD2	2.15	0.82
1:A:72:ILE:HD13	1:A:72:ILE:H	1.43	0.81
1:A:162:ILE:HD11	3:H:57:LYS:HZ1	1.44	0.81
1:A:158:GLU:HG2	3:H:57:LYS:HE3	1.62	0.81
1:B:60:LYS:HD2	4:B:163:LMT:O2'	1.80	0.80
3:H:11:LEU:HB2	3:H:155:PRO:HG3	1.66	0.76
3:I:208:HIS:CD2	3:I:210:PRO:HD2	2.21	0.76
3:H:20:LEU:HD22	3:H:83:MET:HE2	1.69	0.74
3:I:152:ASP:HB3	3:I:183:LEU:HD13	1.69	0.72
1:A:72:ILE:HD13	1:A:72:ILE:N	2.04	0.71
1:B:37:ALA:HB3	1:B:40:ARG:HB2	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:LEU:CD1	3:H:58:THR:HG22	2.21	0.70
3:H:156:GLU:HB3	3:H:157:PRO:HA	1.75	0.69
3:I:51:LEU:CD1	3:I:58:THR:HG22	2.22	0.69
2:M:39:LYS:HB2	2:M:42:LYS:HD2	1.75	0.69
3:I:22:CYS:HB3	3:I:79:LEU:HB3	1.74	0.68
1:A:90:ASN:HD21	1:A:109:ASN:HD21	1.40	0.67
1:A:37:ALA:HB3	1:A:40:ARG:HB2	1.76	0.67
2:L:190:LYS:HE2	2:L:191:VAL:HG23	1.76	0.66
3:H:83:MET:HE1	3:H:117:VAL:HG21	1.77	0.66
3:H:152:ASP:HB3	3:H:183:LEU:HD13	1.77	0.66
3:H:127:PRO:HB2	3:H:150:VAL:HG12	1.78	0.65
1:B:19:TRP:O	3:I:101:ARG:NH2	2.30	0.65
1:A:59:GLN:HE22	2:L:32:ARG:NH2	1.94	0.65
3:H:64:VAL:HG13	3:H:68:PHE:HB2	1.79	0.64
1:B:72:ILE:HD13	1:B:72:ILE:H	1.62	0.64
3:I:87:ARG:O	3:I:119:VAL:HG11	1.97	0.64
2:L:79:GLN:HB3	2:L:80:PRO:HD2	1.79	0.64
2:M:187:GLU:HA	2:M:211:ARG:HH21	1.63	0.64
1:A:93:LEU:HD22	1:A:93:LEU:N	2.13	0.64
2:M:207:LYS:HE3	3:I:137:LYS:HD3	1.80	0.64
1:A:19:TRP:O	3:H:101:ARG:NH2	2.32	0.63
3:H:127:PRO:HB3	3:H:153:TYR:HB3	1.79	0.63
2:M:40:PRO:HG2	2:M:165:GLU:HG2	1.80	0.63
2:L:155:GLN:HG3	2:L:158:ASN:ND2	2.09	0.63
1:A:29:ILE:HG22	1:A:33:ASP:HB2	1.78	0.63
1:A:88:ASN:CB	1:A:109:ASN:HD22	2.11	0.63
3:H:87:ARG:O	3:H:119:VAL:HG11	1.99	0.63
1:A:81:VAL:HG22	1:A:93:LEU:HD12	1.80	0.63
1:B:7:MET:HE3	1:B:96:ASP:HA	1.80	0.62
3:I:20:LEU:HD22	3:I:83:MET:HE2	1.81	0.62
3:I:127:PRO:HB3	3:I:153:TYR:HB3	1.80	0.62
1:B:93:LEU:N	1:B:93:LEU:HD22	2.14	0.62
3:I:156:GLU:HB3	3:I:157:PRO:HA	1.81	0.62
2:M:79:GLN:HB3	2:M:80:PRO:HD2	1.82	0.61
1:A:49:THR:HB	1:A:50:PRO:HD2	1.83	0.61
1:B:72:ILE:HD13	1:B:72:ILE:N	2.16	0.61
3:H:35:THR:HG21	3:H:108:PHE:CE1	2.36	0.61
3:I:2:VAL:HA	3:I:26:GLY:HA3	1.83	0.61
3:I:35:THR:HG21	3:I:108:PHE:CE1	2.36	0.61
3:I:41:PRO:O	3:I:43:LYS:HG2	2.00	0.61
1:B:49:THR:HB	1:B:50:PRO:HD2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:158:ASN:O	2:M:179:LEU:HD12	2.00	0.61
1:B:81:VAL:HG22	1:B:93:LEU:HD12	1.83	0.60
1:B:24:MET:HB3	1:B:120:GLN:HG2	1.83	0.60
3:I:127:PRO:HB2	3:I:150:VAL:HG12	1.83	0.60
1:B:112:GLU:HB3	1:B:115:GLN:HE21	1.67	0.60
3:I:83:MET:HE1	3:I:117:VAL:HG21	1.84	0.60
1:B:90:ASN:HD21	1:B:109:ASN:HD21	1.48	0.60
1:B:148:ARG:C	1:B:149:LEU:HD12	2.27	0.60
1:A:143:LEU:HB3	1:A:145:MET:HE3	1.84	0.59
1:A:108:GLU:HA	1:A:116:SER:O	2.02	0.59
1:B:92:VAL:HG11	4:B:163:LMT:H92	1.85	0.59
3:I:69:THR:HG23	3:I:82:GLN:CB	2.23	0.59
2:L:187:GLU:HG3	2:L:211:ARG:NH2	2.17	0.59
1:A:7:MET:HE3	1:A:96:ASP:HA	1.82	0.59
1:B:29:ILE:HG22	1:B:33:ASP:HB2	1.85	0.59
2:M:175:LEU:C	2:M:175:LEU:HD23	2.28	0.59
1:B:20:TYR:OH	3:I:102:VAL:HG22	2.03	0.59
1:B:60:LYS:HE2	1:B:69:LYS:HD2	1.85	0.59
2:L:46:LEU:HD13	2:L:55:GLN:HB2	1.84	0.58
2:L:125:LEU:HD22	2:L:183:LYS:HG2	1.85	0.58
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.85	0.58
1:B:61:TRP:HE1	1:B:64:GLY:HA2	1.68	0.58
3:H:36:TRP:NE1	3:H:81:LEU:HB2	2.18	0.58
2:L:185:ASP:HA	2:L:188:LYS:HG2	1.86	0.58
1:A:152:ASN:N	1:A:152:ASN:HD22	2.00	0.58
3:I:51:LEU:HD21	3:I:72:ARG:HB3	1.85	0.58
1:B:70:LYS:NZ	2:M:52:SER:OG	2.36	0.57
1:B:88:ASN:CB	1:B:109:ASN:HD22	2.17	0.57
2:M:137:ASN:ND2	2:M:138:ASN:ND2	2.52	0.57
2:M:36:TYR:CE1	2:M:46:LEU:HD23	2.40	0.57
1:B:36:SER:HA	1:B:61:TRP:HB3	1.86	0.57
2:M:125:LEU:HD22	2:M:183:LYS:HG2	1.87	0.57
1:A:33:ASP:O	1:A:34:ALA:HB3	2.04	0.56
2:L:39:LYS:HB2	2:L:42:LYS:HD2	1.85	0.56
1:A:114:GLU:HB2	1:A:115:GLN:NE2	2.21	0.56
1:A:90:ASN:ND2	1:A:109:ASN:ND2	2.53	0.56
2:L:125:LEU:O	2:L:183:LYS:HG3	2.05	0.56
1:B:143:LEU:HB3	1:B:145:MET:HE3	1.87	0.56
3:I:51:LEU:HD12	3:I:58:THR:HG22	1.88	0.56
2:M:32:ARG:HD2	2:M:92:HIS:HA	1.87	0.56
2:M:155:GLN:HG3	2:M:158:ASN:ND2	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TRP:HE1	1:A:64:GLY:HA2	1.70	0.56
2:M:29:ILE:O	2:M:30:SER:HB3	2.06	0.56
2:M:190:LYS:HE2	2:M:191:VAL:HG23	1.86	0.56
2:M:137:ASN:ND2	2:M:138:ASN:HD22	2.03	0.55
1:A:110:SER:O	1:A:113:PRO:HD3	2.07	0.55
1:B:114:GLU:HB2	1:B:115:GLN:NE2	2.21	0.55
2:M:38:GLN:HE22	3:I:39:GLN:HE22	1.54	0.55
3:I:203:ILE:HG23	3:I:217:LYS:O	2.07	0.55
2:L:78:LEU:HD11	2:L:104:LEU:HD21	1.89	0.55
1:B:108:GLU:HA	1:B:116:SER:O	2.06	0.55
1:B:126:PRO:HG3	3:I:102:VAL:HG13	1.89	0.54
2:L:198:HIS:CD2	2:L:200:GLY:H	2.25	0.54
2:L:46:LEU:HB2	3:H:108:PHE:O	2.08	0.54
3:I:209:LYS:HB2	3:I:210:PRO:HD3	1.90	0.54
1:B:112:GLU:HB3	1:B:115:GLN:HG2	1.90	0.54
3:I:6:GLU:CD	3:I:114:GLY:H	2.16	0.54
2:L:190:LYS:O	2:L:210:ASN:HA	2.07	0.54
2:M:22:THR:HG21	2:M:24:ARG:NH2	2.23	0.53
2:L:158:ASN:O	2:L:179:LEU:HD12	2.07	0.53
2:L:159:SER:HA	2:L:178:THR:O	2.08	0.53
3:H:51:LEU:HD21	3:H:72:ARG:HB3	1.91	0.53
2:M:3:VAL:H	2:M:26:SER:HB3	1.74	0.53
2:M:175:LEU:HD23	2:M:176:SER:N	2.22	0.53
2:L:137:ASN:ND2	2:L:138:ASN:HD22	2.07	0.53
2:M:2:ILE:HD13	2:M:29:ILE:HG22	1.90	0.53
2:L:187:GLU:HG3	2:L:211:ARG:CZ	2.39	0.53
2:M:46:LEU:HD13	2:M:55:GLN:HB2	1.91	0.53
3:I:35:THR:HG21	3:I:108:PHE:CZ	2.44	0.53
1:A:24:MET:HB3	1:A:120:GLN:HG2	1.89	0.53
1:A:106:CYS:HA	1:A:119:CYS:HA	1.91	0.53
3:I:136:SER:C	3:I:138:SER:H	2.16	0.53
1:A:36:SER:HA	1:A:61:TRP:HB3	1.89	0.53
2:M:108:ARG:HH21	2:M:111:ALA:HB2	1.73	0.53
1:A:90:ASN:ND2	1:A:109:ASN:HD21	2.07	0.53
2:M:159:SER:HA	2:M:178:THR:O	2.08	0.53
1:A:88:ASN:HB2	1:A:109:ASN:HD22	1.71	0.53
3:H:36:TRP:NE1	3:H:79:LEU:CD1	2.72	0.53
2:L:108:ARG:HH21	2:L:111:ALA:HB2	1.73	0.52
3:H:6:GLU:CD	3:H:114:GLY:H	2.17	0.52
3:I:9:GLY:H	3:I:115:THR:HG21	1.73	0.52
3:I:36:TRP:NE1	3:I:81:LEU:HB2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:HB3	1:A:115:GLN:HG2	1.91	0.52
3:H:41:PRO:O	3:H:43:LYS:HG2	2.10	0.52
1:A:152:ASN:N	1:A:152:ASN:ND2	2.56	0.52
2:L:142:ARG:HD3	2:L:173:TYR:CE2	2.44	0.52
2:M:142:ARG:HD3	2:M:173:TYR:CE2	2.44	0.52
2:L:137:ASN:ND2	2:L:138:ASN:ND2	2.57	0.52
1:A:60:LYS:CE	1:A:69:LYS:HD2	2.39	0.52
3:H:12:VAL:O	3:H:119:VAL:HA	2.09	0.52
1:B:60:LYS:CE	1:B:69:LYS:HD2	2.40	0.52
2:L:83:PHE:CZ	2:L:165:GLU:HG3	2.45	0.51
1:B:90:ASN:ND2	1:B:109:ASN:ND2	2.58	0.51
2:M:185:ASP:HA	2:M:188:LYS:HG2	1.92	0.51
3:H:136:SER:C	3:H:138:SER:H	2.18	0.51
1:B:106:CYS:HA	1:B:119:CYS:HA	1.92	0.51
1:A:92:VAL:O	1:A:93:LEU:HD13	2.10	0.51
1:A:103:LEU:C	1:A:103:LEU:HD23	2.36	0.51
1:B:84:ILE:HG22	1:B:86:ALA:H	1.76	0.51
1:B:110:SER:O	1:B:113:PRO:HD3	2.09	0.51
2:L:175:LEU:HD23	2:L:176:SER:N	2.25	0.51
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.93	0.51
2:M:187:GLU:HA	2:M:211:ARG:NH2	2.24	0.51
1:B:88:ASN:HB2	1:B:109:ASN:HD22	1.75	0.51
1:B:91:LYS:O	1:B:107:MET:HA	2.11	0.51
1:A:112:GLU:HB3	1:A:115:GLN:HE21	1.76	0.51
3:H:177:VAL:HG22	3:H:185:SER:O	2.11	0.51
1:A:90:ASN:HD21	1:A:109:ASN:ND2	2.07	0.50
1:A:28:ASP:H	1:A:31:LEU:HD12	1.76	0.50
1:B:103:LEU:C	1:B:103:LEU:HD23	2.36	0.50
3:H:73:ASP:HB3	3:H:76:ASN:OD1	2.11	0.50
2:L:108:ARG:HD2	2:L:170:ASP:O	2.12	0.50
3:I:12:VAL:O	3:I:119:VAL:HA	2.12	0.50
1:A:60:LYS:HE2	1:A:69:LYS:HD2	1.94	0.50
2:L:151:ASP:HA	2:L:191:VAL:HB	1.94	0.50
1:B:33:ASP:O	1:B:34:ALA:HB3	2.11	0.50
3:I:147:GLY:HA2	3:I:162:TRP:CZ2	2.46	0.50
1:B:80:ALA:HB1	1:B:94:VAL:HB	1.93	0.50
3:I:64:VAL:HG13	3:I:68:PHE:HB2	1.92	0.50
2:L:30:SER:OG	2:L:31:SER:N	2.43	0.50
1:B:131:GLU:O	1:B:134:GLU:HB2	2.12	0.50
3:I:88:ASP:HA	3:I:119:VAL:HG13	1.93	0.49
2:L:83:PHE:HZ	2:L:165:GLU:HG3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:83:PHE:O	2:L:84:ALA:HB2	2.11	0.49
3:H:27:PHE:CZ	3:H:98:LYS:HD2	2.47	0.49
1:A:58:LEU:C	1:A:58:LEU:HD12	2.37	0.49
3:H:27:PHE:CE1	3:H:98:LYS:HD2	2.46	0.49
3:H:51:LEU:HD12	3:H:58:THR:HG22	1.92	0.49
2:M:59:PRO:HG2	2:M:62:PHE:HD1	1.77	0.49
1:B:29:ILE:HA	1:B:147:ILE:HG21	1.95	0.49
1:B:32:LEU:HD23	1:B:149:LEU:HD13	1.93	0.49
1:B:28:ASP:H	1:B:31:LEU:HD12	1.77	0.49
1:B:90:ASN:ND2	1:B:109:ASN:HD21	2.11	0.49
2:M:125:LEU:O	2:M:183:LYS:HG3	2.12	0.49
1:A:31:LEU:O	1:A:37:ALA:HB1	2.13	0.49
2:L:36:TYR:OH	3:H:107:TYR:HA	2.13	0.49
2:M:78:LEU:HD11	2:M:104:LEU:HD21	1.95	0.49
2:M:190:LYS:HA	2:M:211:ARG:HD3	1.95	0.49
2:L:175:LEU:HD23	2:L:175:LEU:C	2.38	0.49
3:H:36:TRP:NE1	3:H:79:LEU:HD11	2.28	0.49
2:M:30:SER:OG	2:M:31:SER:N	2.41	0.49
2:M:167:ASP:HB3	2:M:170:ASP:OD2	2.13	0.49
2:L:133:VAL:HG21	3:H:132:LEU:HD21	1.93	0.49
3:H:87:ARG:HD2	3:H:89:GLU:OE1	2.13	0.48
1:A:32:LEU:HD23	1:A:149:LEU:HD13	1.94	0.48
2:M:66:GLY:HA3	2:M:71:PHE:HA	1.95	0.48
1:A:88:ASN:HD21	4:A:163:LMT:H6D	1.78	0.48
2:M:83:PHE:O	2:M:84:ALA:HB2	2.12	0.48
2:M:190:LYS:O	2:M:210:ASN:HA	2.13	0.48
3:H:153:TYR:CZ	3:H:158:VAL:HG11	2.48	0.48
3:I:2:VAL:HA	3:I:25:SER:O	2.13	0.48
3:I:51:LEU:CD2	3:I:72:ARG:HB3	2.43	0.48
3:I:171:VAL:HA	3:I:190:VAL:HG22	1.96	0.48
1:A:148:ARG:O	1:B:147:ILE:HA	2.14	0.48
2:M:151:ASP:HA	2:M:191:VAL:HB	1.95	0.48
1:A:24:MET:HE3	1:A:151:PHE:HE2	1.79	0.47
3:H:91:THR:OG1	3:H:119:VAL:HG12	2.15	0.47
2:M:198:HIS:CD2	2:M:200:GLY:H	2.32	0.47
3:I:203:ILE:HG23	3:I:217:LYS:C	2.39	0.47
1:A:105:PHE:CE1	1:A:120:GLN:HB2	2.49	0.47
3:H:209:LYS:HB2	3:H:210:PRO:HD3	1.95	0.47
3:I:51:LEU:HD11	3:I:55:GLY:HA2	1.97	0.47
2:L:32:ARG:HD2	2:L:92:HIS:HA	1.97	0.47
1:B:87:LEU:C	1:B:89:GLU:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:C	1:A:149:LEU:HD12	2.39	0.47
3:H:89:GLU:H	3:H:89:GLU:CD	2.21	0.47
2:M:54:LEU:HD11	2:M:58:VAL:CG1	2.44	0.47
3:I:34:MET:HG2	3:I:72:ARG:NH2	2.29	0.47
3:I:87:ARG:HD2	3:I:89:GLU:OE1	2.15	0.47
2:M:115:VAL:HA	2:M:135:LEU:O	2.15	0.47
2:M:83:PHE:HB2	2:M:106:ILE:HG12	1.97	0.47
2:L:49:TYR:CZ	3:H:100:LYS:HE3	2.50	0.46
1:B:126:PRO:HG3	3:I:102:VAL:CG1	2.44	0.46
2:L:97:THR:HG22	2:L:98:PHE:N	2.31	0.46
1:A:88:ASN:ND2	4:A:163:LMT:H6D	2.29	0.46
3:H:35:THR:HG21	3:H:108:PHE:CZ	2.50	0.46
1:B:20:TYR:O	1:B:122:LEU:HA	2.16	0.46
1:B:58:LEU:HD12	1:B:58:LEU:C	2.40	0.46
1:A:84:ILE:HG22	1:A:86:ALA:H	1.79	0.46
2:L:13:ALA:HB1	2:L:17:ASP:OD1	2.16	0.46
2:M:211:ARG:HH11	2:M:211:ARG:HB2	1.81	0.46
3:I:171:VAL:HG22	3:I:190:VAL:HG22	1.96	0.46
2:L:66:GLY:HA3	2:L:71:PHE:HA	1.97	0.46
2:M:125:LEU:C	2:M:127:SER:H	2.24	0.46
3:I:152:ASP:HB3	3:I:183:LEU:CD1	2.43	0.46
2:L:167:ASP:HB3	2:L:170:ASP:OD2	2.16	0.46
3:H:2:VAL:HA	3:H:25:SER:O	2.16	0.46
1:B:44:GLU:HA	3:I:101:ARG:NH2	2.31	0.46
1:A:59:GLN:NE2	2:L:32:ARG:HH22	2.14	0.46
1:A:157:GLU:HG2	3:H:102:VAL:HB	1.97	0.46
2:L:2:ILE:HD13	2:L:29:ILE:HG22	1.97	0.46
1:B:112:GLU:C	1:B:114:GLU:H	2.23	0.46
1:A:29:ILE:HA	1:A:147:ILE:HG21	1.98	0.46
1:A:151:PHE:C	1:A:152:ASN:HD22	2.24	0.46
3:I:171:VAL:HG22	3:I:190:VAL:CG2	2.46	0.46
1:A:72:ILE:N	1:A:72:ILE:CD1	2.74	0.45
3:I:179:GLN:CD	3:I:185:SER:HB2	2.41	0.45
2:L:176:SER:HB3	3:H:174:PHE:CZ	2.51	0.45
1:B:92:VAL:O	1:B:93:LEU:HD13	2.16	0.45
2:M:108:ARG:HD2	2:M:170:ASP:O	2.16	0.45
1:B:152:ASN:N	1:B:152:ASN:ND2	2.63	0.45
2:L:29:ILE:O	2:L:30:SER:HB3	2.15	0.45
1:B:20:TYR:CZ	3:I:102:VAL:HG22	2.51	0.45
2:L:59:PRO:HG2	2:L:62:PHE:HD1	1.81	0.45
1:A:80:ALA:HB1	1:A:94:VAL:HB	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LEU:C	1:A:89:GLU:H	2.25	0.45
1:A:91:LYS:O	1:A:107:MET:HA	2.17	0.45
2:M:59:PRO:HG2	2:M:62:PHE:CD1	2.52	0.45
2:M:83:PHE:HZ	2:M:165:GLU:HG3	1.82	0.45
3:H:51:LEU:CD2	3:H:72:ARG:HB3	2.46	0.45
3:I:89:GLU:CD	3:I:89:GLU:H	2.25	0.45
3:H:39:GLN:C	3:H:92:ALA:HB1	2.42	0.45
3:H:100:LYS:HD2	3:H:107:TYR:HE1	1.81	0.45
3:H:211:SER:O	3:H:213:THR:HG23	2.17	0.45
1:B:149:LEU:HD12	1:B:149:LEU:N	2.32	0.45
2:M:148:TRP:O	2:M:155:GLN:HB2	2.17	0.45
3:I:27:PHE:CZ	3:I:98:LYS:HD2	2.52	0.45
3:I:17:SER:HB3	3:I:84:ASP:HA	1.99	0.44
2:L:54:LEU:HD11	2:L:58:VAL:CG1	2.48	0.44
3:H:127:PRO:CB	3:H:150:VAL:HG12	2.47	0.44
3:I:158:VAL:O	3:I:158:VAL:HG13	2.17	0.44
1:B:152:ASN:N	1:B:152:ASN:HD22	2.15	0.44
2:M:6:GLN:O	2:M:100:GLN:NE2	2.50	0.44
2:M:118:PHE:CD1	3:I:132:LEU:HB3	2.53	0.44
2:M:135:LEU:HD22	3:I:189:VAL:HG21	1.98	0.44
2:L:190:LYS:CE	2:L:191:VAL:HG23	2.44	0.44
1:B:46:LEU:CD2	1:B:56:ILE:HG12	2.48	0.44
3:I:133:ALA:HA	3:I:134:PRO:HD3	1.83	0.44
1:A:83:LYS:HD2	1:A:89:GLU:OE2	2.17	0.44
3:H:34:MET:HG2	3:H:72:ARG:NH2	2.32	0.44
3:H:158:VAL:O	3:H:158:VAL:HG13	2.17	0.44
3:H:51:LEU:HD13	3:H:58:THR:HG22	1.99	0.44
3:I:51:LEU:CD1	3:I:55:GLY:HA2	2.48	0.44
3:I:134:PRO:HD2	3:I:221:PRO:HA	2.00	0.43
3:H:32:HIS:O	3:H:72:ARG:NH2	2.51	0.43
2:M:187:GLU:HG3	2:M:211:ARG:HH21	1.83	0.43
3:I:36:TRP:NE1	3:I:79:LEU:CD1	2.81	0.43
2:L:83:PHE:HD1	2:L:104:LEU:O	2.01	0.43
2:M:91:TYR:HA	2:M:96:TRP:CD1	2.53	0.43
1:A:105:PHE:CZ	1:A:120:GLN:HB2	2.53	0.43
1:A:162:ILE:HD11	3:H:57:LYS:HZ2	1.80	0.43
2:L:115:VAL:HA	2:L:135:LEU:O	2.18	0.43
1:B:26:ALA:HB2	1:B:32:LEU:HD13	2.00	0.43
2:M:149:LYS:HA	2:M:153:ALA:O	2.17	0.43
3:I:186:LEU:HD23	3:I:186:LEU:C	2.44	0.43
2:L:36:TYR:CE1	2:L:46:LEU:HD23	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:NE2	2:L:32:ARG:NH2	2.65	0.42
3:H:133:ALA:HA	3:H:134:PRO:HD3	1.84	0.42
2:L:83:PHE:HB2	2:L:106:ILE:HG12	2.01	0.42
2:M:13:ALA:HB1	2:M:17:ASP:OD1	2.18	0.42
3:I:73:ASP:HB3	3:I:76:ASN:OD1	2.20	0.42
1:A:68:GLN:HB2	2:L:32:ARG:CZ	2.50	0.42
1:A:112:GLU:C	1:A:114:GLU:H	2.28	0.42
1:A:147:ILE:HA	1:B:148:ARG:O	2.18	0.42
2:L:125:LEU:CD2	2:L:130:ALA:HB2	2.49	0.42
3:H:36:TRP:CE2	3:H:81:LEU:HB2	2.54	0.42
1:A:98:ASP:O	1:A:99:TYR:HB2	2.19	0.42
1:A:33:ASP:O	1:A:34:ALA:CB	2.68	0.42
1:A:114:GLU:HB2	1:A:115:GLN:HE22	1.84	0.42
2:M:125:LEU:CD2	2:M:130:ALA:HB2	2.50	0.42
2:M:115:VAL:O	2:M:207:LYS:HE2	2.20	0.42
2:M:187:GLU:CA	2:M:211:ARG:HH21	2.32	0.42
1:A:29:ILE:O	1:A:33:ASP:HB2	2.18	0.42
2:M:124:GLN:HE22	2:M:131:SER:CB	2.33	0.42
3:I:60:PHE:CZ	3:I:70:ILE:HG22	2.54	0.42
2:L:97:THR:HG22	2:L:98:PHE:O	2.20	0.42
2:L:148:TRP:O	2:L:155:GLN:HB2	2.20	0.42
2:M:83:PHE:HD1	2:M:104:LEU:O	2.02	0.42
3:I:153:TYR:CZ	3:I:158:VAL:HG11	2.55	0.42
3:I:208:HIS:ND1	3:I:211:SER:HB3	2.35	0.42
1:A:26:ALA:HB2	1:A:32:LEU:HD13	2.02	0.42
2:L:156:SER:H	2:L:158:ASN:ND2	2.18	0.42
2:L:59:PRO:HG2	2:L:62:PHE:CD1	2.55	0.41
2:L:61:ARG:HB2	2:L:76:SER:HB2	2.01	0.41
3:H:51:LEU:HD11	3:H:55:GLY:HA2	2.01	0.41
2:M:108:ARG:HG2	2:M:109:THR:H	1.83	0.41
1:A:20:TYR:O	1:A:122:LEU:HA	2.19	0.41
2:M:2:ILE:HD13	2:M:29:ILE:CG2	2.50	0.41
3:I:2:VAL:H	3:I:2:VAL:HG12	1.62	0.41
3:I:64:VAL:HG21	3:I:68:PHE:CD2	2.56	0.41
2:L:46:LEU:CD1	2:L:55:GLN:HB2	2.50	0.41
1:B:16:ALA:HB2	1:B:48:PRO:HD3	2.02	0.41
3:H:88:ASP:HA	3:H:119:VAL:HG13	2.02	0.41
1:A:92:VAL:C	1:A:93:LEU:HD13	2.46	0.41
2:L:25:ALA:O	2:L:69:THR:HG23	2.21	0.41
1:B:76:THR:C	1:B:78:ILE:H	2.29	0.41
3:H:9:GLY:H	3:H:115:THR:HG21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:135:LEU:CD2	3:I:189:VAL:HG21	2.50	0.41
2:M:190:LYS:CE	2:M:191:VAL:HG23	2.51	0.41
3:I:91:THR:OG1	3:I:119:VAL:HG12	2.21	0.41
2:L:11:LEU:HG	2:L:12:SER:N	2.36	0.41
3:H:156:GLU:HB3	3:H:157:PRO:CA	2.48	0.41
1:B:83:LYS:HD2	1:B:89:GLU:OE2	2.21	0.41
2:M:187:GLU:HA	2:M:211:ARG:HE	1.86	0.41
3:I:192:VAL:HB	3:I:193:PRO:HD2	2.03	0.41
2:L:125:LEU:C	2:L:127:SER:H	2.28	0.40
3:H:17:SER:HB3	3:H:84:ASP:HA	2.03	0.40
1:B:157:GLU:HB2	3:I:57:LYS:HE2	2.03	0.40
1:A:56:ILE:N	1:A:71:ILE:O	2.50	0.40
1:A:88:ASN:HB3	1:A:109:ASN:HD22	1.82	0.40
3:H:36:TRP:CE2	3:H:79:LEU:CD1	3.05	0.40
3:I:67:ARG:NH1	3:I:87:ARG:HG3	2.36	0.40
1:A:84:ILE:HD13	4:A:163:LMT:H52	2.03	0.40
3:H:147:GLY:HA2	3:H:162:TRP:CZ2	2.56	0.40
2:M:48:ILE:HD13	2:M:54:LEU:HA	2.03	0.40
2:M:108:ARG:HG2	2:M:109:THR:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	157/162 (97%)	133 (85%)	18 (12%)	6 (4%)	2 9
1	B	157/162 (97%)	135 (86%)	18 (12%)	4 (2%)	4 16
2	L	209/211 (99%)	193 (92%)	14 (7%)	2 (1%)	12 38
2	M	209/211 (99%)	194 (93%)	11 (5%)	4 (2%)	6 22
3	H	219/221 (99%)	196 (90%)	21 (10%)	2 (1%)	14 41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	41
All	All	1170/1188 (98%)	1053 (90%)	97 (8%)	20 (2%)	7	25

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	79	PRO
1	A	161	HIS
1	B	8	LYS
1	B	79	PRO
2	M	76	SER
2	L	76	SER
1	B	161	HIS
2	M	138	ASN
2	L	138	ASN
3	I	75	SER
1	A	116	SER
1	B	34	ALA
2	M	154	LEU
1	A	34	ALA
1	A	147	ILE
3	H	75	SER
2	M	84	ALA
3	I	158	VAL
3	H	158	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	140/143 (98%)	129 (92%)	11 (8%)	11	35
1	B	140/143 (98%)	128 (91%)	12 (9%)	10	31
2	L	185/185 (100%)	177 (96%)	8 (4%)	26	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	185/185 (100%)	175 (95%)	10 (5%)	20	51
3	H	183/183 (100%)	167 (91%)	16 (9%)	9	30
3	I	183/183 (100%)	164 (90%)	19 (10%)	7	22
All	All	1016/1022 (99%)	940 (92%)	76 (8%)	12	37

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	45	GLU
1	A	51	GLU
1	A	72	ILE
1	A	75	LYS
1	A	79	PRO
1	A	93	LEU
1	A	127	GLU
1	A	152	ASN
1	A	159	GLN
1	A	160	CYS
2	L	9	SER
2	L	15	VAL
2	L	46	LEU
2	L	81	GLU
2	L	105	GLU
2	L	122	ASP
2	L	155	GLN
2	L	187	GLU
3	H	2	VAL
3	H	6	GLU
3	H	20	LEU
3	H	64	VAL
3	H	69	THR
3	H	72	ARG
3	H	79	LEU
3	H	102	VAL
3	H	115	THR
3	H	157	PRO
3	H	159	THR
3	H	167	LEU
3	H	186	LEU
3	H	205	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	206	VAL
3	H	216	ASP
1	B	22	LEU
1	B	45	GLU
1	B	51	GLU
1	B	72	ILE
1	B	75	LYS
1	B	79	PRO
1	B	93	LEU
1	B	127	GLU
1	B	138	LYS
1	B	152	ASN
1	B	159	GLN
1	B	160	CYS
2	M	9	SER
2	M	15	VAL
2	M	46	LEU
2	M	81	GLU
2	M	105	GLU
2	M	108	ARG
2	M	122	ASP
2	M	155	GLN
2	M	187	GLU
2	M	211	ARG
3	I	2	VAL
3	I	6	GLU
3	I	20	LEU
3	I	41	PRO
3	I	64	VAL
3	I	69	THR
3	I	71	SER
3	I	72	ARG
3	I	79	LEU
3	I	88	ASP
3	I	102	VAL
3	I	115	THR
3	I	157	PRO
3	I	159	THR
3	I	167	LEU
3	I	175	PRO
3	I	186	LEU
3	I	205	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	206	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	59	GLN
1	A	63	ASN
1	A	68	GLN
1	A	88	ASN
1	A	109	ASN
1	A	115	GLN
1	A	152	ASN
2	L	38	GLN
2	L	124	GLN
2	L	137	ASN
2	L	138	ASN
2	L	158	ASN
2	L	210	ASN
3	H	39	GLN
3	H	77	ASN
3	H	207	ASN
1	B	59	GLN
1	B	63	ASN
1	B	88	ASN
1	B	109	ASN
1	B	115	GLN
1	B	152	ASN
2	M	38	GLN
2	M	55	GLN
2	M	124	GLN
2	M	137	ASN
2	M	138	ASN
2	M	158	ASN
2	M	210	ASN
3	I	31	HIS
3	I	77	ASN
3	I	85	ASN
3	I	207	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LMT	A	163	-	36,36,36	1.12	4 (11%)	47,47,47	0.91	0
4	LMT	B	163	-	36,36,36	1.14	3 (8%)	47,47,47	0.90	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	A	163	-	-	2/21/61/61	0/2/2/2
4	LMT	B	163	-	-	2/21/61/61	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	163	LMT	O5B-C1B	2.75	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	163	LMT	O5B-C1B	2.58	1.48	1.41
4	B	163	LMT	O1B-C1B	2.30	1.48	1.41
4	A	163	LMT	C4'-C5'	2.09	1.58	1.52
4	B	163	LMT	C4'-C5'	2.09	1.58	1.52
4	A	163	LMT	O1B-C4'	2.06	1.49	1.43
4	A	163	LMT	O1B-C1B	2.05	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	163	LMT	C4-C3-C2	-2.13	103.58	114.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

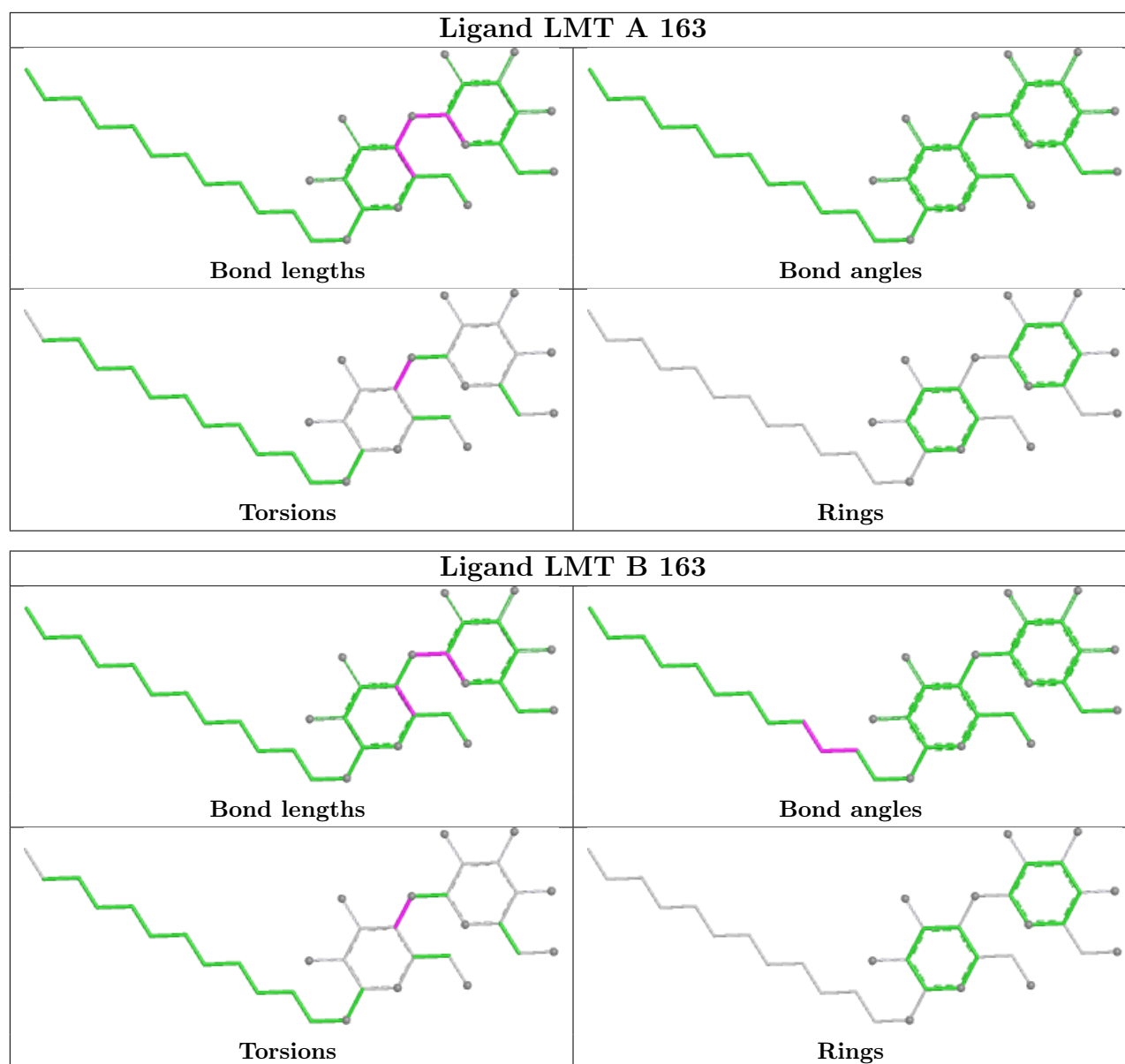
Mol	Chain	Res	Type	Atoms
4	A	163	LMT	C3'-C4'-O1B-C1B
4	B	163	LMT	C3'-C4'-O1B-C1B
4	B	163	LMT	C5'-C4'-O1B-C1B
4	A	163	LMT	C5'-C4'-O1B-C1B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	163	LMT	3	0
4	B	163	LMT	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.



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	159/162 (98%)	0.63	21 (13%)	7 6	3, 29, 69, 79	0
1	B	159/162 (98%)	0.59	19 (11%)	9 7	3, 29, 68, 79	0
2	L	211/211 (100%)	0.29	5 (2%)	59 49	2, 25, 54, 61	0
2	M	211/211 (100%)	0.30	5 (2%)	59 49	3, 26, 54, 59	0
3	H	221/221 (100%)	0.11	7 (3%)	50 40	2, 17, 54, 87	0
3	I	221/221 (100%)	0.17	15 (6%)	23 17	2, 17, 54, 86	0
All	All	1182/1188 (99%)	0.32	72 (6%)	27 20	2, 23, 59, 87	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	SER	6.3
1	A	64	GLY	5.5
1	B	113	PRO	4.9
1	A	162	ILE	4.8
1	A	88	ASN	4.8
1	B	110	SER	4.7
1	A	111	ALA	4.7
1	A	4	THR	4.5
3	I	139	THR	4.3
3	H	136	SER	4.2
1	A	110	SER	4.1
3	H	139	THR	4.1
1	A	161	HIS	4.1
3	I	138	SER	4.0
1	B	4	THR	3.7
1	A	87	LEU	3.6
3	I	135	SER	3.5
3	H	140	SER	3.5
1	A	63	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	134	PRO	3.4
1	A	61	TRP	3.4
3	I	195	SER	3.3
1	A	65	GLU	3.2
3	I	140	SER	3.2
1	B	116	SER	3.2
1	B	87	LEU	3.2
1	B	111	ALA	3.1
3	H	141	GLY	3.1
1	B	79	PRO	3.1
3	I	143	THR	3.0
3	I	137	LYS	3.0
3	I	196	SER	3.0
1	A	159	GLN	2.9
1	A	86	ALA	2.9
1	B	115	GLN	2.8
1	B	114	GLU	2.8
2	L	190	LYS	2.8
3	I	141	GLY	2.8
2	L	130	ALA	2.7
1	A	9	GLY	2.7
3	H	137	LYS	2.6
2	M	83	PHE	2.6
3	I	88	ASP	2.6
2	M	184	ALA	2.6
1	A	36	SER	2.6
1	A	89	GLU	2.5
1	B	12	ILE	2.5
1	A	8	LYS	2.4
1	A	158	GLU	2.4
1	A	85	ASP	2.4
1	B	77	LYS	2.3
3	I	1	GLN	2.3
2	M	168	SER	2.3
1	B	112	GLU	2.3
1	B	78	ILE	2.3
2	M	121	SER	2.3
3	I	199	THR	2.3
1	B	86	ALA	2.2
1	A	109	ASN	2.2
2	L	127	SER	2.2
2	M	193	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	187	GLU	2.1
3	I	213	THR	2.1
1	B	159	GLN	2.1
1	B	73	ALA	2.1
1	A	35	GLN	2.1
3	H	1	GLN	2.1
1	B	76	THR	2.1
1	B	160	CYS	2.0
3	I	212	ASN	2.0
2	L	184	ALA	2.0
1	B	8	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

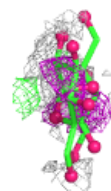
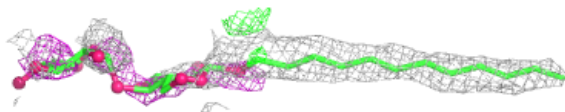
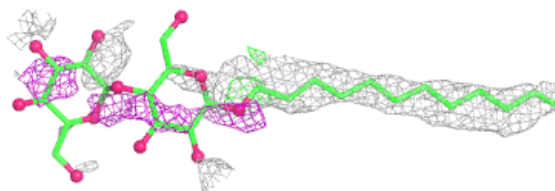
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LMT	B	163	35/35	0.42	0.22	28,67,75,75	0
4	LMT	A	163	35/35	0.65	0.19	26,66,75,76	0

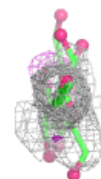
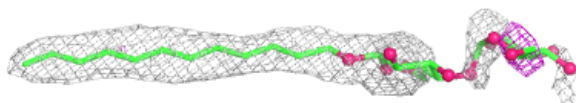
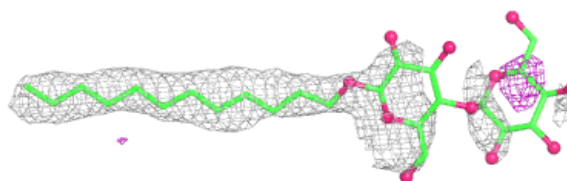
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 163:

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

**Electron density around LMT A 163:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.