



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:30 pm GMT

PDB ID : 8CJ8
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 mutant A651V
in complex with L-malate
Authors : Haesaerts, S.; Loris, R.; Larsen, P.B.
Deposited on : 2023-02-12
Resolution : 3.49 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

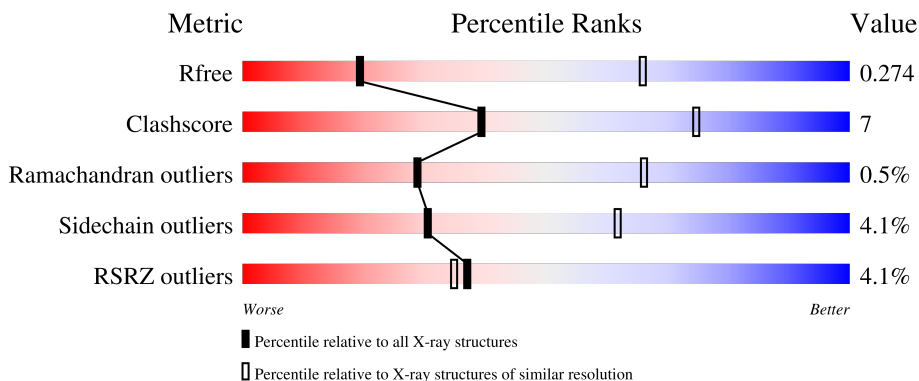
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	974	 5% 77% 17% . .
1	B	974	 5% 76% 18% . .
1	C	974	 % 76% 19% . .

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
2	LMR	A	1002	-	-	-	X
2	LMR	B	1002	-	-	X	-
2	LMR	C	1002	-	-	X	-
3	CL	A	1003	-	-	-	X
3	CL	A	1004	-	-	-	X
3	CL	B	1003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22657 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 Phosphoenolpyruvate carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	932	Total 7495	C 4753	N 1310	O 1402	S 30	0	3	0
1	B	935	Total 7533	C 4776	N 1319	O 1408	S 30	0	2	0
1	C	938	Total 7563	C 4795	N 1325	O 1413	S 30	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

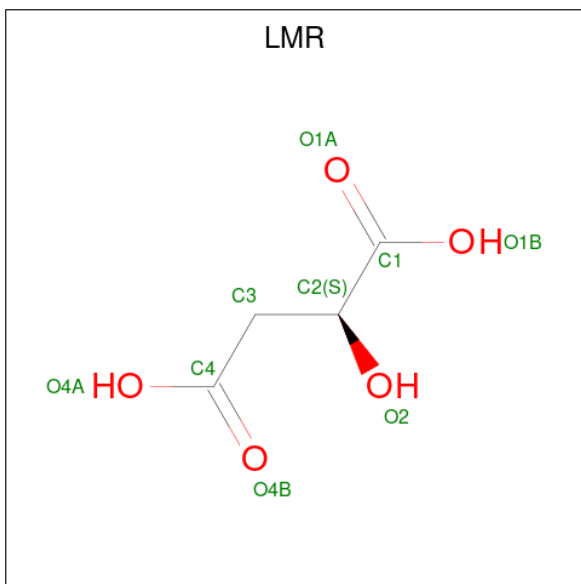
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
A	651	VAL	ALA	engineered mutation	UNP Q9MAH0
B	-6	MET	-	initiating methionine	UNP Q9MAH0
B	-5	HIS	-	expression tag	UNP Q9MAH0
B	-4	HIS	-	expression tag	UNP Q9MAH0
B	-3	HIS	-	expression tag	UNP Q9MAH0
B	-2	HIS	-	expression tag	UNP Q9MAH0
B	-1	HIS	-	expression tag	UNP Q9MAH0
B	0	HIS	-	expression tag	UNP Q9MAH0
B	651	VAL	ALA	engineered mutation	UNP Q9MAH0
C	-6	MET	-	initiating methionine	UNP Q9MAH0
C	-5	HIS	-	expression tag	UNP Q9MAH0
C	-4	HIS	-	expression tag	UNP Q9MAH0
C	-3	HIS	-	expression tag	UNP Q9MAH0
C	-2	HIS	-	expression tag	UNP Q9MAH0
C	-1	HIS	-	expression tag	UNP Q9MAH0
C	0	HIS	-	expression tag	UNP Q9MAH0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	651	VAL	ALA	engineered mutation	UNP Q9MAH0

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C₄H₆O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0
2	A	1	Total C O 9 4 5	0	0
2	B	1	Total C O 9 4 5	0	0
2	B	1	Total C O 9 4 5	0	0
2	C	1	Total C O 9 4 5	0	0
2	C	1	Total C O 9 4 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	B	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

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

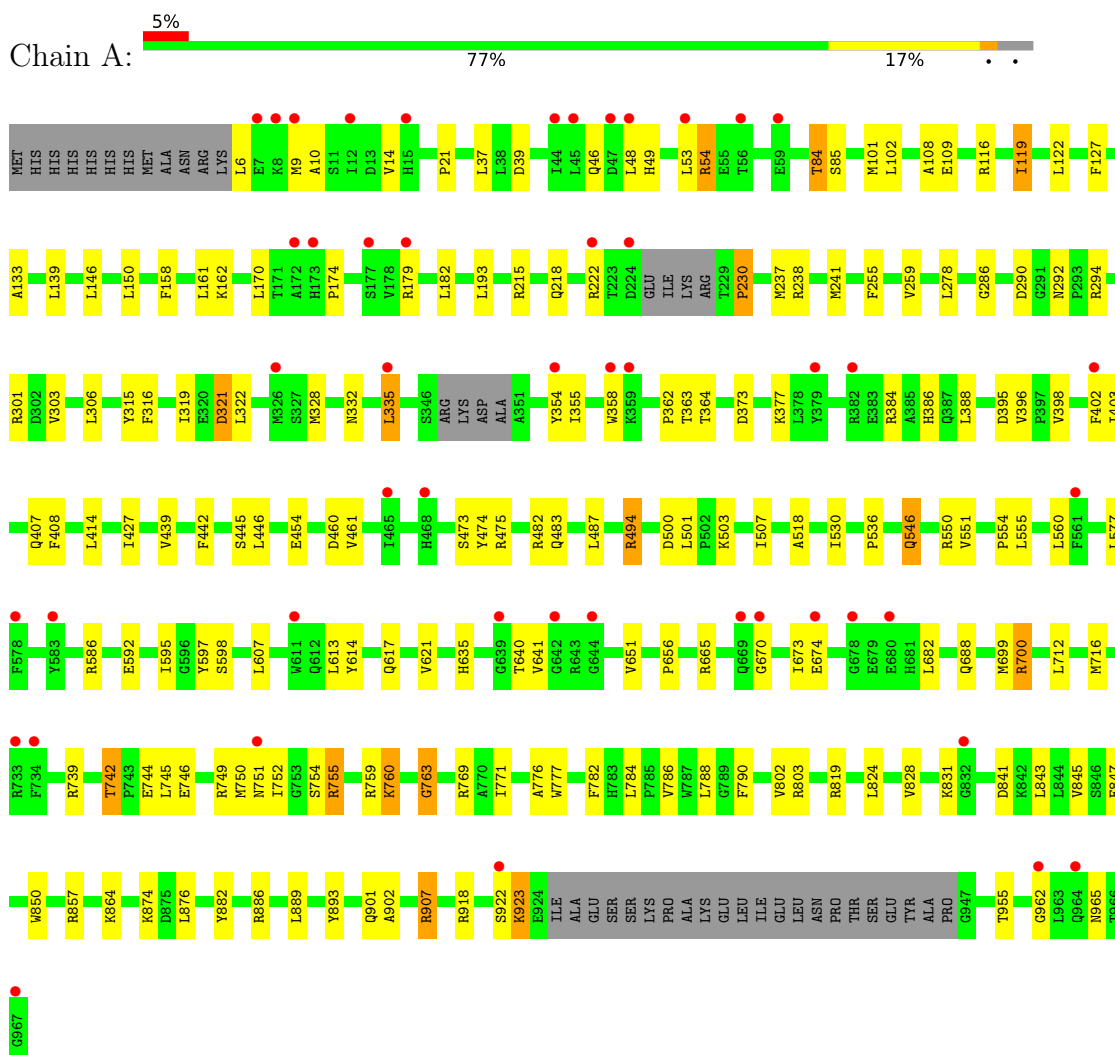
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	2	Total O 2 2	0	0

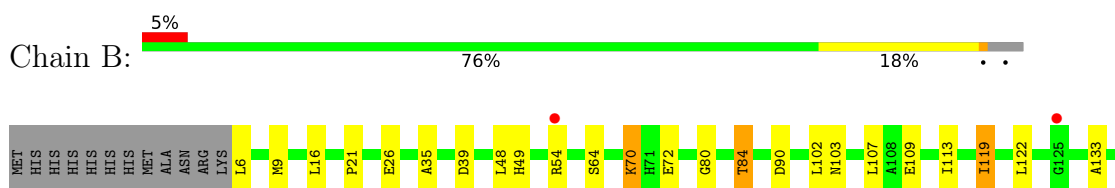
3 Residue-property plots i

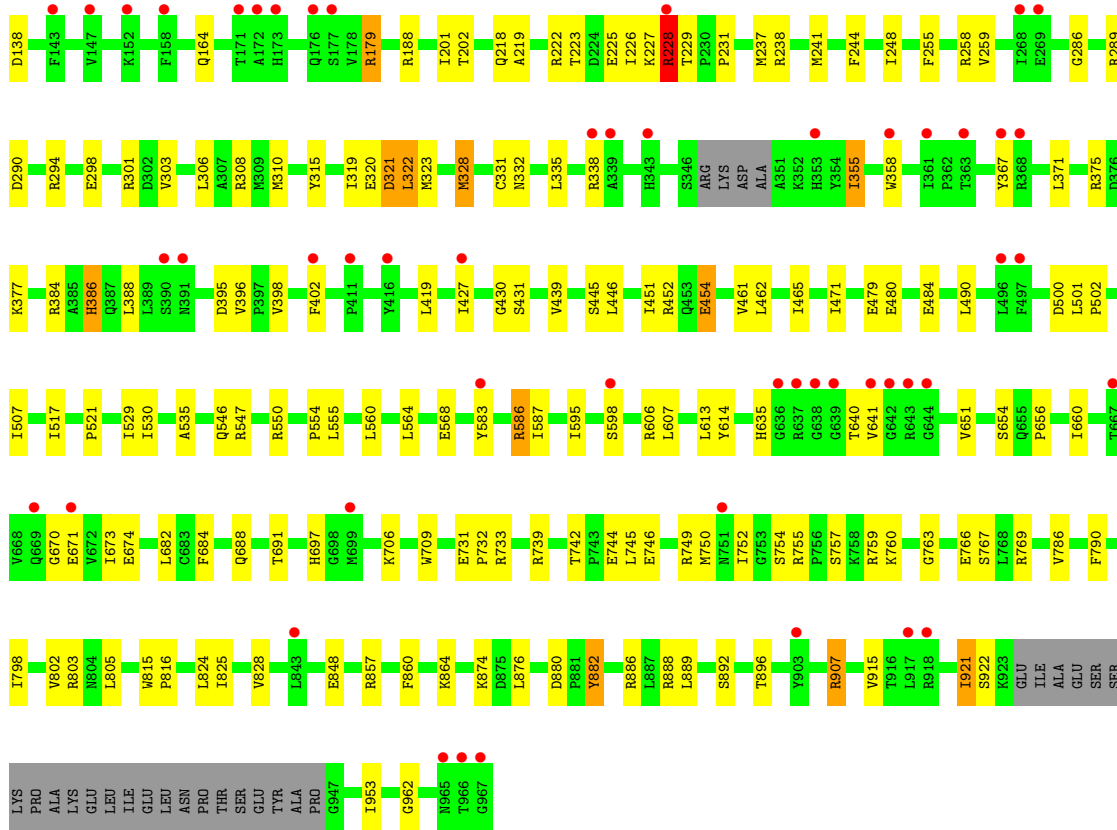
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphoenolpyruvate carboxylase 1

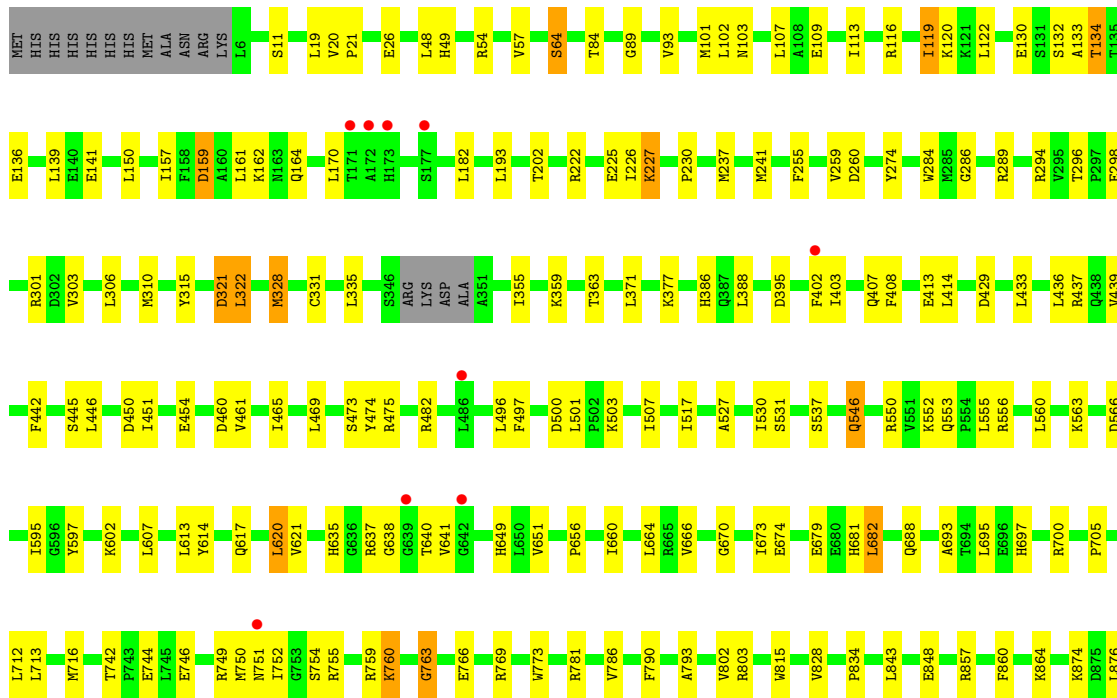
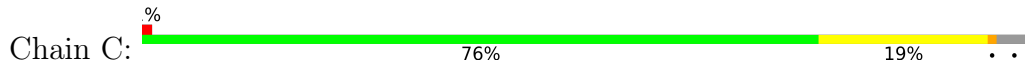


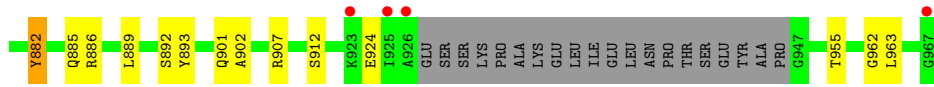
- Molecule 1: Phosphoenolpyruvate carboxylase 1





● Molecule 1: Phosphoenolpyruvate carboxylase 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	245.38Å 245.38Å 397.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.49 49.72 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.72-3.49) 86.6 (49.72-3.49)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.244 , 0.274 0.244 , 0.274	Depositor DCC
R_{free} test set	3803 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	100.9	Xtrriage
Anisotropy	0.446	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22657	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1770e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/7663	0.60	0/10369
1	B	0.36	0/7699	0.59	0/10415
1	C	0.43	0/7732	0.67	2/10459 (0.0%)
All	All	0.39	0/23094	0.62	2/31243 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	620	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	C	436	LEU	CA-CB-CG	-5.09	103.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7495	0	7458	109	0
1	B	7533	0	7515	119	0
1	C	7563	0	7550	116	0
2	A	18	0	8	3	0
2	B	18	0	8	6	0
2	C	18	0	8	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	6	0	0	0	0
4	B	2	0	0	0	0
All	All	22657	0	22547	332	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (332) 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:B:384:ARG:HG3	1:B:396:VAL:HB	1.55	0.88
1:B:746:GLU:O	1:B:750:MET:HB2	1.75	0.87
1:A:460:ASP:OD1	1:A:475:ARG:NH2	2.07	0.86
1:B:886:ARG:NH1	2:B:1002:LMR:O2	2.10	0.84
1:C:886:ARG:NH1	2:C:1002:LMR:O2	2.11	0.82
1:C:133:ALA:HB3	2:C:1002:LMR:H3	1.64	0.80
1:C:119:ILE:HD12	1:C:122:LEU:HD22	1.63	0.79
1:A:133:ALA:HB3	2:A:1002:LMR:H3	1.64	0.78
1:A:845:VAL:O	1:A:850:TRP:NE1	2.18	0.77
1:B:641:VAL:HA	1:B:651:VAL:HG11	1.69	0.75
1:B:290:ASP:OD1	1:B:759:ARG:NH2	2.21	0.74
1:A:746:GLU:O	1:A:750:MET:HB2	1.90	0.72
1:C:150:LEU:HD21	1:C:700:ARG:HE	1.55	0.70
1:B:864:LYS:HE2	1:B:876:LEU:HD11	1.74	0.70
1:B:298:GLU:OE2	1:B:301:ARG:NH1	2.24	0.70
1:A:84:THR:O	1:A:907:ARG:NH2	2.25	0.69
1:C:746:GLU:O	1:C:750:MET:HB2	1.92	0.69
1:C:460:ASP:OD1	1:C:475:ARG:NH2	2.26	0.69
1:C:760:LYS:HD3	1:C:763:GLY:H	1.58	0.69
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.74	0.69
1:B:733:ARG:NH2	1:B:848:GLU:OE2	2.25	0.69
1:B:48:LEU:HD13	1:B:222:ARG:HD3	1.75	0.69
1:A:373:ASP:OD2	1:A:377:LYS:NZ	2.27	0.68
1:A:760:LYS:HD3	1:A:763:GLY:H	1.59	0.68
1:C:546:GLN:OE1	1:C:555:LEU:N	2.27	0.67
1:A:179:ARG:NH2	1:B:358:TRP:HE1	1.93	0.66
1:A:786:VAL:HG11	1:A:828:VAL:HG21	1.76	0.66
1:B:546:GLN:OE1	1:B:555:LEU:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HG3	1:A:396:VAL:HB	1.79	0.64
1:C:641:VAL:HA	1:C:651:VAL:HG11	1.79	0.64
1:A:48:LEU:HD13	1:A:222:ARG:HD3	1.80	0.64
1:C:461:VAL:HG22	1:C:507:ILE:HG23	1.79	0.64
1:A:546:GLN:OE1	1:A:555:LEU:N	2.32	0.63
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.81	0.63
1:B:802:VAL:HG23	1:B:803:ARG:HG3	1.82	0.62
1:C:48:LEU:HD13	1:C:222:ARG:HD3	1.80	0.62
1:A:364:THR:OG1	1:B:228:ARG:NE	2.33	0.62
1:B:331:CYS:HB2	1:B:335:LEU:HD23	1.82	0.62
1:A:49:HIS:ND1	1:A:923:LYS:HA	2.15	0.62
1:C:109:GLU:HG2	1:C:886:ARG:HD2	1.82	0.62
1:A:641:VAL:HA	1:A:651:VAL:HG11	1.83	0.61
1:C:864:LYS:HE2	1:C:876:LEU:HD11	1.83	0.60
1:B:746:GLU:HG3	1:B:749:ARG:NH2	2.16	0.60
1:C:294:ARG:NH1	1:C:754:SER:O	2.35	0.60
1:B:886:ARG:NH1	2:B:1002:LMR:HO2	2.00	0.59
1:A:882:TYR:O	1:A:886:ARG:HG3	2.03	0.59
1:B:49:HIS:O	1:B:922:SER:HB3	2.02	0.59
1:C:20:VAL:HG11	1:C:885:GLN:HG3	1.84	0.59
1:B:454:GLU:CD	1:B:759:ARG:HH12	2.06	0.59
1:A:364:THR:H	1:B:228:ARG:HH21	1.50	0.59
1:B:90:ASP:CG	1:B:921:ILE:HG12	2.22	0.59
1:C:857:ARG:O	1:C:860:PHE:HB3	2.03	0.59
1:C:301:ARG:NH2	1:C:388:LEU:O	2.35	0.59
1:A:116:ARG:NH1	2:A:1002:LMR:O1B	2.34	0.58
1:C:882:TYR:O	1:C:886:ARG:HG3	2.02	0.58
1:A:802:VAL:HG23	1:A:803:ARG:HG3	1.85	0.58
1:B:907:ARG:HE	1:B:915:VAL:HG21	1.67	0.58
1:A:474:TYR:CZ	1:A:482:ARG:HD3	2.39	0.58
1:A:597:TYR:HH	1:A:635:HIS:CE1	2.22	0.58
1:A:301:ARG:NH2	1:A:388:LEU:O	2.37	0.57
1:B:750:MET:HB3	1:B:752:ILE:HG12	1.85	0.57
1:C:660:ILE:HD12	1:C:697:HIS:CG	2.40	0.57
1:B:739:ARG:HG2	1:B:745:LEU:HD21	1.87	0.57
1:A:635:HIS:HB3	1:A:641:VAL:HG21	1.86	0.56
1:C:284:TRP:CD1	1:C:450:ASP:HB2	2.40	0.56
1:A:127:PHE:HE1	1:A:819:ARG:HD2	1.71	0.56
1:C:802:VAL:HG23	1:C:803:ARG:HG3	1.88	0.56
1:B:750:MET:HB3	1:B:752:ILE:CG1	2.35	0.56
1:B:857:ARG:O	1:B:860:PHE:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD21	1:A:700:ARG:HE	1.70	0.56
1:A:750:MET:HB3	1:A:752:ILE:HG12	1.88	0.56
1:B:286:GLY:HA3	1:B:303:VAL:HG21	1.86	0.55
1:C:335:LEU:HA	1:C:414:LEU:HD21	1.88	0.55
1:A:290:ASP:CG	1:A:769:ARG:HH12	2.10	0.55
1:A:595:ILE:HD12	1:A:613:LEU:HD22	1.88	0.55
1:C:649:HIS:CD2	1:C:693:ALA:HB2	2.41	0.55
1:B:255:PHE:O	1:B:259:VAL:HG23	2.07	0.55
1:C:237:MET:O	1:C:241:MET:HG2	2.06	0.55
1:C:286:GLY:HA3	1:C:303:VAL:HG21	1.88	0.55
1:A:403:ILE:HG22	1:A:407:GLN:OE1	2.07	0.54
1:B:320:GLU:HB3	1:B:375:ARG:NH1	2.23	0.54
1:C:746:GLU:HG3	1:C:749:ARG:HH21	1.73	0.54
1:A:49:HIS:O	1:A:922:SER:HB3	2.07	0.54
1:B:635:HIS:HB3	1:B:641:VAL:HG21	1.90	0.54
1:B:500:ASP:OD1	1:B:500:ASP:N	2.37	0.54
1:C:750:MET:HB3	1:C:752:ILE:HG12	1.90	0.54
1:A:335:LEU:HD12	1:A:414:LEU:HG	1.89	0.53
1:B:614:TYR:CD2	1:B:656:PRO:HG3	2.44	0.53
1:C:501:LEU:O	1:C:503:LYS:HG3	2.09	0.53
1:A:218:GLN:HG2	1:B:427:ILE:HD11	1.89	0.53
1:B:119:ILE:HD12	1:B:122:LEU:HD22	1.89	0.53
1:A:554:PRO:HG2	1:A:586:ARG:CZ	2.39	0.53
1:A:10:ALA:O	1:A:14:VAL:HG23	2.09	0.53
1:A:864:LYS:HE2	1:A:876:LEU:HD11	1.91	0.53
1:A:750:MET:HB3	1:A:752:ILE:CG1	2.39	0.52
1:B:70:LYS:HB3	1:B:72:GLU:HG3	1.92	0.52
1:B:90:ASP:OD2	1:B:921:ILE:HG12	2.09	0.52
1:A:119:ILE:HD12	1:A:122:LEU:HD22	1.92	0.52
1:B:746:GLU:HG3	1:B:749:ARG:HH21	1.74	0.52
1:A:831:LYS:NZ	1:A:965:ASN:O	2.41	0.52
1:A:501:LEU:O	1:A:503:LYS:HG3	2.10	0.52
1:B:306:LEU:O	1:B:310:MET:HG3	2.10	0.52
1:A:640:THR:HA	1:A:824:LEU:HD12	1.91	0.51
1:B:490:LEU:O	1:B:547:ARG:NH1	2.42	0.51
1:C:635:HIS:HB3	1:C:641:VAL:HG21	1.91	0.51
1:C:19:LEU:HD21	1:C:892:SER:HB3	1.92	0.51
1:A:362:PRO:HB2	1:B:228:ARG:NH2	2.26	0.51
1:A:841:ASP:OD2	1:A:857:ARG:NH1	2.41	0.51
1:A:292:ASN:ND2	1:A:755:ARG:HB3	2.25	0.51
1:A:46:GLN:OE1	1:A:54:ARG:NH1	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ILE:HG22	1:C:682:LEU:HD11	1.91	0.51
1:C:474:TYR:CZ	1:C:482:ARG:HD3	2.46	0.51
1:B:660:ILE:HD12	1:B:697:HIS:CG	2.46	0.51
1:A:238:ARG:NE	1:B:355:ILE:O	2.40	0.50
1:C:746:GLU:HG3	1:C:749:ARG:NH2	2.26	0.50
1:C:750:MET:HB3	1:C:752:ILE:CG1	2.41	0.50
1:B:226:ILE:HG13	1:B:227:LYS:N	2.27	0.50
1:B:739:ARG:HB3	1:B:745:LEU:HD11	1.92	0.50
1:C:750:MET:O	1:C:752:ILE:N	2.42	0.50
1:A:139:LEU:HD21	1:A:259:VAL:HG22	1.94	0.50
1:C:306:LEU:O	1:C:310:MET:HG3	2.11	0.50
1:A:536:PRO:HB3	1:A:577:LEU:HG	1.93	0.49
1:B:244:PHE:HA	1:B:248:ILE:HB	1.94	0.49
1:B:64:SER:HB3	1:B:892:SER:O	2.13	0.49
1:C:403:ILE:HG22	1:C:407:GLN:OE1	2.12	0.49
1:C:335:LEU:HD12	1:C:414:LEU:HG	1.94	0.49
1:A:37:LEU:HD12	1:A:108:ALA:HB2	1.93	0.49
1:A:237:MET:O	1:A:241:MET:HG2	2.13	0.49
1:C:113:ILE:HG12	2:C:1002:LMR:O1A	2.12	0.49
1:C:64:SER:HB3	1:C:892:SER:O	2.12	0.49
1:A:294:ARG:NH1	1:A:754:SER:O	2.46	0.49
1:B:237:MET:O	1:B:241:MET:HG2	2.12	0.49
1:B:757:SER:O	1:B:769:ARG:HG2	2.12	0.49
1:A:614:TYR:CD2	1:A:656:PRO:HG3	2.48	0.48
1:B:607:LEU:HB2	1:B:790:PHE:CZ	2.48	0.48
1:C:49:HIS:CD2	1:C:924:GLU:HG3	2.48	0.48
1:B:133:ALA:H	2:B:1002:LMR:H3	1.78	0.48
1:C:901:GLN:HB2	1:C:955:THR:HB	1.95	0.48
1:C:226:ILE:HG13	1:C:227:LYS:N	2.29	0.48
1:C:712:LEU:O	1:C:716:MET:HG3	2.14	0.48
1:C:781:ARG:HD2	1:C:963:LEU:HD11	1.94	0.48
1:C:298:GLU:OE2	1:C:301:ARG:NH1	2.47	0.48
1:A:230:PRO:HG3	1:A:751:ASN:HB2	1.96	0.47
1:B:80:GLY:O	1:B:84:THR:OG1	2.32	0.47
1:B:766:GLU:H	1:B:766:GLU:CD	2.17	0.47
1:C:230:PRO:HG3	1:C:751:ASN:ND2	2.29	0.47
1:C:597:TYR:HH	1:C:635:HIS:CE1	2.27	0.47
1:A:358:TRP:HE1	1:B:179:ARG:NH2	2.11	0.47
1:B:606:ARG:HB3	1:B:790:PHE:HE1	1.79	0.47
1:B:480:GLU:O	1:B:484:GLU:HG2	2.14	0.47
1:C:607:LEU:HD13	1:C:790:PHE:CE2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:HIS:C	1:B:922:SER:HB3	2.35	0.47
1:A:109:GLU:CG	1:A:886:ARG:HD2	2.44	0.47
1:A:442:PHE:HB3	1:A:446:LEU:HD23	1.96	0.47
1:B:319:ILE:O	1:B:323:MET:HG3	2.15	0.47
1:C:255:PHE:CE1	1:C:688:GLN:HA	2.50	0.47
1:C:843:LEU:HD12	1:C:902:ALA:HB1	1.97	0.47
1:A:377:LYS:HD2	1:A:402:PHE:CE1	2.50	0.47
1:B:102:LEU:HD21	1:B:962:GLY:CA	2.45	0.47
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.97	0.47
1:B:882:TYR:O	1:B:886:ARG:HG3	2.15	0.47
1:B:301:ARG:NH2	1:B:388:LEU:O	2.48	0.46
1:C:530:ILE:O	1:C:560:LEU:HB3	2.15	0.46
1:A:742:THR:HG21	1:A:776:ALA:HB1	1.97	0.46
1:B:315:TYR:OH	1:B:439:VAL:HA	2.15	0.46
1:C:552:LYS:HE3	1:C:553:GLN:HG3	1.97	0.46
1:C:103:ASN:O	1:C:107:LEU:HG	2.16	0.46
1:C:133:ALA:HA	1:C:136:GLU:HG2	1.96	0.46
1:C:164:GLN:HE22	1:C:695:LEU:HB2	1.81	0.46
1:C:874:LYS:HA	1:C:874:LYS:HD3	1.75	0.46
1:B:320:GLU:HG3	1:B:321[A]:ASP:OD1	2.15	0.46
1:B:451:ILE:HG13	1:B:517:ILE:HD11	1.97	0.46
1:A:315:TYR:OH	1:A:439:VAL:HA	2.15	0.46
1:C:157:ILE:HG23	1:C:695:LEU:HD21	1.98	0.46
1:C:315:TYR:OH	1:C:439:VAL:HA	2.16	0.46
1:A:286:GLY:HA3	1:A:303:VAL:HG21	1.98	0.46
1:A:454:GLU:HB2	1:A:759:ARG:NH2	2.30	0.46
1:B:9:MET:HG2	1:B:39:ASP:OD1	2.16	0.46
1:A:769:ARG:HE	1:A:769:ARG:HB3	1.53	0.46
1:B:530:ILE:O	1:B:560:LEU:HB3	2.16	0.46
1:C:563:LYS:HB2	1:C:566:ASP:OD2	2.16	0.46
1:C:132:SER:OG	1:C:134:THR:HG23	2.15	0.46
1:C:182:LEU:HA	1:C:182:LEU:HD12	1.67	0.46
1:B:322:LEU:HD13	1:B:371:LEU:HD13	1.98	0.45
1:B:554:PRO:HG2	1:B:586:ARG:NH1	2.31	0.45
1:C:500:ASP:OD1	1:C:500:ASP:N	2.49	0.45
1:C:595:ILE:HD12	1:C:613:LEU:HD22	1.98	0.45
1:B:133:ALA:HB3	2:B:1002:LMR:H3	1.97	0.45
1:C:322:LEU:HD13	1:C:371:LEU:HD13	1.98	0.45
1:C:451:ILE:HG13	1:C:517:ILE:HD11	1.98	0.45
1:C:465:ILE:O	1:C:469:LEU:HG	2.16	0.45
1:C:260:ASP:CG	1:C:437:ARG:HH22	2.18	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:GLY:O	1:C:673:ILE:HG22	2.16	0.45
1:C:716:MET:HB3	1:C:793:ALA:HB1	1.99	0.45
1:B:614:TYR:CE2	1:B:656:PRO:HG3	2.52	0.45
1:C:834:PRO:HD3	1:C:860:PHE:CE1	2.52	0.45
1:A:592:GLU:OE2	1:A:665:ARG:NH1	2.49	0.45
1:C:130:GLU:O	1:C:649:HIS:HB3	2.17	0.45
1:C:496:LEU:HB3	1:C:497:PHE:HD1	1.81	0.45
1:B:113:ILE:HG12	2:B:1002:LMR:O1A	2.16	0.45
1:C:109:GLU:CD	1:C:886:ARG:HB3	2.37	0.45
1:A:777:TRP:CE3	1:A:782:PHE:HD2	2.35	0.45
1:A:784:LEU:HD21	1:A:788:LEU:HD22	1.99	0.45
1:B:103:ASN:O	1:B:107:LEU:HG	2.17	0.45
1:C:786:VAL:HG11	1:C:828:VAL:HG21	1.99	0.45
1:A:607:LEU:HD13	1:A:790:PHE:CE2	2.53	0.44
1:B:113:ILE:HG23	2:B:1002:LMR:O1A	2.17	0.44
1:C:664:LEU:HG	1:C:666:VAL:HG23	2.00	0.44
1:B:462:LEU:HD23	1:B:465:ILE:HD12	1.99	0.44
1:B:322:LEU:HD23	1:B:431:SER:HB3	2.00	0.44
1:B:109:GLU:CD	1:B:886:ARG:HB3	2.38	0.44
1:C:769:ARG:HE	1:C:769:ARG:HB3	1.40	0.44
1:B:294:ARG:NH1	1:B:754:SER:O	2.50	0.44
1:A:742:THR:CG2	1:A:776:ALA:HB1	2.47	0.44
1:B:119:ILE:CD1	1:B:122:LEU:HD22	2.48	0.44
1:A:255:PHE:CE1	1:A:688:GLN:HA	2.52	0.44
1:B:64:SER:OG	1:B:896:THR:OG1	2.22	0.44
1:C:614:TYR:CD2	1:C:656:PRO:HG3	2.53	0.44
1:C:912:SER:O	1:C:912:SER:OG	2.36	0.44
1:C:162:LYS:HB3	1:C:162:LYS:HE2	1.78	0.43
1:C:274:TYR:OH	1:C:413:GLU:HG2	2.17	0.43
1:A:377:LYS:HD2	1:A:402:PHE:CZ	2.53	0.43
1:A:483:GLN:O	1:A:487:LEU:HG	2.18	0.43
1:A:640:THR:HA	1:A:824:LEU:CD1	2.48	0.43
1:A:739:ARG:HB3	1:A:745:LEU:HD11	1.99	0.43
1:B:377:LYS:HD2	1:B:402:PHE:CE1	2.53	0.43
1:C:116:ARG:HD2	2:C:1002:LMR:O1B	2.18	0.43
1:A:746:GLU:O	1:A:750:MET:CB	2.64	0.43
1:A:174:PRO:HB3	1:A:771:ILE:CG2	2.49	0.43
1:B:164:GLN:NE2	1:B:691:THR:HG23	2.33	0.43
1:A:518:ALA:HB2	1:A:551:VAL:HG22	1.99	0.43
1:C:331:CYS:HB2	1:C:335:LEU:HD22	2.01	0.43
1:A:146:LEU:HD22	1:A:699:MET:SD	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:ARG:HD3	1:B:825:ILE:HD11	2.01	0.43
1:B:874:LYS:HD3	1:B:874:LYS:HA	1.79	0.43
1:A:355:ILE:O	1:B:238:ARG:NE	2.49	0.43
1:B:219:ALA:O	1:B:223:THR:HG23	2.19	0.43
1:A:670:GLY:O	1:A:673:ILE:HG22	2.18	0.43
1:C:20:VAL:CG1	1:C:885:GLN:HG3	2.47	0.43
1:C:139:LEU:HD21	1:C:259:VAL:HG22	2.00	0.43
1:C:617:GLN:O	1:C:621:VAL:HG23	2.19	0.43
1:A:886:ARG:NH1	2:A:1002:LMR:O2	2.52	0.43
1:B:16:LEU:HD12	1:B:35:ALA:HB2	2.01	0.42
1:C:226:ILE:HG13	1:C:227:LYS:HG3	2.01	0.42
1:C:255:PHE:O	1:C:259:VAL:HG23	2.18	0.42
1:C:637[B]:ARG:HG2	1:C:638:GLY:H	1.84	0.42
1:A:215:ARG:HD2	1:B:430:GLY:HA3	2.00	0.42
1:C:89:GLY:O	1:C:93:VAL:HG23	2.20	0.42
1:C:120:LYS:NZ	1:C:141:GLU:OE2	2.43	0.42
1:C:294:ARG:O	1:C:296:THR:HG23	2.19	0.42
1:A:750:MET:O	1:A:752:ILE:N	2.51	0.42
1:C:159:ASP:HA	1:C:162:LYS:HD3	2.01	0.42
1:A:427:ILE:HD11	1:B:218:GLN:HG2	2.01	0.42
1:A:874:LYS:HD3	1:A:874:LYS:HA	1.77	0.42
1:B:479:GLU:CD	1:B:535:ALA:HB1	2.39	0.42
1:B:670:GLY:O	1:B:673:ILE:HG22	2.20	0.42
1:B:815:TRP:HD1	1:B:816:PRO:HD2	1.85	0.42
1:C:377:LYS:HD2	1:C:402:PHE:CE1	2.55	0.42
1:B:102:LEU:HD21	1:B:962:GLY:HA3	2.01	0.42
1:C:161:LEU:HD23	1:C:161:LEU:HA	1.83	0.42
1:C:230:PRO:HG3	1:C:751:ASN:HD22	1.85	0.42
1:B:258:ARG:HG2	1:B:684:PHE:HZ	1.84	0.42
1:B:328:MET:SD	1:B:328:MET:N	2.93	0.42
1:C:660:ILE:HD12	1:C:697:HIS:ND1	2.35	0.42
1:A:316:PHE:O	1:A:319:ILE:HG22	2.19	0.42
1:A:901:GLN:HB2	1:A:955:THR:HB	2.01	0.42
1:B:229:THR:HG23	1:B:231:PRO:HA	2.02	0.42
1:B:445:SER:O	1:B:446:LEU:HB2	2.19	0.42
1:C:230:PRO:HG3	1:C:751:ASN:HB2	2.02	0.42
1:A:102:LEU:HD21	1:A:962:GLY:CA	2.50	0.42
1:A:847:GLU:HA	1:A:850:TRP:CD2	2.55	0.42
1:B:880:ASP:OD1	1:B:882:TYR:HD1	2.02	0.42
1:A:712:LEU:O	1:A:716:MET:HG3	2.20	0.42
1:B:367:TYR:CE1	1:B:419:LEU:HG	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:ARG:HB2	1:B:767:SER:O	2.19	0.42
1:A:230:PRO:CG	1:A:751:ASN:HB2	2.50	0.42
1:B:706:LYS:HD2	1:B:709:TRP:CZ2	2.54	0.42
1:C:766:GLU:CD	1:C:766:GLU:H	2.22	0.42
1:A:161:LEU:O	1:A:278:LEU:HD11	2.20	0.41
1:A:292:ASN:CG	1:A:755:ARG:HB3	2.40	0.41
1:A:355:ILE:HD13	1:B:386:HIS:CE1	2.55	0.41
1:A:617:GLN:O	1:A:621:VAL:HG23	2.20	0.41
1:B:138:ASP:HB2	1:B:688:GLN:OE1	2.19	0.41
1:B:332:ASN:HB3	1:B:335:LEU:H	1.84	0.41
1:B:201:ILE:HD12	1:B:201:ILE:HA	1.81	0.41
1:A:158:PHE:CE2	1:A:162:LYS:HD2	2.54	0.41
1:C:102:LEU:HD21	1:C:962:GLY:CA	2.49	0.41
1:C:442:PHE:HB3	1:C:446:LEU:HA	2.03	0.41
1:C:49:HIS:NE2	1:C:924:GLU:HG3	2.35	0.41
1:C:445:SER:O	1:C:446:LEU:HB2	2.21	0.41
1:A:101:MET:HB3	1:A:893:TYR:CE1	2.55	0.41
1:B:595:ILE:HD12	1:B:613:LEU:HD22	2.01	0.41
1:C:705:PRO:HB3	1:C:815:TRP:CZ2	2.55	0.41
1:A:9:MET:HG2	1:A:39:ASP:CG	2.41	0.41
1:B:731:GLU:HA	1:B:732:PRO:HD3	1.96	0.41
1:B:798:ILE:HD11	1:B:805:LEU:HD13	2.02	0.41
1:C:531:SER:HA	1:C:560:LEU:HD23	2.03	0.41
1:A:332:ASN:HB3	1:A:335:LEU:H	1.86	0.41
1:C:101:MET:HB3	1:C:893:TYR:CE1	2.56	0.41
1:C:454:GLU:HB2	1:C:759:ARG:NH2	2.36	0.41
1:C:679:GLU:OE1	1:C:681:HIS:N	2.53	0.41
1:A:445:SER:O	1:A:446:LEU:HB2	2.21	0.41
1:A:530:ILE:O	1:A:560:LEU:HB3	2.21	0.41
1:C:713:LEU:HD23	1:C:713:LEU:HA	1.86	0.41
1:A:102:LEU:HD21	1:A:962:GLY:HA3	2.03	0.40
1:B:750:MET:O	1:B:752:ILE:N	2.50	0.40
1:C:328:MET:SD	1:C:328:MET:N	2.94	0.40
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.90	0.40
1:A:321[B]:ASP:OD2	1:B:188:ARG:NH2	2.54	0.40
1:A:843:LEU:HD12	1:A:902:ALA:HB1	2.03	0.40
1:B:452:ARG:HA	1:B:529:ILE:O	2.21	0.40
1:B:564:LEU:O	1:B:568:GLU:HG3	2.21	0.40
1:B:706:LYS:HD2	1:B:709:TRP:CE2	2.56	0.40
1:C:57:VAL:HG11	1:C:101:MET:HE1	2.02	0.40
1:A:494:ARG:H	1:A:494:ARG:HG2	1.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:CZ	1:B:521:PRO:HG2	2.51	0.40
1:C:429:ASP:HA	1:C:433:LEU:HB2	2.04	0.40
1:A:255:PHE:O	1:A:259:VAL:HG23	2.22	0.40
1:B:501:LEU:HA	1:B:502:PRO:HD2	1.98	0.40
1:B:583:TYR:CE2	1:B:587:ILE:HG21	2.56	0.40
1:B:640:THR:HA	1:B:824:LEU:CD1	2.52	0.40
1:C:527:ALA:HB2	1:C:556:ARG:CZ	2.52	0.40
1:C:620:LEU:HA	1:C:620:LEU:HD23	1.90	0.40
1:A:85:SER:O	1:A:918:ARG:N	2.51	0.40
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.96	0.40
1:A:500:ASP:OD1	1:A:500:ASP:N	2.46	0.40
1:B:752:ILE:HD11	1:B:953:ILE:HG12	2.03	0.40
1:C:602:LYS:HG3	1:C:773:TRP:CD1	2.56	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	927/974 (95%)	888 (96%)	33 (4%)	6 (1%)	25	63
1	B	931/974 (96%)	889 (96%)	37 (4%)	5 (0%)	29	66
1	C	935/974 (96%)	892 (95%)	39 (4%)	4 (0%)	34	70
All	All	2793/2922 (96%)	2669 (96%)	109 (4%)	15 (0%)	29	66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	395	ASP
1	A	923	LYS
1	B	395	ASP
1	C	395	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	763	GLY
1	B	763	GLY
1	C	763	GLY
1	B	21	PRO
1	C	227	LYS
1	A	21	PRO
1	B	228	ARG
1	A	354	TYR
1	B	921	ILE
1	C	21	PRO
1	A	230	PRO

5.3.2 Protein sidechains [i](#)

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	812/850 (96%)	781 (96%)	31 (4%)	33	64
1	B	818/850 (96%)	782 (96%)	36 (4%)	28	60
1	C	821/850 (97%)	784 (96%)	37 (4%)	27	60
All	All	2451/2550 (96%)	2347 (96%)	104 (4%)	30	61

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	53	LEU
1	A	54	ARG
1	A	84	THR
1	A	119	ILE
1	A	170	LEU
1	A	193	LEU
1	A	321[A]	ASP
1	A	321[B]	ASP
1	A	322	LEU
1	A	328	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	335	LEU
1	A	363	THR
1	A	386	HIS
1	A	398	VAL
1	A	408	PHE
1	A	473	SER
1	A	494	ARG
1	A	546	GLN
1	A	550	ARG
1	A	598	SER
1	A	674	GLU
1	A	682	LEU
1	A	700	ARG
1	A	742	THR
1	A	744	GLU
1	A	749	ARG
1	A	755	ARG
1	A	760	LYS
1	A	889	LEU
1	A	907	ARG
1	B	6	LEU
1	B	26	GLU
1	B	54	ARG
1	B	70	LYS
1	B	84	THR
1	B	119	ILE
1	B	179	ARG
1	B	202	THR
1	B	225	GLU
1	B	228	ARG
1	B	289	ARG
1	B	321[A]	ASP
1	B	321[B]	ASP
1	B	322	LEU
1	B	328	MET
1	B	338	ARG
1	B	355	ILE
1	B	386	HIS
1	B	398	VAL
1	B	454	GLU
1	B	471	ILE
1	B	550	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	586	ARG
1	B	598	SER
1	B	654	SER
1	B	671	GLU
1	B	674	GLU
1	B	682	LEU
1	B	742	THR
1	B	744	GLU
1	B	755	ARG
1	B	760	LYS
1	B	882	TYR
1	B	888	ARG
1	B	889	LEU
1	B	907	ARG
1	C	11	SER
1	C	26	GLU
1	C	54	ARG
1	C	64	SER
1	C	84	THR
1	C	119	ILE
1	C	134	THR
1	C	159	ASP
1	C	170	LEU
1	C	193	LEU
1	C	202	THR
1	C	225	GLU
1	C	289	ARG
1	C	321[A]	ASP
1	C	321[B]	ASP
1	C	322	LEU
1	C	328	MET
1	C	355	ILE
1	C	359	LYS
1	C	363	THR
1	C	386	HIS
1	C	408	PHE
1	C	473	SER
1	C	537	SER
1	C	546	GLN
1	C	550	ARG
1	C	640	THR
1	C	674	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	682	LEU
1	C	742	THR
1	C	744	GLU
1	C	755	ARG
1	C	760	LYS
1	C	848	GLU
1	C	882	TYR
1	C	889	LEU
1	C	907	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
2	LMR	C	1002	-	8,8,8	1.57	1 (12%)	10,10,10	1.93	3 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMR	C	1001	-	8,8,8	1.57	1 (12%)	10,10,10	1.64	1 (10%)
2	LMR	B	1001	-	8,8,8	1.54	1 (12%)	10,10,10	1.53	1 (10%)
2	LMR	A	1001	-	8,8,8	1.43	1 (12%)	10,10,10	1.59	1 (10%)
2	LMR	A	1002	-	8,8,8	1.42	1 (12%)	10,10,10	1.47	3 (30%)
2	LMR	B	1002	-	8,8,8	1.44	1 (12%)	10,10,10	2.07	2 (20%)

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
2	LMR	C	1002	-	-	3/8/8/8	-
2	LMR	C	1001	-	-	1/8/8/8	-
2	LMR	B	1001	-	-	6/8/8/8	-
2	LMR	A	1001	-	-	1/8/8/8	-
2	LMR	A	1002	-	-	6/8/8/8	-
2	LMR	B	1002	-	-	1/8/8/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	LMR	C2-C1	-3.55	1.47	1.52
2	B	1001	LMR	C2-C1	-3.44	1.47	1.52
2	C	1002	LMR	C2-C1	-3.36	1.47	1.52
2	A	1001	LMR	C2-C1	-2.70	1.48	1.52
2	A	1002	LMR	C2-C1	-2.25	1.48	1.52
2	B	1002	LMR	C2-C1	-2.22	1.48	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1002	LMR	O1B-C1-C2	4.63	122.90	112.72
2	C	1002	LMR	O1B-C1-C2	4.27	122.10	112.72
2	A	1001	LMR	O1B-C1-C2	3.45	120.31	112.72
2	C	1001	LMR	O1B-C1-C2	3.30	119.96	112.72
2	B	1001	LMR	O1B-C1-C2	3.00	119.32	112.72
2	B	1002	LMR	O1B-C1-O1A	-2.74	117.86	124.09
2	A	1002	LMR	O1B-C1-C2	2.72	118.69	112.72
2	A	1002	LMR	O4A-C4-C3	2.30	121.44	114.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1002	LMR	O1B-C1-O1A	-2.17	119.17	124.09
2	C	1002	LMR	O1B-C1-O1A	-2.16	119.18	124.09
2	C	1002	LMR	O4A-C4-C3	2.14	120.92	114.07

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	LMR	O2-C2-C3-C4
2	C	1002	LMR	O1A-C1-C2-O2
2	C	1002	LMR	O1B-C1-C2-O2
2	B	1001	LMR	C1-C2-C3-C4
2	A	1002	LMR	O1A-C1-C2-O2
2	A	1002	LMR	O1B-C1-C2-C3
2	B	1001	LMR	O1A-C1-C2-C3
2	B	1001	LMR	O1B-C1-C2-C3
2	B	1002	LMR	O1B-C1-C2-C3
2	A	1002	LMR	C2-C3-C4-O4A
2	A	1002	LMR	C2-C3-C4-O4B
2	A	1002	LMR	O1B-C1-C2-O2
2	B	1001	LMR	O1A-C1-C2-O2
2	B	1001	LMR	O1B-C1-C2-O2
2	C	1001	LMR	O1B-C1-C2-O2
2	A	1001	LMR	O1B-C1-C2-C3
2	A	1002	LMR	O1A-C1-C2-C3
2	C	1002	LMR	O1A-C1-C2-C3

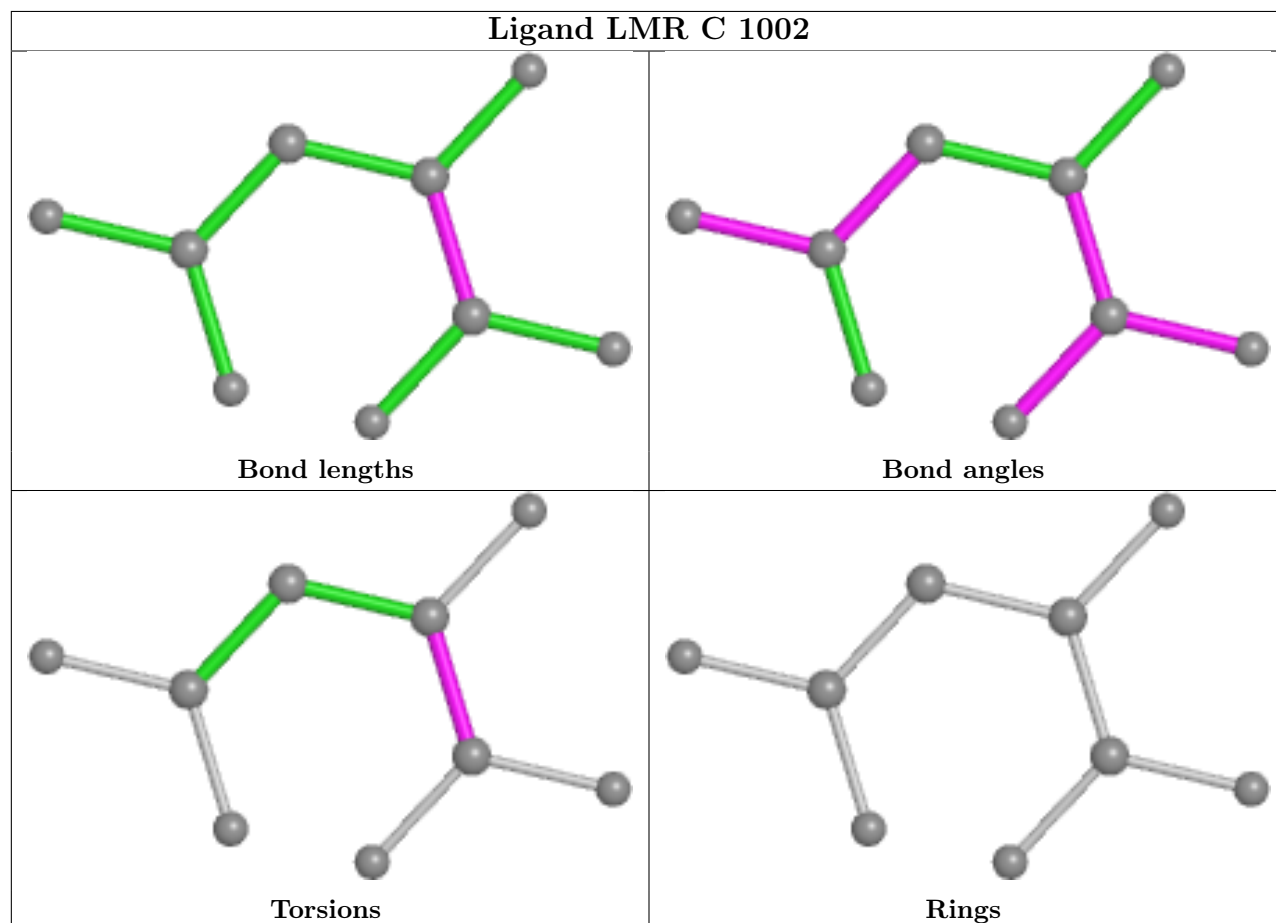
There are no ring outliers.

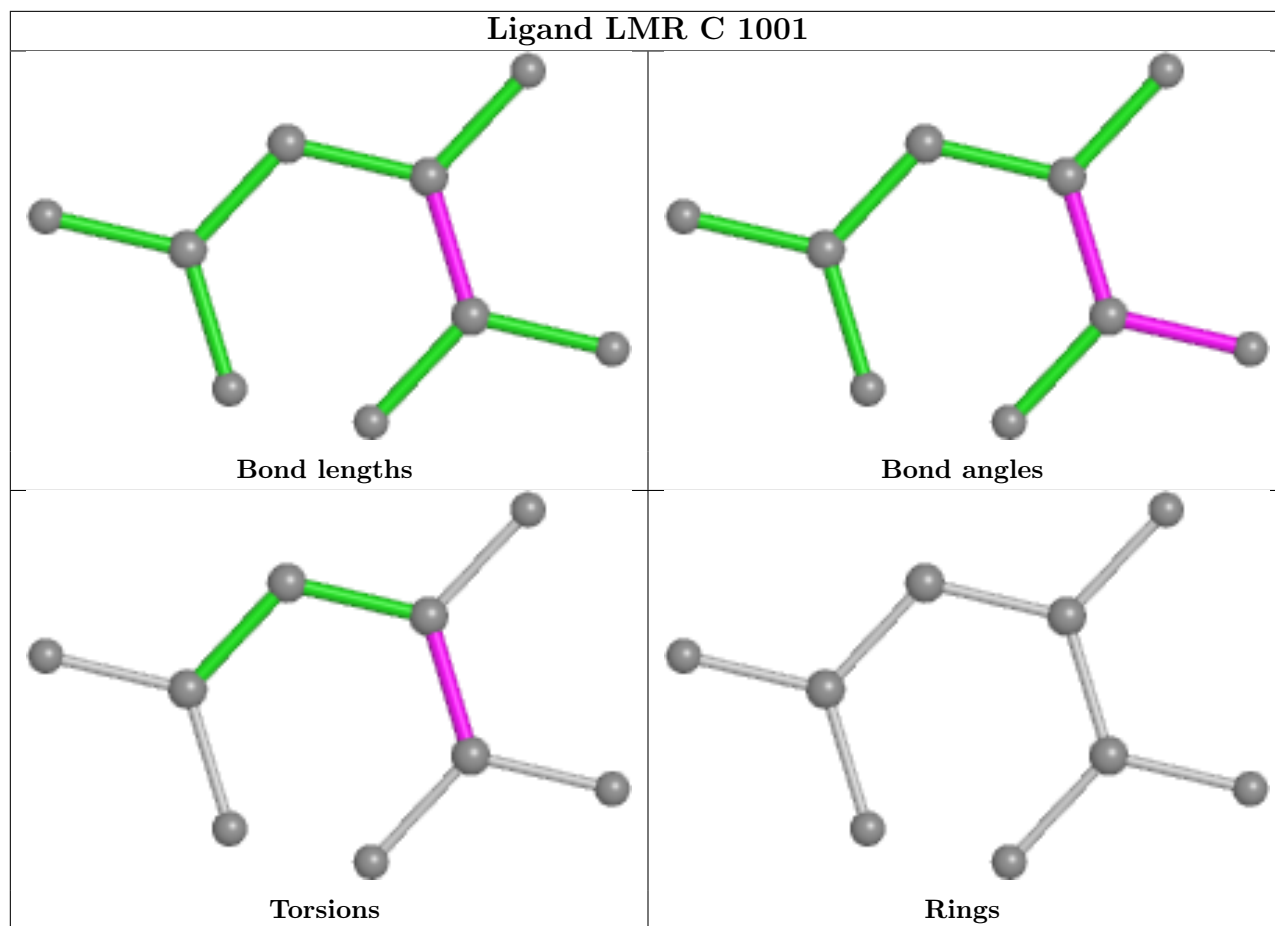
3 monomers are involved in 13 short contacts:

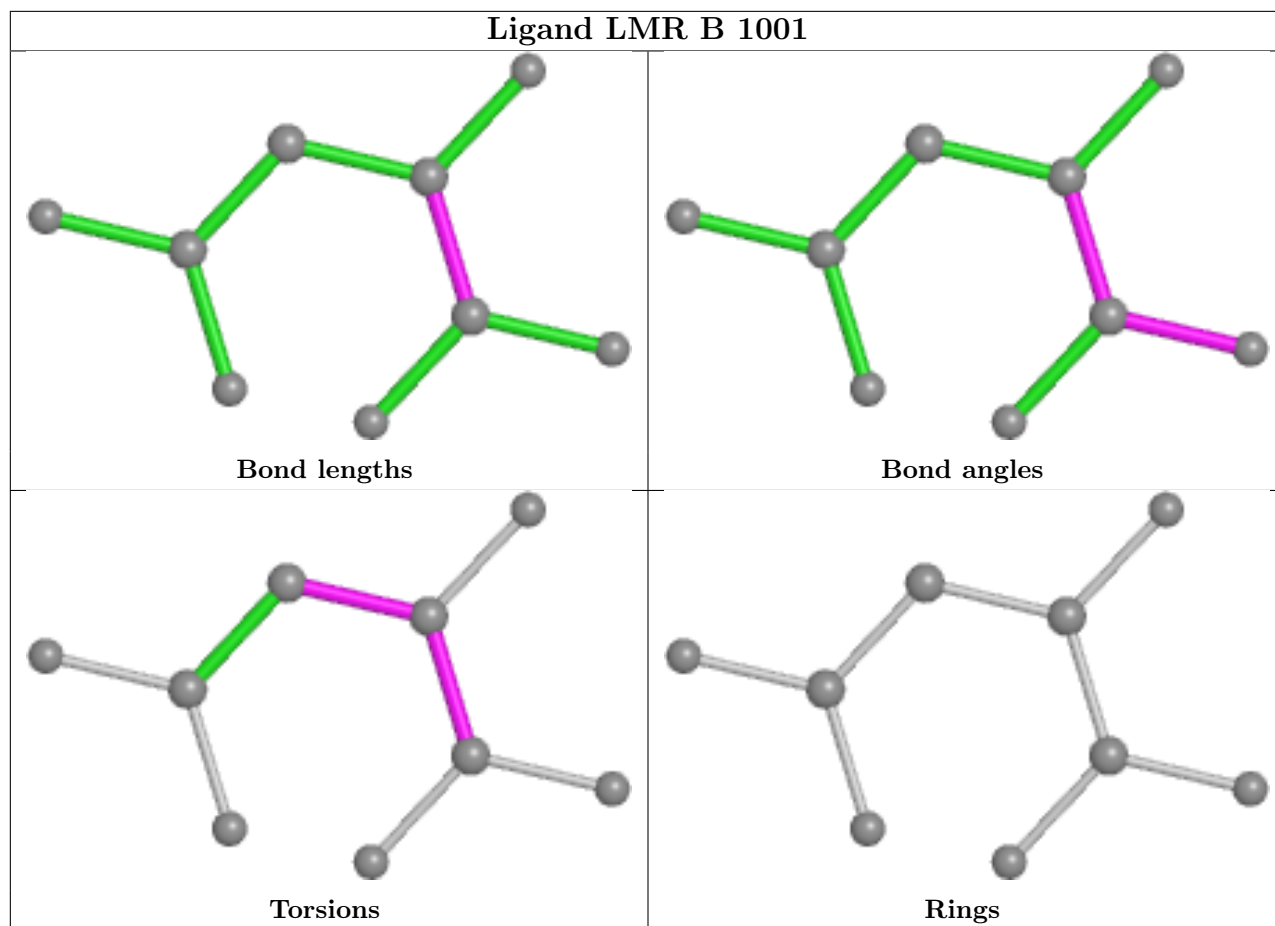
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1002	LMR	4	0
2	A	1002	LMR	3	0
2	B	1002	LMR	6	0

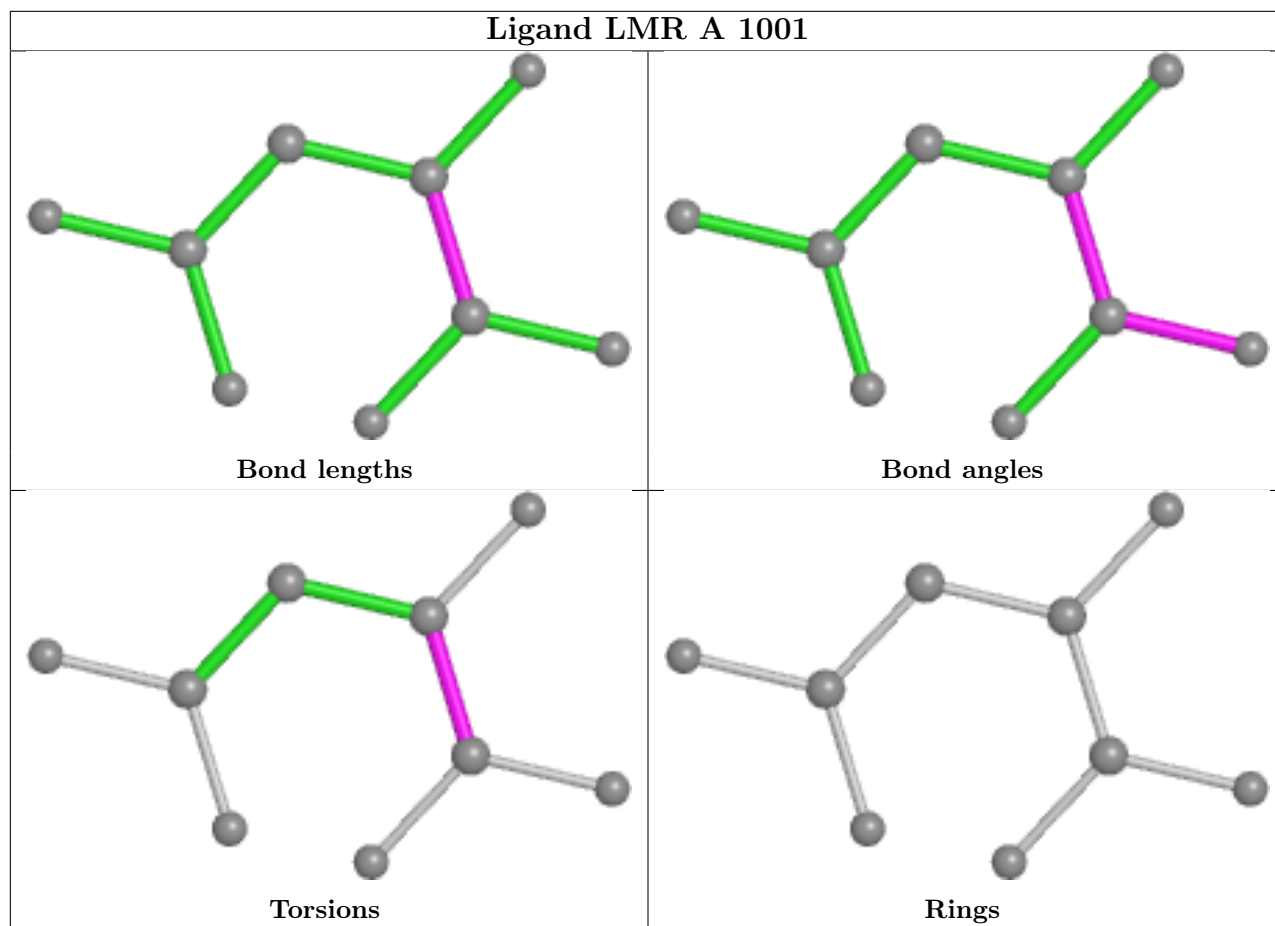
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

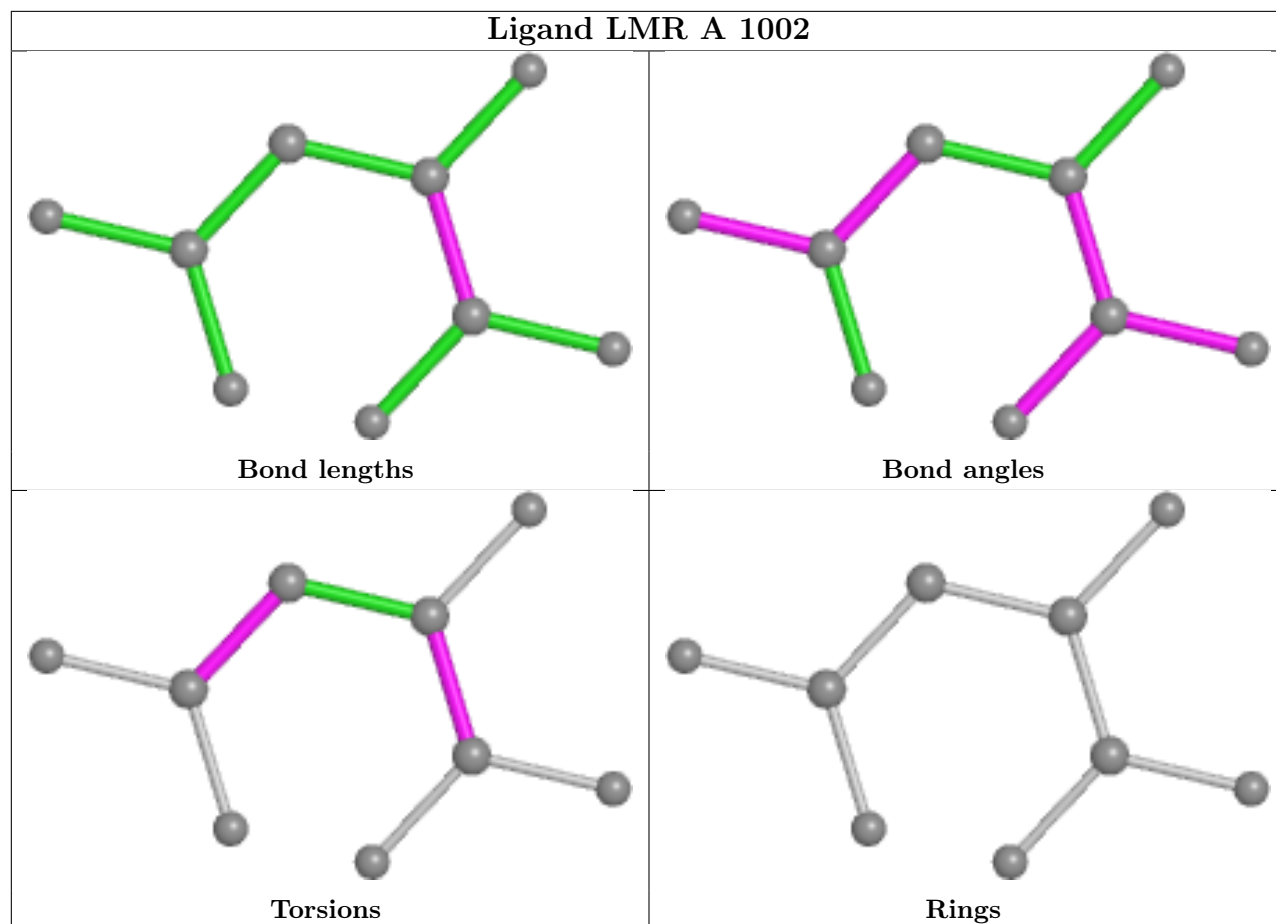
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

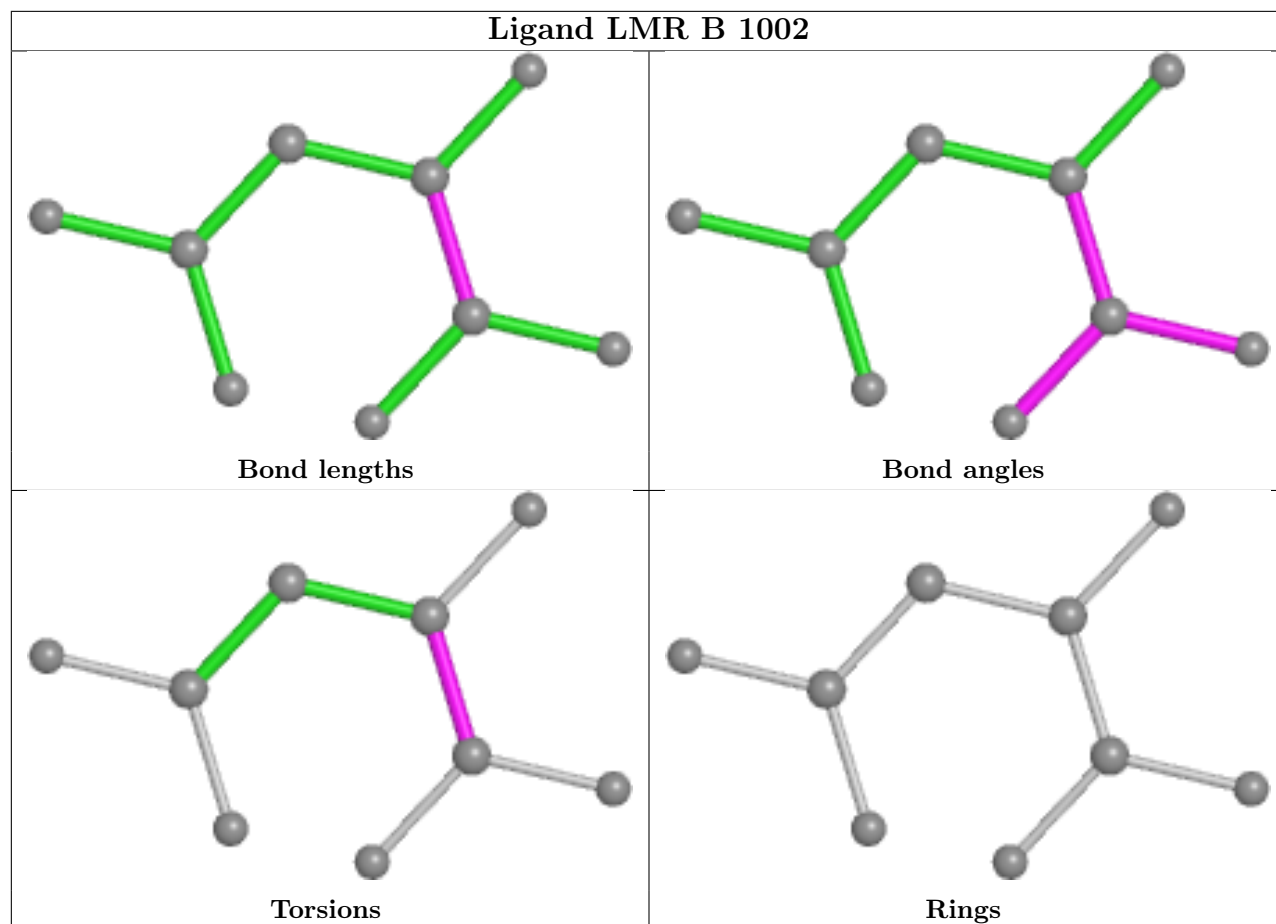












5.7 Other polymers [i](#)

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	932/974 (95%)	0.23	48 (5%) 27 26	90, 139, 205, 283	0
1	B	935/974 (95%)	0.36	53 (5%) 23 22	103, 153, 203, 280	0
1	C	938/974 (96%)	-0.07	13 (1%) 75 71	62, 97, 155, 289	0
All	All	2805/2922 (95%)	0.17	114 (4%) 37 35	62, 134, 195, 289	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	642	GLY	8.0
1	B	637[A]	ARG	5.6
1	C	172	ALA	4.9
1	C	926	ALA	4.5
1	B	171	THR	4.5
1	B	152	LYS	4.3
1	B	143	PHE	4.3
1	A	751	ASN	4.2
1	B	967	GLY	4.1
1	A	47	ASP	4.1
1	B	172	ALA	4.1
1	C	177	SER	4.0
1	B	669	GLN	4.0
1	A	642	GLY	4.0
1	B	966	THR	4.0
1	A	177	SER	3.9
1	B	402	PHE	3.8
1	A	639	GLY	3.8
1	C	642	GLY	3.8
1	B	639	GLY	3.6
1	B	917	LEU	3.6
1	B	965	ASN	3.6
1	A	8	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	224	ASP	3.4
1	A	48	LEU	3.4
1	B	269	GLU	3.4
1	C	402	PHE	3.4
1	A	56	THR	3.4
1	A	402	PHE	3.3
1	B	268	ILE	3.2
1	B	843	LEU	3.2
1	A	335	LEU	3.2
1	B	353	HIS	3.2
1	B	361	ILE	3.1
1	B	644	GLY	3.1
1	B	173	HIS	3.1
1	B	638	GLY	3.1
1	C	171	THR	3.1
1	B	497	PHE	3.1
1	B	636	GLY	3.1
1	B	147	VAL	3.0
1	B	177	SER	3.0
1	B	427	ILE	3.0
1	B	363	THR	2.9
1	C	751	ASN	2.9
1	A	359	LYS	2.9
1	A	53	LEU	2.9
1	A	45	LEU	2.9
1	B	54	ARG	2.8
1	A	680	GLU	2.8
1	A	922	SER	2.8
1	A	44	ILE	2.8
1	B	643	ARG	2.8
1	B	699	MET	2.8
1	B	391	ASN	2.7
1	C	925	ILE	2.7
1	B	125	GLY	2.7
1	B	598	SER	2.7
1	A	9	MET	2.7
1	B	496	LEU	2.7
1	A	358	TRP	2.7
1	C	923	LYS	2.6
1	A	465	ILE	2.5
1	A	964	GLN	2.5
1	A	962	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	12	ILE	2.5
1	A	382	ARG	2.5
1	B	338	ARG	2.5
1	A	15	HIS	2.4
1	B	358	TRP	2.4
1	A	7	GLU	2.4
1	C	173	HIS	2.4
1	B	903	TYR	2.4
1	A	669	GLN	2.4
1	C	967	GLY	2.3
1	C	486	LEU	2.3
1	A	561	PHE	2.3
1	A	222	ARG	2.3
1	A	59	GLU	2.3
1	B	583	TYR	2.3
1	A	326	MET	2.3
1	B	176	GLN	2.3
1	B	667	THR	2.3
1	B	411	PRO	2.3
1	A	172	ALA	2.3
1	B	390	SER	2.2
1	A	967	GLY	2.2
1	B	416	TYR	2.2
1	B	751	ASN	2.2
1	B	671	GLU	2.2
1	B	367	TYR	2.2
1	A	733	ARG	2.2
1	A	578	PHE	2.2
1	A	173	HIS	2.2
1	A	379	TYR	2.2
1	A	832	GLY	2.2
1	C	639	GLY	2.1
1	B	158	PHE	2.1
1	A	468	HIS	2.1
1	B	641	VAL	2.1
1	A	670	GLY	2.1
1	B	368	ARG	2.1
1	B	228	ARG	2.1
1	B	918	ARG	2.1
1	A	611	TRP	2.0
1	A	644	GLY	2.0
1	A	678	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	ARG	2.0
1	A	354	TYR	2.0
1	B	339	ALA	2.0
1	A	734	PHE	2.0
1	A	674	GLU	2.0
1	B	343	HIS	2.0
1	A	583	TYR	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](#)

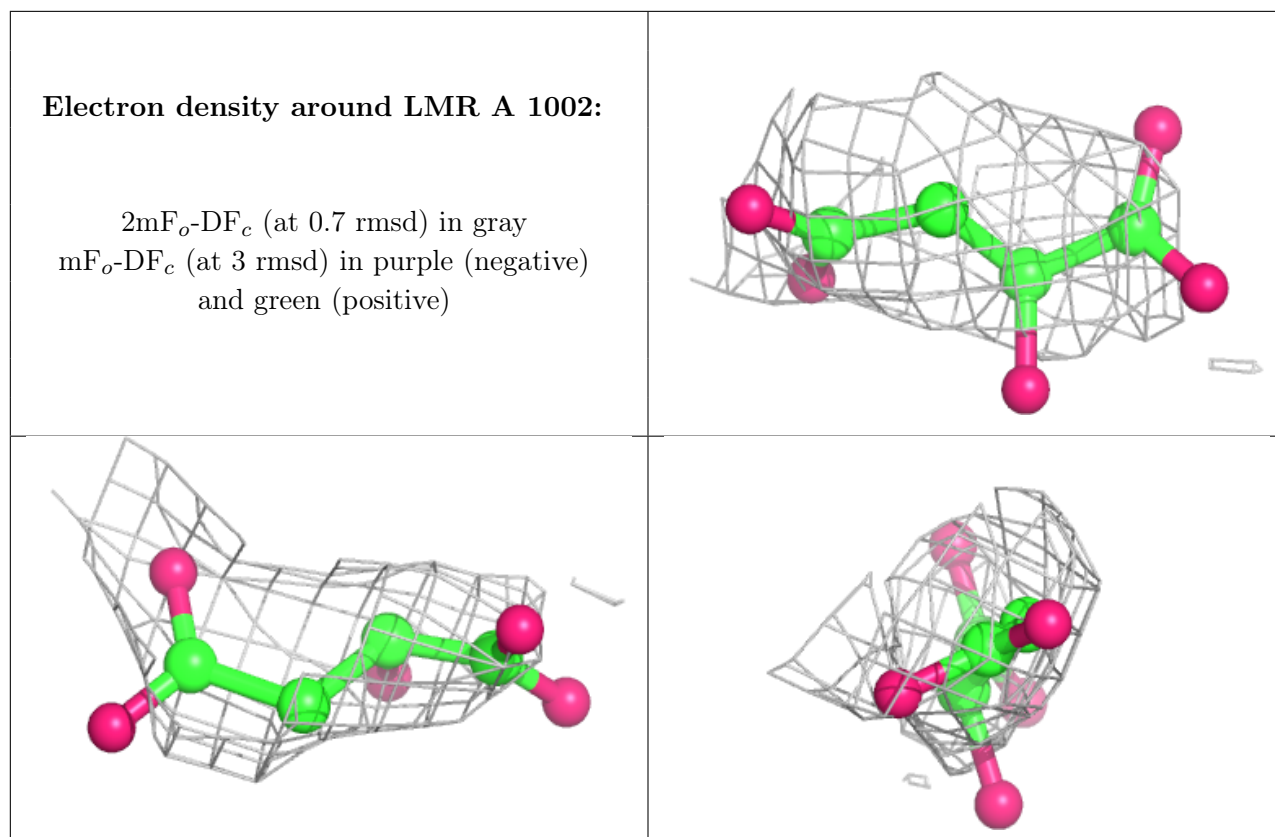
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

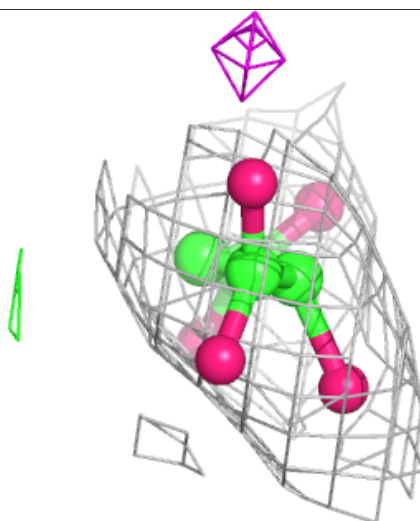
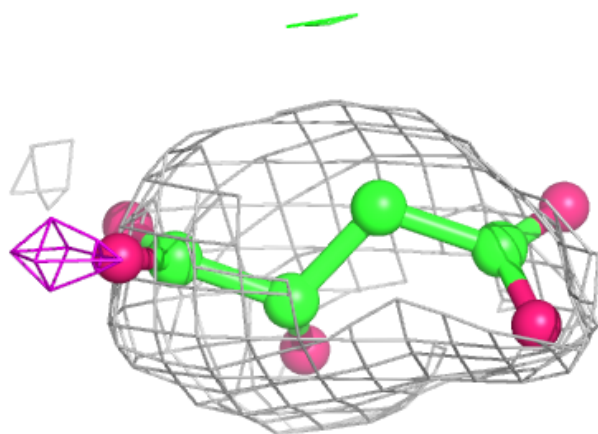
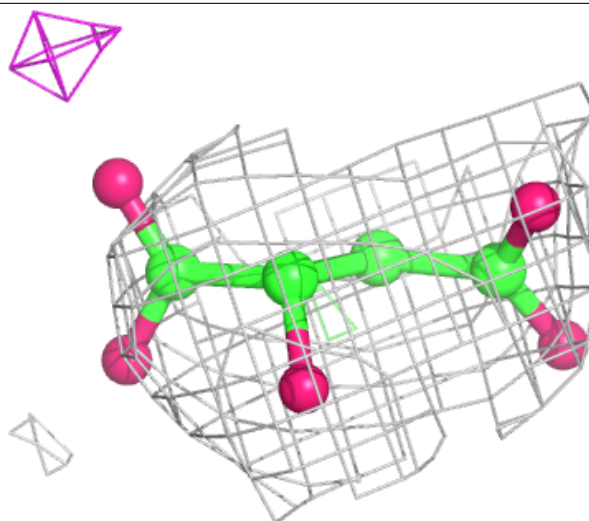
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMR	A	1002	9/9	0.69	0.49	159,161,169,171	0
3	CL	B	1003	1/1	0.69	1.20	128,128,128,128	0
3	CL	A	1004	1/1	0.70	0.59	104,104,104,104	0
3	CL	A	1003	1/1	0.70	0.46	166,166,166,166	0
2	LMR	B	1002	9/9	0.80	0.33	97,129,140,141	0
2	LMR	C	1002	9/9	0.81	0.35	120,129,137,139	0
3	CL	C	1003	1/1	0.88	0.94	96,96,96,96	0
2	LMR	A	1001	9/9	0.90	0.54	165,176,186,202	0
2	LMR	C	1001	9/9	0.94	0.38	117,124,132,136	0
2	LMR	B	1001	9/9	0.94	0.57	154,156,164,171	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.



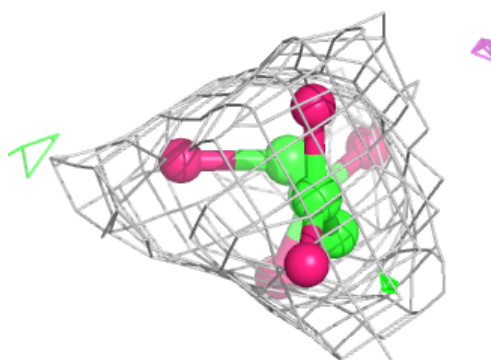
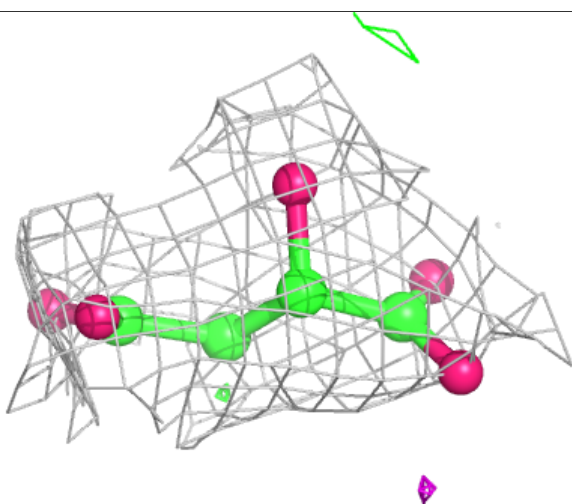
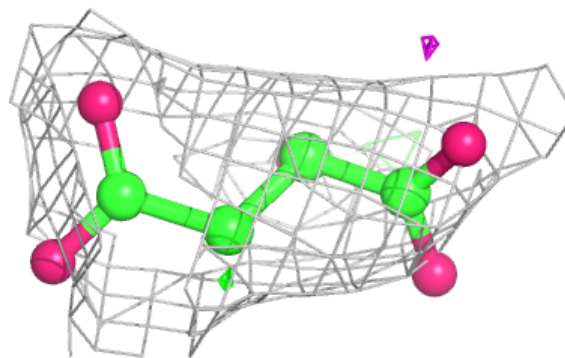
Electron density around LMR B 1002:

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



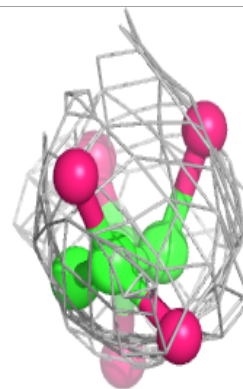
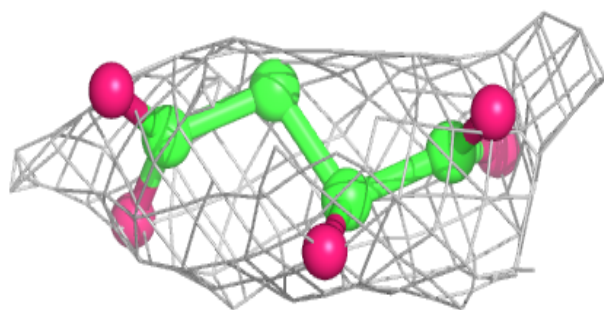
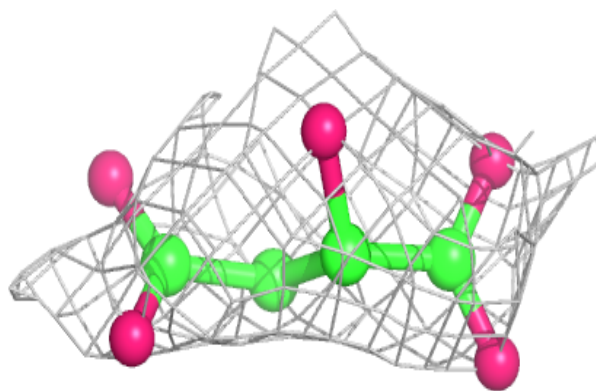
Electron density around LMR C 1002:

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



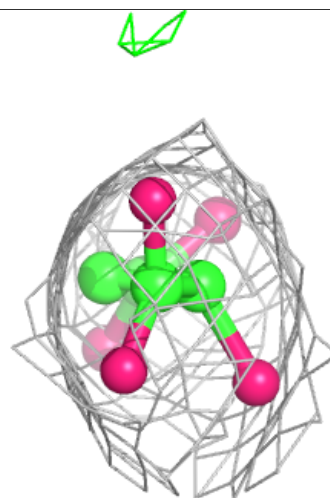
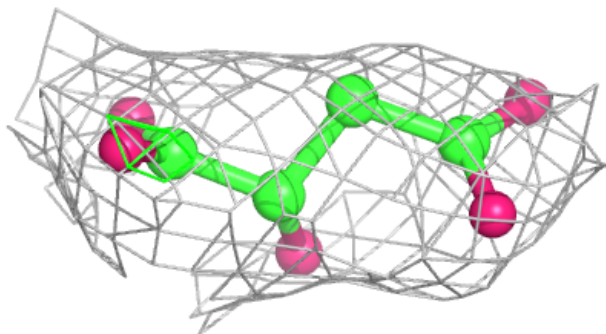
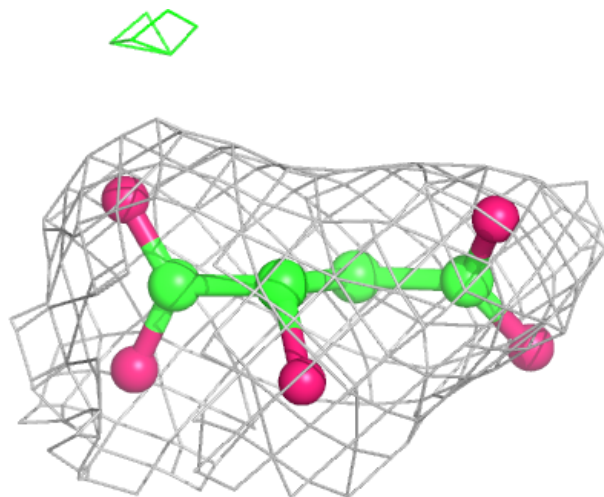
Electron density around LMR A 1001:

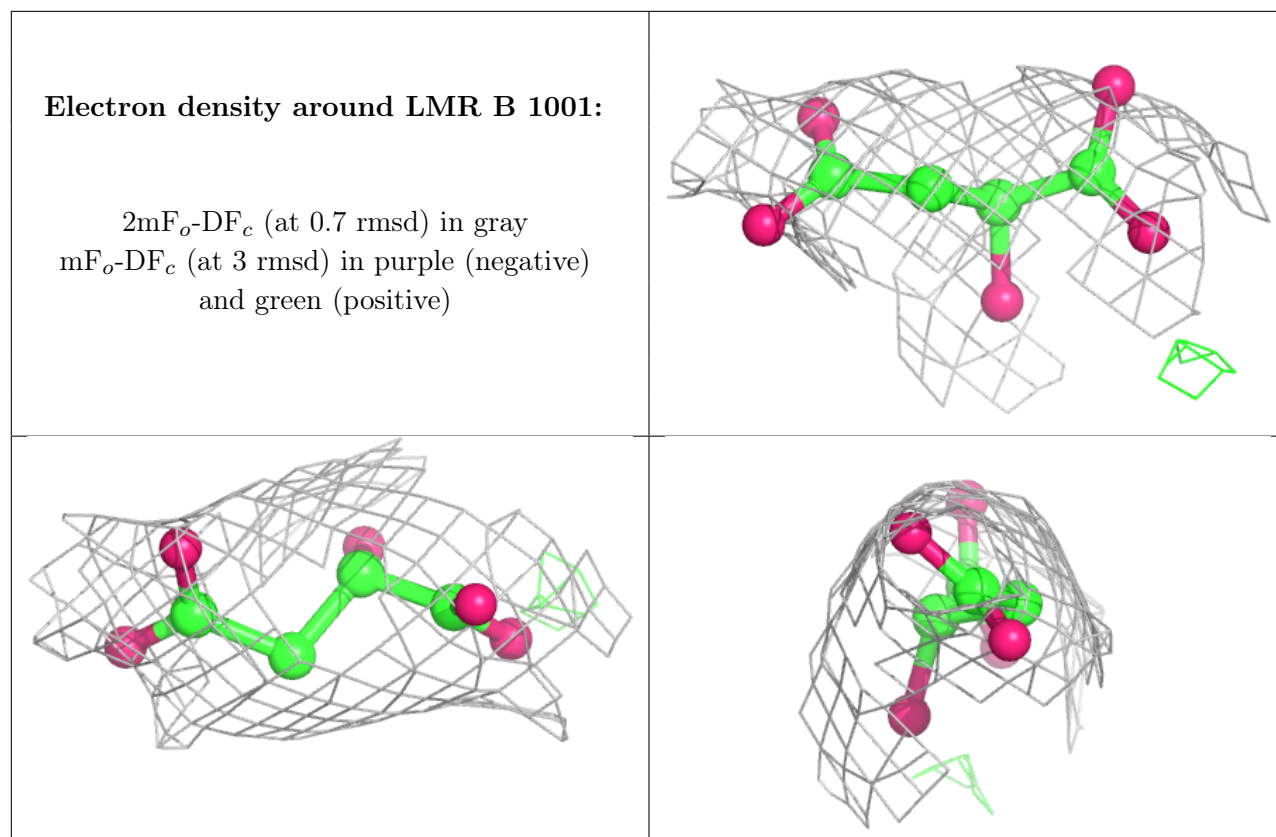
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMR C 1001:

$2mF_o-DF_c$ (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.