



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:23 PM UTC

PDB ID : 8OJY / pdb_00008ojy
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 T778 mutant with bound malate
Authors : Loris, R.; Haesaerts, S.; Larsen, P.B.
Deposited on : 2023-03-25
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

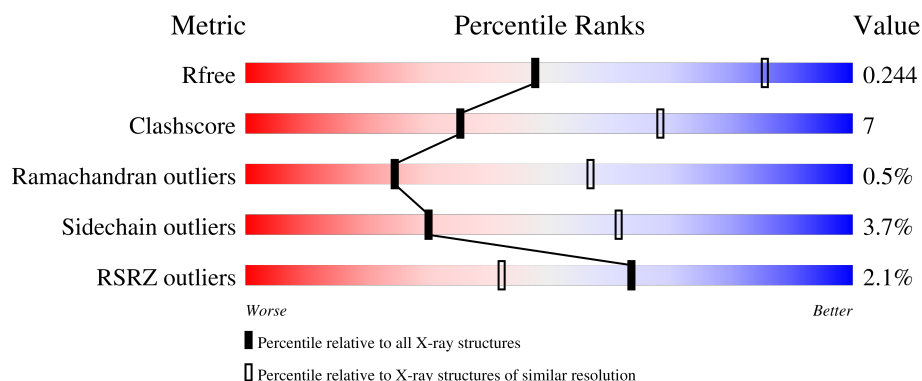
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

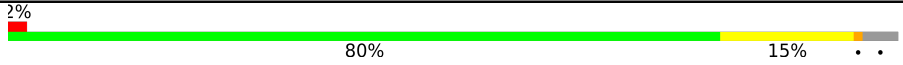
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	
1	B	974	
1	C	974	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22324 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
1	A	935	Total	C	N	O	S	0	5	0
			7244	4615	1252	1347	30			
1	B	948	Total	C	N	O	S	0	3	0
			7340	4677	1256	1377	30			
1	C	952	Total	C	N	O	S	0	4	0
			7513	4777	1302	1404	30			

There are 24 discrepancies between the modelled and reference sequences:

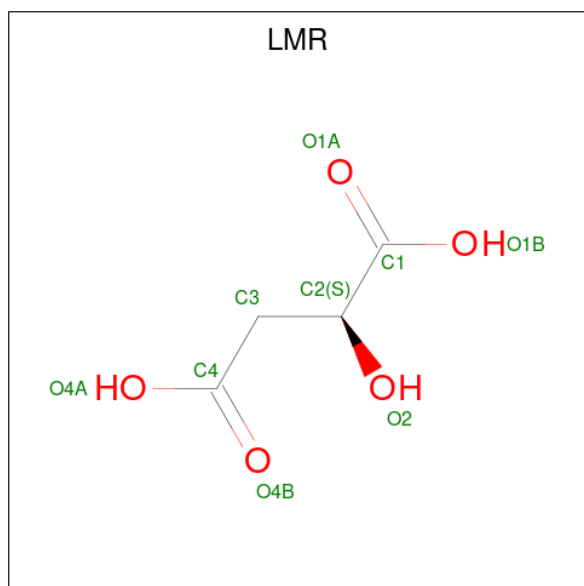
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9MAH0
A	-5	HIS	-	expression tag	UNP Q9MAH0
A	-4	HIS	-	expression tag	UNP Q9MAH0
A	-3	HIS	-	expression tag	UNP Q9MAH0
A	-2	HIS	-	expression tag	UNP Q9MAH0
A	-1	HIS	-	expression tag	UNP Q9MAH0
A	0	HIS	-	expression tag	UNP Q9MAH0
A	778	ILE	THR	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	778	ILE	THR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	ILE	THR	engineered mutation	UNP Q9MAH0

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: 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	B	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 (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			6	4	2		
4	B	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			3	2	1		
4	C	1	Total	C	O	0	0
			6	4	2		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		

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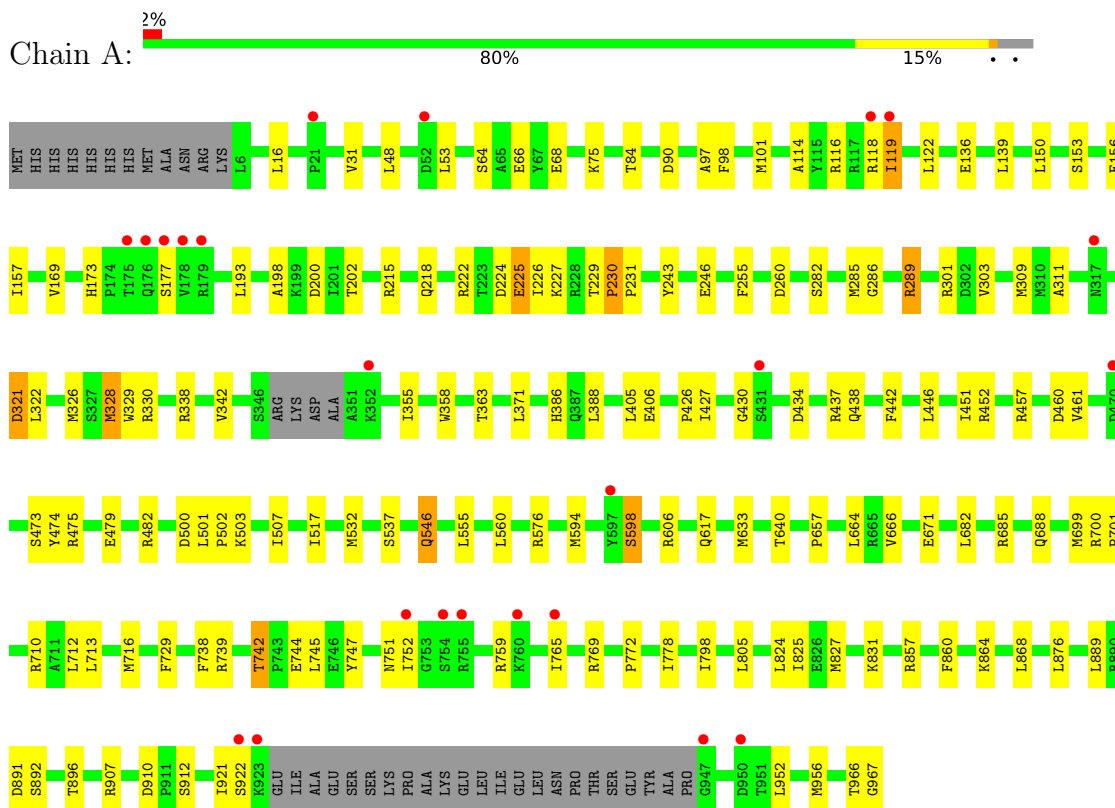
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	28	Total	O	0	0
			28	28		
5	C	62	Total	O	0	0
			62	62		

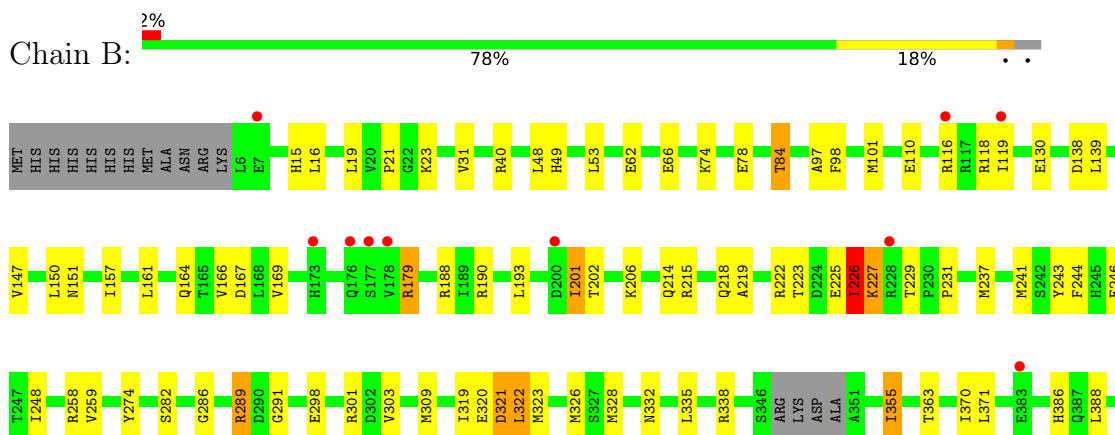
3 Residue-property plots [i](#)

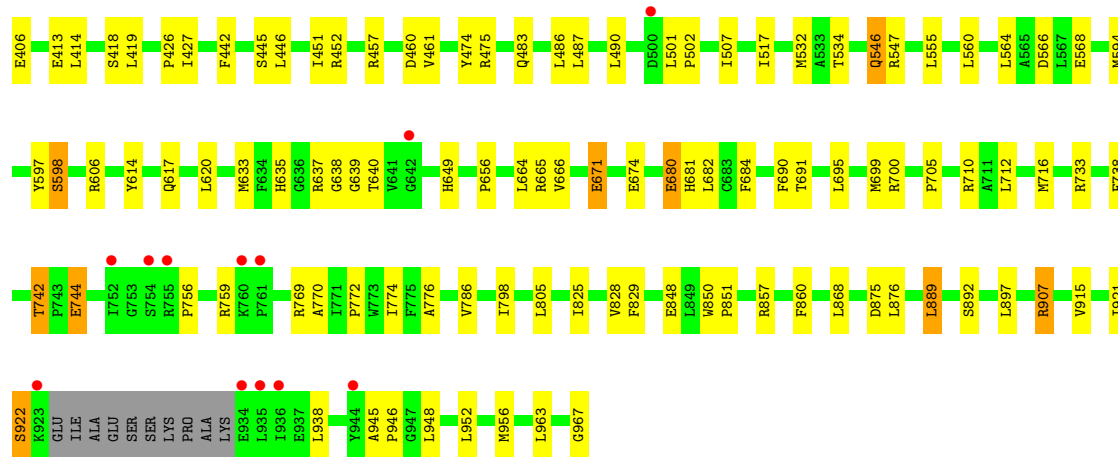
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

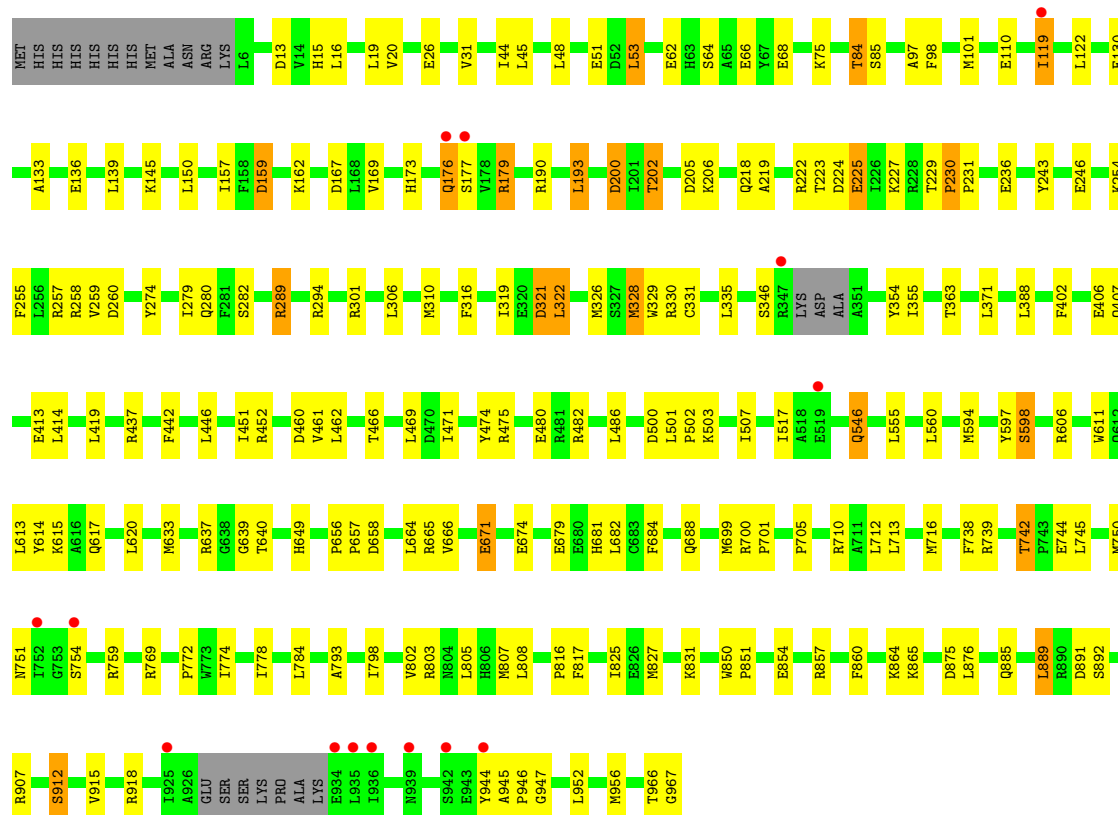
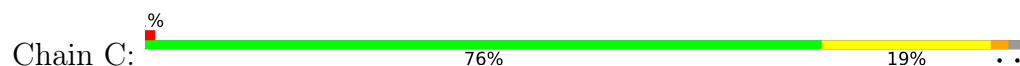


• Molecule 1: Phosphoenolpyruvate carboxylase 1





• 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	241.78Å 241.78Å 394.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 3.10 48.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.4 (48.00-3.10) 80.4 (48.00-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.197 , 0.245 0.197 , 0.244	Depositor DCC
R_{free} test set	1989 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 89.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22324	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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 66.39 % 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 6.0908e-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: PEG, 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	0.37	0/7418	0.56	0/10089
1	B	0.36	0/7509	0.55	2/10217 (0.0%)
1	C	0.52	0/7689	0.70	0/10436
All	All	0.42	0/22616	0.61	2/30742 (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	B	921	ILE	CA-C-N	5.22	131.51	121.54
1	B	921	ILE	C-N-CA	5.22	131.51	121.54

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	7244	0	6939	93	1
1	B	7340	0	7012	116	0
1	C	7513	0	7307	125	1
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	2	0
4	A	13	0	17	0	0
4	B	16	0	19	2	0
4	C	36	0	45	2	0
5	A	40	0	0	2	0
5	B	28	0	0	1	0
5	C	62	0	0	4	0
All	All	22324	0	21351	321	1

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 (321) 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:C:952:LEU:HG	1:C:956:MET:HE2	1.58	0.85
1:B:952:LEU:HG	1:B:956:MET:HE2	1.58	0.85
1:A:952:LEU:HG	1:A:956:MET:HE2	1.64	0.80
1:C:68:GLU:OE1	5:C:1101:HOH:O	1.99	0.79
1:C:461:VAL:HG22	1:C:507:ILE:HG23	1.65	0.79
1:C:501:LEU:HD12	1:C:502:PRO:HD2	1.66	0.77
1:A:301:ARG:NH2	1:A:388:LEU:O	2.18	0.77
1:A:309:MET:HE1	1:B:355:ILE:HD13	1.68	0.76
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.68	0.75
1:C:301:ARG:NH2	1:C:388:LEU:O	2.20	0.75
1:B:301:ARG:NH2	1:B:388:LEU:O	2.20	0.75
1:A:321[B]:ASP:OD2	1:B:188:ARG:NH2	2.19	0.74
1:C:480:GLU:HG3	4:C:1009:PEG:H21	1.71	0.73
1:C:460:ASP:OD1	1:C:475:ARG:NH2	2.22	0.72
1:C:658:ASP:HA	3:C:1004:CL:CL	2.29	0.70
1:B:298:GLU:OE2	1:B:301:ARG:NH1	2.26	0.68
1:C:169:VAL:HG22	1:C:282:SER:HB2	1.75	0.68
1:C:546:GLN:OE1	1:C:555:LEU:N	2.26	0.68
1:C:606:ARG:NH1	5:C:1103:HOH:O	2.27	0.68
1:A:451:ILE:HG13	1:A:517:ILE:HD11	1.74	0.68
1:C:254:LYS:NZ	5:C:1102:HOH:O	2.13	0.67
1:B:501:LEU:HD12	1:B:502:PRO:HD2	1.76	0.67
1:A:169:VAL:HG22	1:A:282:SER:HB2	1.77	0.66
1:C:206:LYS:HE2	4:C:1008:PEG:O2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:LEU:HD13	1:C:222:ARG:HD3	1.77	0.66
1:B:206:LYS:HE3	4:B:1005:PEG:H31	1.78	0.66
1:C:85:SER:HB2	1:C:918:ARG:HG3	1.78	0.65
1:A:218:GLN:HG2	1:B:427:ILE:HD11	1.79	0.65
1:C:802:VAL:HG23	1:C:803:ARG:HG3	1.80	0.64
1:C:98:PHE:HA	1:C:101:MET:HE3	1.80	0.64
1:A:426:PRO:O	1:B:215:ARG:HD3	1.97	0.64
1:B:532:MET:HG3	1:B:759:ARG:HH12	1.63	0.64
1:A:739:ARG:HB3	1:A:745:LEU:HD11	1.79	0.63
1:A:460:ASP:OD1	1:A:475:ARG:NH2	2.30	0.63
1:B:169:VAL:HG22	1:B:282:SER:HB2	1.78	0.63
1:C:451:ILE:HG13	1:C:517:ILE:HD11	1.79	0.62
1:B:110:GLU:OE1	1:B:190:ARG:NH1	2.31	0.62
1:A:442:PHE:HB3	1:A:446:LEU:HA	1.82	0.62
1:B:637[B]:ARG:NH2	1:B:671:GLU:OE2	2.29	0.62
1:A:118[B]:ARG:HH22	1:A:685:ARG:HD3	1.64	0.61
1:A:546:GLN:OE1	1:A:555:LEU:N	2.33	0.61
1:B:798:ILE:HD11	1:B:805:LEU:HD13	1.83	0.61
1:C:778:ILE:HD11	1:C:966:THR:OG1	2.01	0.61
1:A:857:ARG:O	1:A:860:PHE:HB3	2.01	0.60
1:B:680:GLU:HG3	1:B:681:HIS:N	2.16	0.60
1:A:48:LEU:HD13	1:A:222:ARG:HD3	1.84	0.60
1:A:729:PHE:HE1	1:A:765:ILE:HB	1.67	0.60
1:C:110:GLU:OE1	1:C:190:ARG:NH1	2.35	0.59
1:B:546:GLN:OE1	1:B:555:LEU:N	2.33	0.59
1:A:98:PHE:HA	1:A:101:MET:HE3	1.84	0.59
1:A:617:GLN:HG2	1:A:633:MET:HE2	1.83	0.59
1:A:215:ARG:HD3	1:B:426:PRO:O	2.02	0.59
1:B:945:ALA:HB1	1:B:946:PRO:HD2	1.84	0.59
1:C:501:LEU:O	1:C:503:LYS:HG3	2.03	0.59
1:A:118[B]:ARG:NH2	1:A:685:ARG:HD3	2.19	0.57
1:A:501:LEU:O	1:A:503:LYS:HG3	2.04	0.57
1:B:606:ARG:HD3	1:B:825:ILE:HD11	1.87	0.57
1:C:119:ILE:HD12	1:C:122:LEU:HD22	1.85	0.57
1:B:48:LEU:HD13	1:B:222:ARG:HD3	1.85	0.57
1:C:469:LEU:HB2	1:C:471:ILE:HG12	1.86	0.57
1:A:355:ILE:HD13	1:B:386:HIS:CE1	2.39	0.56
1:B:738:PHE:CE1	1:B:742:THR:HG21	2.40	0.56
1:C:20:VAL:HG21	1:C:885:GLN:HG3	1.86	0.56
1:A:712:LEU:O	1:A:716:MET:HG3	2.06	0.56
1:C:637[A]:ARG:NH2	1:C:671:GLU:OE2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:O	1:C:101:MET:HG3	2.06	0.55
1:C:133:ALA:HA	1:C:136:GLU:HG2	1.88	0.55
1:A:328:MET:SD	1:A:328:MET:N	2.79	0.55
1:C:289:ARG:HG3	1:C:452:ARG:O	2.05	0.55
1:C:738:PHE:CE1	1:C:742:THR:HG21	2.41	0.55
1:A:173:HIS:HB2	1:A:177:SER:HB3	1.87	0.55
1:B:289:ARG:HG3	1:B:452:ARG:O	2.07	0.55
1:B:490:LEU:O	1:B:547:ARG:NH1	2.40	0.55
1:C:617:GLN:HG2	1:C:633:MET:HE2	1.89	0.55
1:B:733:ARG:NH2	1:B:848:GLU:OE2	2.33	0.54
1:C:329:TRP:CZ3	1:C:330:ARG:HG3	2.42	0.54
1:B:16:LEU:HB3	1:B:31:VAL:HG13	1.88	0.54
1:C:739:ARG:HB3	1:C:745:LEU:HD11	1.90	0.54
1:A:68:GLU:CD	1:A:891:ASP:HB3	2.33	0.54
1:B:319:ILE:O	1:B:323:MET:HG3	2.08	0.54
1:B:617:GLN:HG2	1:B:633:MET:HE2	1.90	0.53
1:A:501:LEU:HD12	1:A:502:PRO:HD2	1.90	0.53
1:C:769:ARG:O	1:C:772:PRO:HD2	2.09	0.53
1:B:857:ARG:O	1:B:860:PHE:HB3	2.09	0.53
1:B:226:ILE:HD12	1:B:227:LYS:H	1.73	0.53
1:C:705:PRO:HG2	1:C:710[B]:ARG:CZ	2.39	0.53
1:B:326:MET:HG3	1:B:371:LEU:HD11	1.91	0.53
1:B:338:ARG:HB3	1:B:370:ILE:HD11	1.91	0.52
1:C:139:LEU:HD21	1:C:259:VAL:HG22	1.89	0.52
1:C:243:TYR:HA	1:C:246:GLU:HB2	1.91	0.52
1:B:179:ARG:HB3	1:B:179:ARG:CZ	2.39	0.52
1:C:857:ARG:O	1:C:860:PHE:HB3	2.09	0.52
1:B:907:ARG:HE	1:B:915:VAL:HG21	1.75	0.52
1:A:118[A]:ARG:NH2	1:A:136:GLU:O	2.44	0.51
1:B:116:ARG:NH1	5:B:1102:HOH:O	2.43	0.51
1:C:560:LEU:HD13	1:C:594:MET:HG2	1.93	0.51
1:A:224:ASP:OD1	1:A:225:GLU:N	2.43	0.51
1:B:460:ASP:OD1	1:B:475:ARG:NH2	2.43	0.51
1:C:20:VAL:HG11	1:C:885:GLN:OE1	2.11	0.51
1:C:606:ARG:HD3	1:C:825:ILE:HD11	1.93	0.51
1:C:66:GLU:OE1	1:C:75:LYS:NZ	2.27	0.51
1:B:219:ALA:O	1:B:223:THR:HG23	2.11	0.50
1:C:173:HIS:HB2	1:C:177:SER:HB3	1.92	0.50
1:B:335:LEU:HD12	1:B:414:LEU:HG	1.91	0.50
1:B:532:MET:CG	1:B:759:ARG:HH12	2.25	0.50
1:A:798:ILE:HD11	1:A:805:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:HIS:CE1	1:B:355:ILE:HG12	2.46	0.50
1:A:560:LEU:HD13	1:A:594:MET:HG2	1.94	0.50
1:A:532:MET:CG	1:A:759:ARG:HH12	2.24	0.50
1:B:49:HIS:O	1:B:922:SER:HB3	2.12	0.50
1:C:945:ALA:HB1	1:C:946:PRO:HD2	1.94	0.50
1:C:150:LEU:HD21	1:C:700:ARG:HE	1.77	0.49
1:A:532:MET:HG2	1:A:759:ARG:HH12	1.76	0.49
1:B:442:PHE:HB3	1:B:446:LEU:HA	1.94	0.49
1:C:328:MET:SD	1:C:328:MET:N	2.86	0.49
1:B:98:PHE:HA	1:B:101:MET:HE3	1.93	0.49
1:A:97:ALA:O	1:A:101:MET:HG3	2.13	0.49
1:A:442:PHE:HB3	1:A:446:LEU:HD23	1.95	0.49
1:A:598:SER:OG	1:A:967:GLY:OXT	2.30	0.49
1:A:606[B]:ARG:HD3	1:A:825:ILE:HD11	1.95	0.49
1:B:322:LEU:HD22	1:B:326:MET:HG2	1.95	0.49
1:B:770:ALA:O	1:B:774:ILE:HG12	2.13	0.49
1:C:62:GLU:O	1:C:66:GLU:HG3	2.12	0.49
1:C:68:GLU:CD	1:C:891:ASP:HB3	2.37	0.49
1:C:712:LEU:O	1:C:716:MET:HG3	2.12	0.48
1:B:945:ALA:HB3	1:B:948:LEU:HB2	1.94	0.48
1:C:15:HIS:CE1	1:C:62:GLU:HG2	2.49	0.48
1:B:139:LEU:HD21	1:B:259:VAL:HG22	1.94	0.48
1:C:219:ALA:O	1:C:223:THR:HG23	2.14	0.48
1:C:335:LEU:HA	1:C:414:LEU:HD21	1.95	0.48
1:A:116:ARG:NH1	5:A:1101:HOH:O	2.47	0.48
1:B:118:ARG:HH12	1:B:138:ASP:HB3	1.79	0.48
1:B:868:LEU:HD21	1:B:876:LEU:HD23	1.95	0.48
1:C:224:ASP:OD1	1:C:225:GLU:N	2.47	0.48
1:A:427:ILE:HD11	1:B:218:GLN:HG2	1.95	0.48
1:A:868:LEU:HD21	1:A:876:LEU:HD23	1.95	0.48
1:B:229:THR:HG23	1:B:231:PRO:HA	1.96	0.48
1:B:742:THR:CG2	1:B:776:ALA:HB1	2.44	0.47
1:A:864:LYS:HE2	1:A:876:LEU:HD11	1.95	0.47
1:B:291:GLY:O	1:B:756:PRO:HD2	2.14	0.47
1:C:157:ILE:HA	1:C:699:MET:HE1	1.95	0.47
1:C:179:ARG:CZ	1:C:179:ARG:HB3	2.44	0.47
1:C:306:LEU:O	1:C:310:MET:HG3	2.14	0.47
1:C:322:LEU:HD22	1:C:326:MET:HG2	1.96	0.47
1:C:664:LEU:HG	1:C:666:VAL:HG23	1.96	0.47
1:C:230:PRO:HG3	1:C:751:ASN:HB3	1.95	0.47
1:C:657:PRO:HG3	1:C:701:PRO:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HD2	1:B:214:GLN:HG2	1.97	0.47
1:B:97:ALA:O	1:B:101:MET:HG3	2.15	0.47
1:B:201:ILE:HD12	1:B:201:ILE:HA	1.73	0.47
1:B:597[B]:TYR:CD2	1:B:639:GLY:HA2	2.49	0.47
1:A:738:PHE:CE1	1:A:742:THR:HG21	2.50	0.47
1:C:331:CYS:HB2	1:C:335:LEU:HD22	1.97	0.47
1:A:430:GLY:CA	1:B:215:ARG:HD2	2.45	0.47
1:B:157:ILE:HA	1:B:699:MET:HE1	1.97	0.47
1:C:665:ARG:HD2	5:C:1117:HOH:O	2.15	0.47
1:B:274:TYR:CE1	1:B:413:GLU:HG2	2.49	0.46
1:C:889:LEU:HD23	1:C:889:LEU:HA	1.75	0.46
1:A:729:PHE:CE1	1:A:765:ILE:HB	2.48	0.46
1:A:229:THR:HG23	1:A:231:PRO:HA	1.97	0.46
1:A:358:TRP:HE1	1:B:179:ARG:NH2	2.13	0.46
1:A:657:PRO:HG3	1:A:701:PRO:HB2	1.96	0.46
1:C:713:LEU:HD23	1:C:713:LEU:HA	1.69	0.46
1:B:19:LEU:HD21	1:B:892:SER:HB3	1.97	0.46
1:B:309:MET:HE2	1:B:309:MET:HB3	1.82	0.46
1:C:500:ASP:OD1	1:C:500:ASP:N	2.45	0.46
1:C:229:THR:HG23	1:C:231:PRO:HA	1.97	0.46
1:C:501:LEU:HD12	1:C:502:PRO:CD	2.42	0.46
1:C:637[B]:ARG:HH22	1:C:774:ILE:HG13	1.81	0.46
1:B:332:ASN:HB2	1:B:418:SER:HA	1.97	0.46
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.97	0.46
1:B:237:MET:O	1:B:241:MET:HG2	2.15	0.46
1:A:434:ASP:O	1:A:438:GLN:HG3	2.15	0.45
1:B:130:GLU:O	1:B:649:HIS:HB3	2.16	0.45
1:A:713:LEU:HD23	1:A:713:LEU:HA	1.79	0.45
1:B:62:GLU:O	1:B:66:GLU:HG3	2.16	0.45
1:C:44:ILE:HD13	1:C:218:GLN:HB2	1.98	0.45
1:B:597[A]:TYR:HH	1:B:635:HIS:CE1	2.34	0.45
1:A:778:ILE:HD11	1:A:966:THR:OG1	2.16	0.45
1:C:759:ARG:HE	1:C:769:ARG:HD2	1.80	0.45
1:C:750:MET:HE2	1:C:944:TYR:HE2	1.81	0.45
1:A:286:GLY:HA3	1:A:303:VAL:HG21	1.99	0.45
1:A:326:MET:HG3	1:A:371:LEU:HD11	1.99	0.45
1:B:598:SER:OG	1:B:967:GLY:OXT	2.32	0.45
1:C:335:LEU:HD12	1:C:414:LEU:HG	1.99	0.45
1:C:159:ASP:HA	1:C:162:LYS:HD3	1.98	0.45
1:B:564:LEU:O	1:B:568:GLU:HG3	2.17	0.45
1:B:664:LEU:HG	1:B:666:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TYR:HA	1:A:246:GLU:HB2	1.99	0.44
1:C:202:THR:HG23	1:C:205:ASP:CG	2.42	0.44
1:B:445:SER:O	1:B:446:LEU:HB2	2.15	0.44
1:C:45:LEU:HA	1:C:45:LEU:HD12	1.80	0.44
1:B:712:LEU:O	1:B:716:MET:HG3	2.18	0.44
1:C:419:LEU:HD23	1:C:419:LEU:HA	1.81	0.44
1:A:664:LEU:HG	1:A:666:VAL:HG23	1.99	0.44
1:B:161:LEU:HG	1:B:695:LEU:HD13	1.98	0.44
1:A:827:MET:SD	1:A:831:LYS:HE3	2.57	0.44
1:B:705:PRO:HG2	1:B:710:ARG:NH1	2.32	0.44
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.99	0.44
1:C:177:SER:OG	1:C:236:GLU:HG2	2.18	0.44
1:C:784:LEU:C	1:C:784:LEU:HD23	2.43	0.44
1:B:258:ARG:HG2	1:B:684:PHE:HZ	1.83	0.44
1:B:742:THR:HG22	1:B:744:GLU:H	1.82	0.44
1:C:130:GLU:O	1:C:649:HIS:HB3	2.17	0.44
1:C:613:LEU:HD23	1:C:613:LEU:HA	1.81	0.44
1:A:285:MET:HE3	1:A:285:MET:HB2	1.88	0.43
1:A:769:ARG:O	1:A:772:PRO:HD2	2.17	0.43
1:B:501:LEU:HD12	1:B:502:PRO:CD	2.44	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.82	0.43
1:B:243:TYR:HA	1:B:246:GLU:HB2	2.00	0.43
1:C:200:ASP:OD1	1:C:200:ASP:N	2.51	0.43
1:A:289:ARG:HG3	1:A:452:ARG:O	2.18	0.43
1:A:752:ILE:HD11	1:A:956:MET:CE	2.49	0.43
1:A:479:GLU:OE2	1:A:537:SER:HB3	2.18	0.43
1:A:311:ALA:HB2	1:A:446:LEU:HG	2.00	0.43
1:C:620:LEU:HD23	1:C:620:LEU:HA	1.84	0.43
1:A:98:PHE:CZ	1:A:896:THR:HG21	2.54	0.43
1:A:153:SER:OG	1:A:156:GLU:HG3	2.18	0.43
1:C:614:TYR:CE2	1:C:656:PRO:HG3	2.54	0.43
1:B:457:ARG:O	1:B:461:VAL:HG23	2.18	0.43
1:B:606:ARG:NH2	1:B:638:GLY:O	2.52	0.43
1:C:19:LEU:HA	1:C:19:LEU:HD12	1.74	0.43
1:C:598:SER:OG	1:C:967:GLY:OXT	2.28	0.43
1:A:355:ILE:HD11	1:B:309:MET:HE1	1.99	0.42
1:B:206:LYS:CE	4:B:1005:PEG:H31	2.48	0.42
1:C:16:LEU:HB3	1:C:31:VAL:HG13	2.01	0.42
1:C:274:TYR:CE1	1:C:413:GLU:HG2	2.54	0.42
1:B:226:ILE:HD12	1:B:227:LYS:N	2.33	0.42
1:B:474:TYR:OH	1:B:486:LEU:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:LEU:HD23	1:B:897:LEU:HA	1.88	0.42
1:B:164:GLN:HE22	1:B:691:THR:HG23	1.83	0.42
1:B:244:PHE:HA	1:B:248:ILE:HB	2.00	0.42
1:B:742:THR:HG23	1:B:776:ALA:HB1	2.01	0.42
1:C:716:MET:HE2	1:C:716:MET:HB3	1.90	0.42
1:C:798:ILE:HD11	1:C:805:LEU:HD13	2.02	0.42
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.87	0.42
1:C:167:ASP:HB3	1:C:665:ARG:HG3	2.02	0.42
1:A:90:ASP:OD2	1:A:921:ILE:HG13	2.19	0.42
1:B:534:THR:HG22	1:B:566:ASP:CG	2.44	0.42
1:C:64:SER:HB3	1:C:892:SER:O	2.19	0.42
1:A:150:LEU:HD21	1:A:700:ARG:HE	1.83	0.42
1:A:474:TYR:CZ	1:A:482:ARG:HD3	2.55	0.42
1:C:176:GLN:H	1:C:176:GLN:HG3	1.48	0.42
1:C:850:TRP:N	1:C:851:PRO:HD2	2.34	0.42
1:A:114:ALA:HB2	1:A:682:LEU:HD13	2.02	0.42
1:A:747:TYR:HA	1:A:752:ILE:HD12	2.01	0.42
1:B:166:VAL:HG11	1:B:690:PHE:HB3	2.02	0.42
1:B:560:LEU:HD13	1:B:594:MET:HG2	2.02	0.42
1:C:294:ARG:HD2	1:C:754:SER:HB2	2.01	0.42
1:A:64:SER:HB3	1:A:892:SER:O	2.19	0.42
1:A:157:ILE:HA	1:A:699:MET:HE1	2.02	0.42
1:C:769:ARG:HE	1:C:769:ARG:HB3	1.60	0.42
1:B:15:HIS:CE1	1:B:62:GLU:HG2	2.55	0.42
1:C:258:ARG:HG2	1:C:684:PHE:HZ	1.85	0.42
1:C:260:ASP:CG	1:C:437:ARG:HH22	2.27	0.42
1:A:260:ASP:CG	1:A:437:ARG:HH22	2.26	0.41
1:B:84:THR:HG22	1:B:915:VAL:HG11	2.02	0.41
1:C:679:GLU:OE1	1:C:681:HIS:N	2.52	0.41
1:A:198:ALA:HB1	1:A:200:ASP:OD1	2.20	0.41
1:A:255:PHE:CE1	1:A:688:GLN:HA	2.55	0.41
1:C:402:PHE:HD1	1:C:407:GLN:HB3	1.85	0.41
1:C:486:LEU:HD23	1:C:486:LEU:HA	1.80	0.41
1:C:912:SER:O	1:C:912:SER:OG	2.31	0.41
1:A:330:ARG:HD3	1:B:222:ARG:CZ	2.50	0.41
1:C:716:MET:HB3	1:C:793:ALA:HB1	2.02	0.41
1:B:167:ASP:HB3	1:B:665:ARG:HG3	2.02	0.41
1:C:611:TRP:CE2	1:C:615:LYS:HD3	2.55	0.41
1:C:712:LEU:HD22	1:C:807:MET:SD	2.60	0.41
1:C:864:LYS:HE2	1:C:876:LEU:HD11	2.02	0.41
1:C:119:ILE:CD1	1:C:122:LEU:HD22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:PHE:HB3	1:C:446:LEU:HD23	2.02	0.41
1:A:338:ARG:O	1:A:342:VAL:HG23	2.20	0.41
1:A:606[B]:ARG:CZ	1:A:824:LEU:HD22	2.51	0.41
1:B:829:PHE:HB3	1:B:876:LEU:HD11	2.03	0.41
1:B:963:LEU:HD23	1:B:963:LEU:HA	1.82	0.41
1:A:66:GLU:OE1	1:A:75:LYS:NZ	2.32	0.41
1:A:119:ILE:HD12	1:A:122:LEU:HD22	2.03	0.41
1:A:710:ARG:HD2	5:A:1104:HOH:O	2.20	0.41
1:A:716:MET:HE2	1:A:716:MET:HB3	1.96	0.41
1:B:614:TYR:CE2	1:B:656:PRO:HG3	2.56	0.41
1:C:255:PHE:CE1	1:C:688:GLN:HA	2.55	0.41
1:C:257:ARG:HD3	3:C:1002:CL:CL	2.57	0.41
1:C:808:LEU:HD23	1:C:808:LEU:HA	1.91	0.41
1:A:16:LEU:HB3	1:A:31:VAL:HG13	2.03	0.41
1:A:139:LEU:HD12	1:A:139:LEU:HA	1.85	0.41
1:A:500:ASP:N	1:A:500:ASP:OD1	2.53	0.41
1:A:752:ILE:HD11	1:A:956:MET:HE1	2.03	0.41
1:B:286:GLY:HA3	1:B:303:VAL:HG21	2.03	0.41
1:B:332:ASN:HB2	1:B:418:SER:CB	2.51	0.41
1:C:597[B]:TYR:CD2	1:C:639:GLY:HA2	2.56	0.41
1:C:827:MET:SD	1:C:831:LYS:HE3	2.60	0.41
1:B:889:LEU:HD23	1:B:889:LEU:HA	1.93	0.41
1:C:53:LEU:HD22	1:C:53:LEU:HA	1.84	0.41
1:C:326:MET:HG3	1:C:371:LEU:HD11	2.02	0.41
1:C:851:PRO:HA	1:C:854:GLU:HB2	2.03	0.41
1:A:457:ARG:O	1:A:461:VAL:HG23	2.22	0.40
1:B:483:GLN:O	1:B:487:LEU:HG	2.21	0.40
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.65	0.40
1:C:474:TYR:CZ	1:C:482:ARG:HD3	2.56	0.40
1:A:329:TRP:CE3	1:B:938:LEU:HD21	2.55	0.40
1:B:451:ILE:HG13	1:B:517:ILE:HD11	2.03	0.40
1:B:620:LEU:HD23	1:B:620:LEU:HA	1.87	0.40
1:B:769:ARG:O	1:B:772:PRO:HD2	2.20	0.40
1:C:289:ARG:HG3	1:C:289:ARG:H	1.67	0.40
1:A:910:ASP:OD1	1:A:912:SER:HB3	2.21	0.40
1:B:74:LYS:O	1:B:78:GLU:HG3	2.21	0.40
1:B:850:TRP:N	1:B:851:PRO:HD2	2.35	0.40
1:C:279:ILE:O	1:C:280:GLN:NE2	2.52	0.40
1:C:466:THR:HG21	1:C:474:TYR:HB2	2.04	0.40
1:A:230:PRO:HG3	1:A:751:ASN:HB3	2.04	0.40
1:C:84:THR:HG22	1:C:915:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:462:LEU:HD23	1:C:462:LEU:HA	1.87	0.40
1:C:614:TYR:CD2	1:C:656:PRO:HG3	2.56	0.40
1:C:816:PRO:O	1:C:817:PHE:C	2.63	0.40
1:B:147:VAL:O	1:B:151:ASN:HA	2.22	0.40
1:B:150:LEU:HD21	1:B:700:ARG:HE	1.86	0.40
1:C:316:PHE:O	1:C:319:ILE:HG22	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ARG:NH2	1:C:480:GLU:OE2[10_665]	2.18	0.02

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	934/974 (96%)	896 (96%)	34 (4%)	4 (0%)	30	61
1	B	945/974 (97%)	903 (96%)	38 (4%)	4 (0%)	30	61
1	C	950/974 (98%)	905 (95%)	39 (4%)	6 (1%)	21	52
All	All	2829/2922 (97%)	2704 (96%)	111 (4%)	14 (0%)	24	57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	922	SER
1	C	227	LYS
1	A	227	LYS
1	A	922	SER
1	B	227	LYS
1	C	346	SER

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Mol	Chain	Res	Type
1	A	226	ILE
1	B	226	ILE
1	C	200	ASP
1	C	354	TYR
1	B	21	PRO
1	A	230	PRO
1	C	230	PRO
1	C	947	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	734/849 (86%)	712 (97%)	22 (3%)	36	65
1	B	742/849 (87%)	712 (96%)	30 (4%)	28	60
1	C	781/849 (92%)	747 (96%)	34 (4%)	25	56
All	All	2257/2547 (89%)	2171 (96%)	86 (4%)	30	60

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	84	THR
1	A	119	ILE
1	A	193	LEU
1	A	202	THR
1	A	225	GLU
1	A	289	ARG
1	A	321[A]	ASP
1	A	321[B]	ASP
1	A	322	LEU
1	A	328	MET
1	A	363	THR
1	A	406	GLU
1	A	473	SER

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Mol	Chain	Res	Type
1	A	546	GLN
1	A	598	SER
1	A	640	THR
1	A	671	GLU
1	A	742	THR
1	A	744	GLU
1	A	889	LEU
1	A	907	ARG
1	B	23	LYS
1	B	53	LEU
1	B	84	THR
1	B	119	ILE
1	B	179	ARG
1	B	193	LEU
1	B	201	ILE
1	B	202	THR
1	B	225	GLU
1	B	226	ILE
1	B	289	ARG
1	B	321[A]	ASP
1	B	321[B]	ASP
1	B	322	LEU
1	B	328	MET
1	B	355	ILE
1	B	363	THR
1	B	406	GLU
1	B	546	GLN
1	B	598	SER
1	B	640	THR
1	B	671	GLU
1	B	674	GLU
1	B	680	GLU
1	B	682	LEU
1	B	742	THR
1	B	744	GLU
1	B	875	ASP
1	B	889	LEU
1	B	907	ARG
1	C	13	ASP
1	C	26	GLU
1	C	51	GLU
1	C	53	LEU

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Mol	Chain	Res	Type
1	C	84	THR
1	C	119	ILE
1	C	145	LYS
1	C	159	ASP
1	C	176	GLN
1	C	179	ARG
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	363	THR
1	C	406	GLU
1	C	546	GLN
1	C	598	SER
1	C	640	THR
1	C	671	GLU
1	C	674	GLU
1	C	682	LEU
1	C	742	THR
1	C	744	GLU
1	C	865	LYS
1	C	875	ASP
1	C	889	LEU
1	C	907	ARG
1	C	912	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
1	A	164	GLN
1	A	207	GLN
1	A	353	HIS
1	A	391	ASN
1	A	591	GLN
1	A	617	GLN
1	A	920	HIS

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Mol	Chain	Res	Type
1	B	49	HIS
1	B	245	HIS
1	B	318	GLN
1	B	391	ASN
1	B	730	GLN
1	B	814	HIS
1	C	71	HIS
1	C	164	GLN
1	C	391	ASN
1	C	617	GLN
1	C	796	HIS
1	C	914	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	1001	-	8,8,8	1.63	1 (12%)	10,10,10	1.26	1 (10%)
4	PEG	C	1008	4	6,6,6	0.57	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	A	1004	-	6,6,6	0.52	0	5,5,5	0.34	0
4	PEG	C	1006	4	2,2,6	0.59	0	1,1,5	0.07	0
4	PEG	A	1003	-	5,5,6	0.64	0	4,4,5	0.91	0
4	PEG	C	1010	-	6,6,6	0.49	0	5,5,5	0.20	0
4	PEG	C	1007	4	5,5,6	0.52	0	4,4,5	0.58	0
4	PEG	B	1003	4	5,5,6	0.60	0	4,4,5	0.17	0
4	PEG	B	1005	-	6,6,6	0.51	0	5,5,5	0.49	0
4	PEG	C	1009	-	6,6,6	0.54	0	5,5,5	0.39	0
2	LMR	A	1001	-	8,8,8	1.47	2 (25%)	10,10,10	1.69	3 (30%)
2	LMR	B	1001	-	8,8,8	1.55	1 (12%)	10,10,10	1.45	1 (10%)
4	PEG	B	1004	4	2,2,6	0.51	0	1,1,5	0.08	0
4	PEG	C	1005	4	5,5,6	0.58	0	4,4,5	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMR	C	1001	-	-	3/8/8/8	-
4	PEG	C	1008	4	-	3/4/4/4	-
4	PEG	A	1004	-	-	3/4/4/4	-
4	PEG	C	1010	-	-	2/4/4/4	-
4	PEG	A	1003	-	-	1/3/3/4	-
4	PEG	C	1007	4	-	1/3/3/4	-
4	PEG	B	1003	4	-	1/3/3/4	-
4	PEG	C	1009	-	-	3/4/4/4	-
2	LMR	A	1001	-	-	1/8/8/8	-
2	LMR	B	1001	-	-	4/8/8/8	-
4	PEG	B	1005	-	-	2/4/4/4	-
4	PEG	C	1005	4	-	2/3/3/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	LMR	C2-C1	-3.66	1.47	1.52
2	B	1001	LMR	C2-C1	-3.27	1.47	1.52
2	A	1001	LMR	C2-C1	-2.36	1.48	1.52
2	A	1001	LMR	O4B-C4	2.02	1.28	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	LMR	O1B-C1-C2	3.79	120.75	112.74
2	B	1001	LMR	O1B-C1-C2	2.97	119.03	112.74
2	C	1001	LMR	O1B-C1-C2	2.05	117.07	112.74
2	A	1001	LMR	O4A-C4-C3	2.05	120.36	114.00
2	A	1001	LMR	O1A-C1-C2	-2.02	118.56	122.60

There are no chirality outliers.

All (26) torsion outliers are listed below:

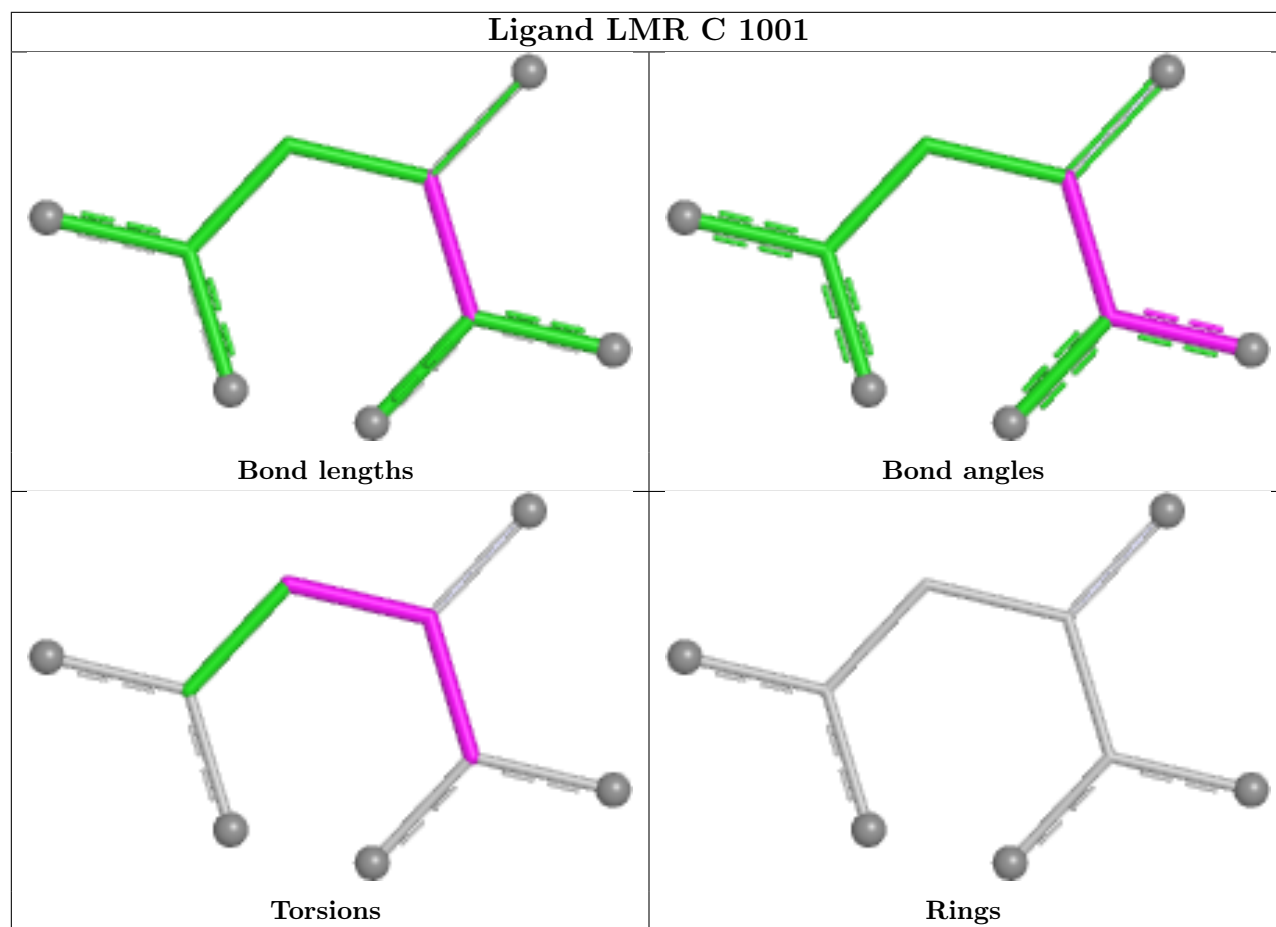
Mol	Chain	Res	Type	Atoms
4	A	1004	PEG	O1-C1-C2-O2
4	C	1008	PEG	O2-C3-C4-O4
4	C	1005	PEG	O2-C3-C4-O4
4	C	1010	PEG	O1-C1-C2-O2
4	B	1005	PEG	O1-C1-C2-O2
4	B	1005	PEG	O2-C3-C4-O4
4	C	1009	PEG	O2-C3-C4-O4
2	B	1001	LMR	O2-C2-C3-C4
2	C	1001	LMR	O2-C2-C3-C4
2	B	1001	LMR	C1-C2-C3-C4
4	B	1003	PEG	O2-C3-C4-O4
4	A	1004	PEG	O2-C3-C4-O4
4	C	1009	PEG	C4-C3-O2-C2
4	C	1005	PEG	C4-C3-O2-C2
4	A	1004	PEG	C4-C3-O2-C2
4	C	1008	PEG	C1-C2-O2-C3
4	C	1008	PEG	C4-C3-O2-C2
4	C	1007	PEG	C4-C3-O2-C2
4	A	1003	PEG	O2-C3-C4-O4
2	C	1001	LMR	O1B-C1-C2-C3
2	C	1001	LMR	C1-C2-C3-C4
4	C	1010	PEG	C1-C2-O2-C3
2	B	1001	LMR	O1B-C1-C2-O2
2	A	1001	LMR	O1B-C1-C2-C3
4	C	1009	PEG	C1-C2-O2-C3
2	B	1001	LMR	O1A-C1-C2-O2

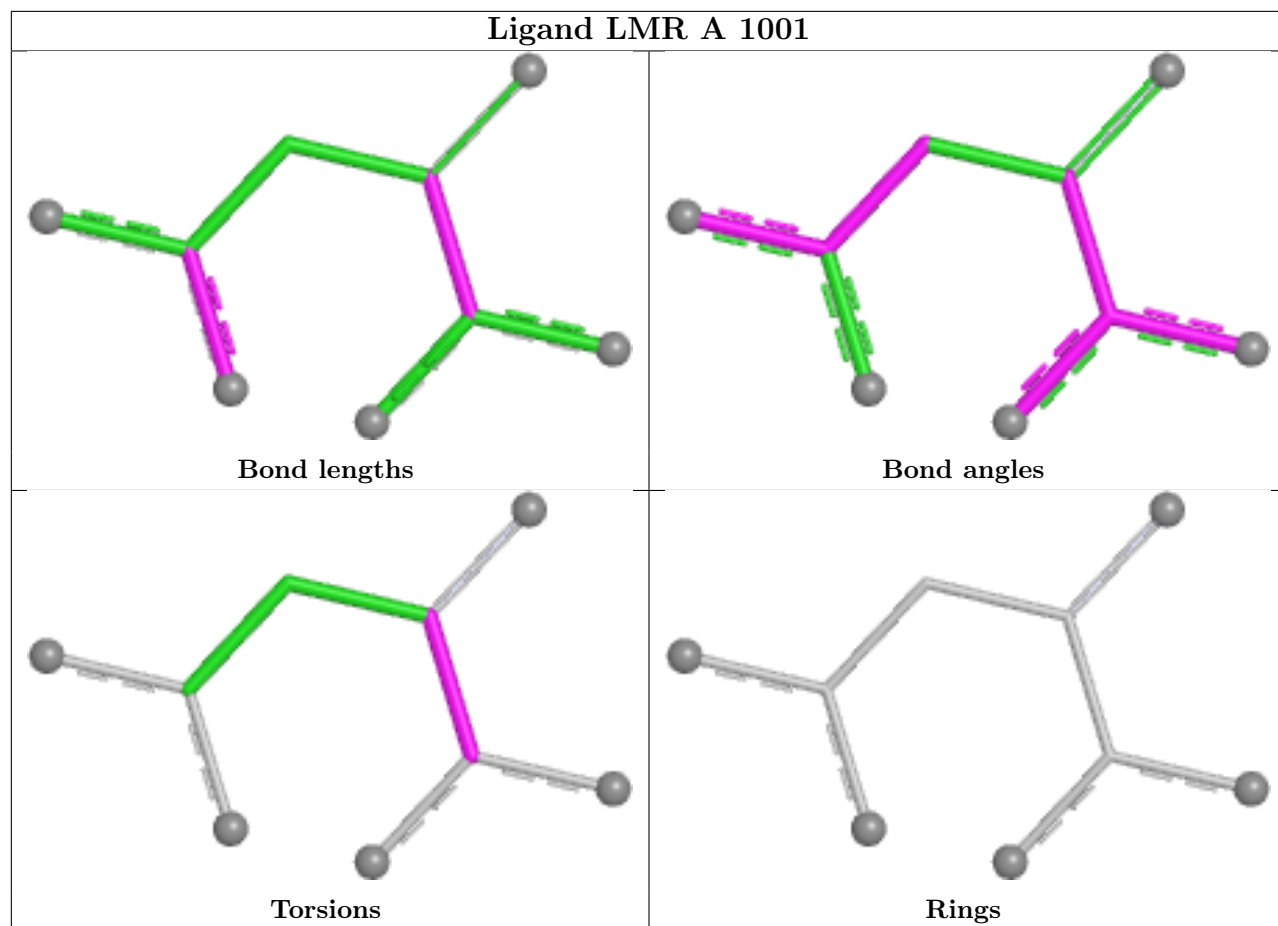
There are no ring outliers.

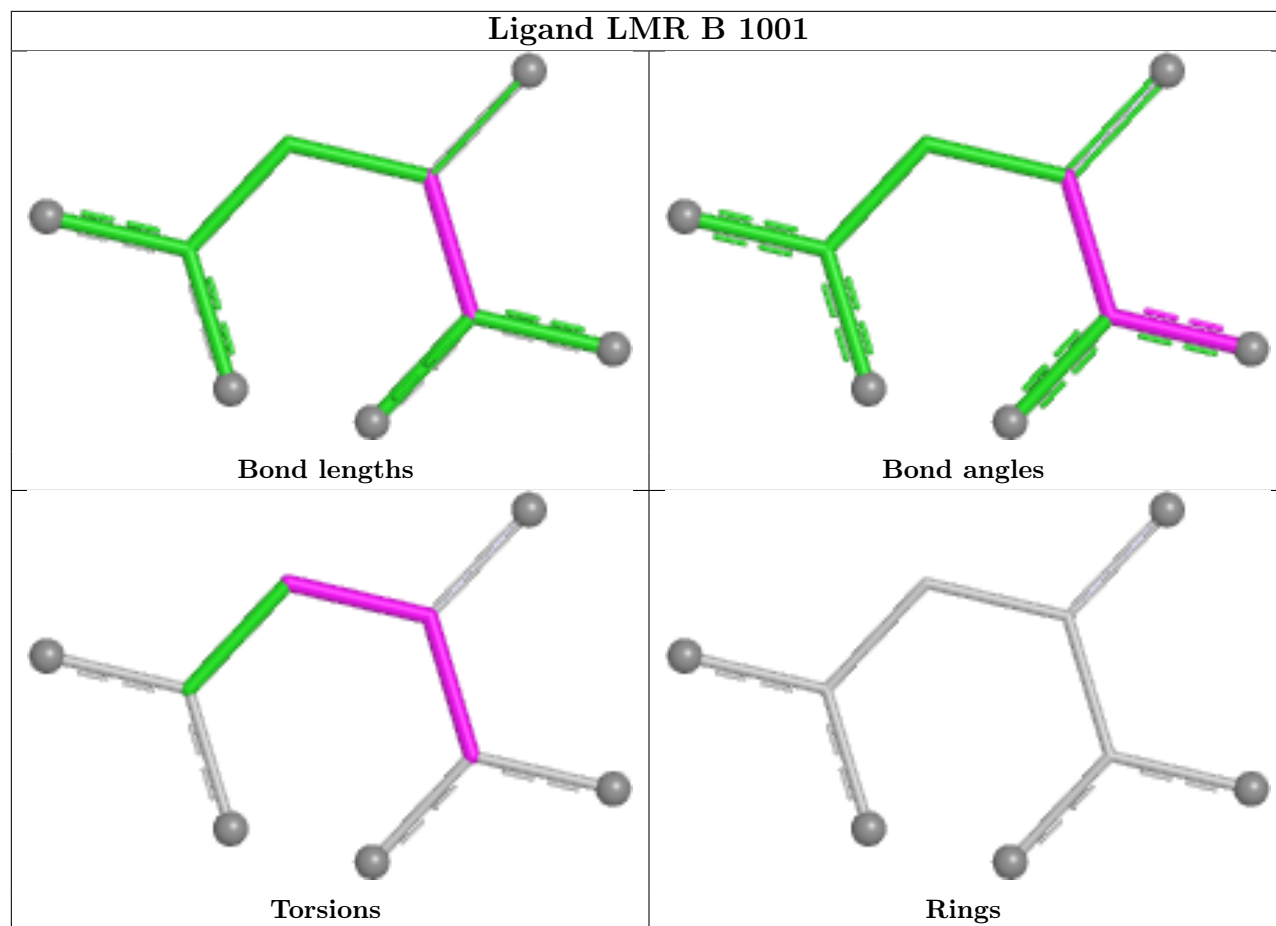
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1008	PEG	1	0
4	B	1005	PEG	2	0
4	C	1009	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	935/974 (95%)	-0.33	23 (2%)	58 37	37, 88, 150, 222	5 (0%)
1	B	948/974 (97%)	-0.25	22 (2%)	61 39	44, 98, 150, 255	3 (0%)
1	C	952/974 (97%)	-0.46	14 (1%)	72 52	27, 62, 127, 238	4 (0%)
All	All	2835/2922 (97%)	-0.35	59 (2%)	63 42	27, 84, 145, 255	12 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	761	PRO	4.1
1	B	176	GLN	3.8
1	B	934	GLU	3.7
1	A	947	GLY	3.6
1	B	500	ASP	3.5
1	B	760	LYS	3.4
1	C	935	LEU	3.4
1	A	175	THR	3.3
1	C	939	ASN	3.3
1	A	177	SER	3.2
1	C	752	ILE	3.2
1	C	942	SER	3.2
1	B	935	LEU	3.2
1	C	934	GLU	3.1
1	B	936	ILE	3.1
1	C	925	ILE	3.0
1	A	752	ILE	3.0
1	A	431	SER	2.9
1	A	922	SER	2.9
1	A	755	ARG	2.9
1	A	597[A]	TYR	2.9
1	B	754	SER	2.9
1	B	119	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	754	SER	2.8
1	A	52	ASP	2.8
1	B	944	TYR	2.8
1	C	347	ARG	2.8
1	A	765	ILE	2.8
1	C	936	ILE	2.8
1	B	7	GLU	2.7
1	C	176	GLN	2.7
1	A	754	SER	2.7
1	B	177	SER	2.7
1	C	944	TYR	2.6
1	A	923	LYS	2.6
1	A	470	ASP	2.6
1	A	118[A]	ARG	2.5
1	B	923	LYS	2.4
1	B	178	VAL	2.4
1	A	352	LYS	2.4
1	A	179	ARG	2.3
1	B	383	GLU	2.3
1	B	755	ARG	2.3
1	A	21	PRO	2.3
1	B	752	ILE	2.3
1	C	177	SER	2.2
1	B	642	GLY	2.2
1	A	119	ILE	2.2
1	B	200	ASP	2.2
1	C	519	GLU	2.2
1	B	173	HIS	2.2
1	A	178	VAL	2.1
1	A	760	LYS	2.1
1	B	116	ARG	2.1
1	A	950	ASP	2.1
1	A	176	GLN	2.1
1	A	317	ASN	2.0
1	B	228	ARG	2.0
1	C	119	ILE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

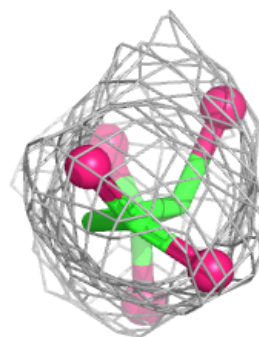
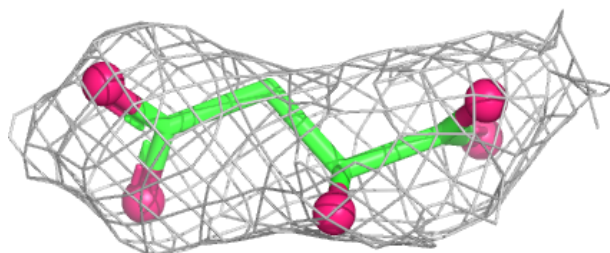
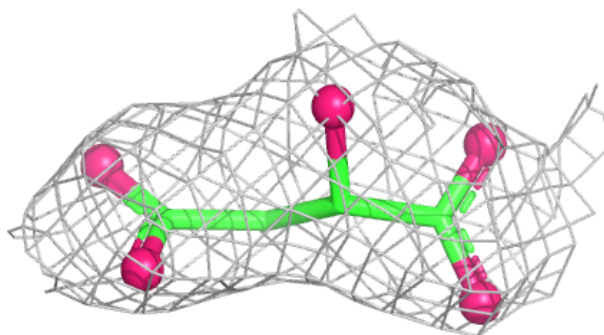
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	C	1006	3/7	0.74	0.21	35,35,66,67	0
4	PEG	B	1004	3/7	0.82	0.18	67,67,85,90	0
4	PEG	C	1009	7/7	0.83	0.15	87,102,111,118	0
4	PEG	A	1003	6/7	0.85	0.27	45,70,86,90	0
4	PEG	C	1008	7/7	0.86	0.15	116,124,136,137	0
3	CL	A	1002	1/1	0.91	0.22	83,83,83,83	0
4	PEG	B	1003	6/7	0.92	0.21	83,101,106,108	0
4	PEG	C	1010	7/7	0.92	0.13	37,60,71,75	0
4	PEG	A	1004	7/7	0.93	0.14	80,85,100,104	0
3	CL	B	1002	1/1	0.94	0.09	89,89,89,89	0
4	PEG	B	1005	7/7	0.94	0.13	81,87,92,93	0
3	CL	C	1002	1/1	0.95	0.07	71,71,71,71	0
2	LMR	A	1001	9/9	0.95	0.13	72,81,86,86	0
2	LMR	B	1001	9/9	0.96	0.07	84,89,101,102	0
4	PEG	C	1005	6/7	0.96	0.10	64,72,87,90	0
3	CL	C	1003	1/1	0.96	0.20	66,66,66,66	0
4	PEG	C	1007	6/7	0.97	0.09	64,74,77,83	0
3	CL	C	1004	1/1	0.98	0.12	73,73,73,73	0
2	LMR	C	1001	9/9	0.98	0.07	52,58,65,66	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.

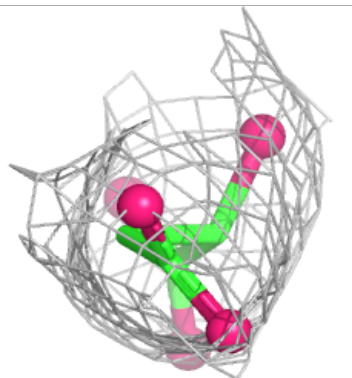
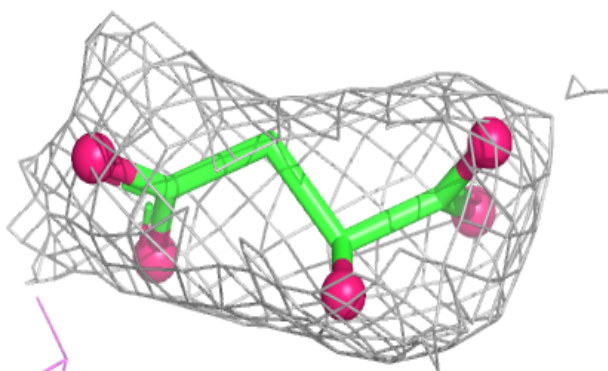
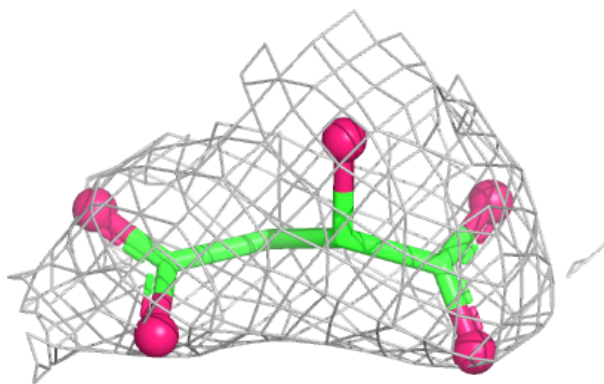
Electron density around LMR A 1001:

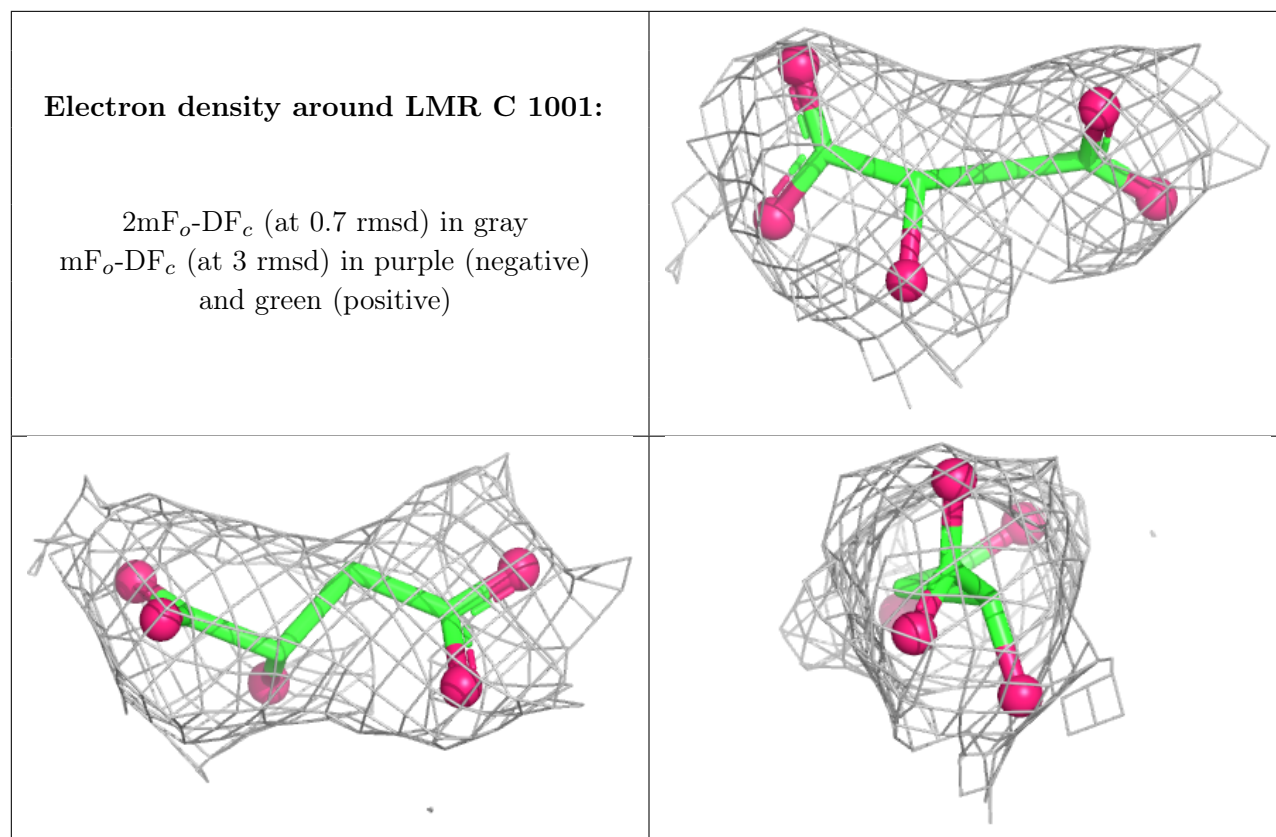
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMR B 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.