



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:53 PM UTC

PDB ID : 8OJE / pdb_00008oje
Title : Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 in complex with L-malate
Authors : Haesaerts, S.; Loris, R.; Larsen, P.B.
Deposited on : 2023-03-24
Resolution : 3.14 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:

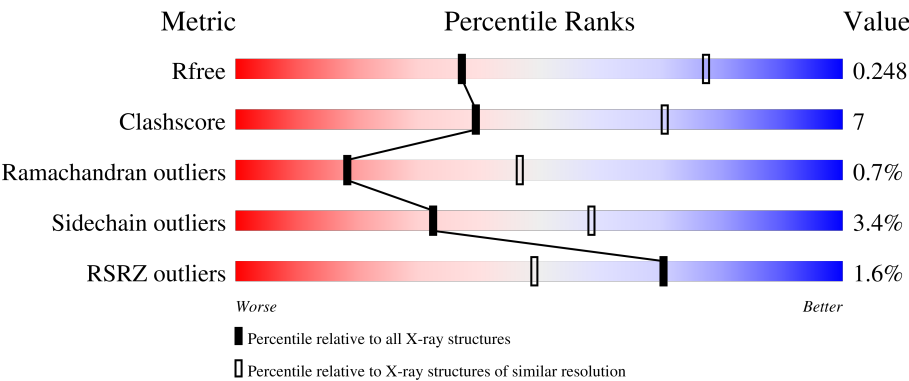
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	2% 80% 14% ..
1	B	974	2% 79% 16% ..
1	C	974	% 78% 16% ..
1	D	974	% 77% 17% ..
1	E	974	2% 78% 16% ..

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Mol	Chain	Length	Quality of chain
1	F	974	 2% 79% 15% . .
1	G	974	 2% 79% 15% . .
1	H	974	 2% 76% 18% . .

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
3	PEG	A	1003	-	-	-	X
3	PEG	C	1003	-	-	-	X
3	PEG	E	1003	-	-	-	X
3	PEG	G	1003	-	-	-	X
4	CL	C	1009	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59093 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	932	Total	C	N	O	S	0	2	0
			7262	4622	1249	1362	29			
1	B	932	Total	C	N	O	S	0	2	2
			7228	4603	1246	1350	29			
1	C	932	Total	C	N	O	S	0	3	1
			7395	4696	1279	1390	30			
1	D	933	Total	C	N	O	S	0	4	0
			7415	4709	1281	1395	30			
1	E	933	Total	C	N	O	S	0	3	0
			7326	4658	1255	1383	30			
1	F	933	Total	C	N	O	S	0	4	0
			7298	4642	1254	1372	30			
1	G	933	Total	C	N	O	S	0	2	1
			7346	4662	1276	1378	30			
1	H	933	Total	C	N	O	S	0	4	0
			7395	4694	1276	1395	30			

There are 56 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
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

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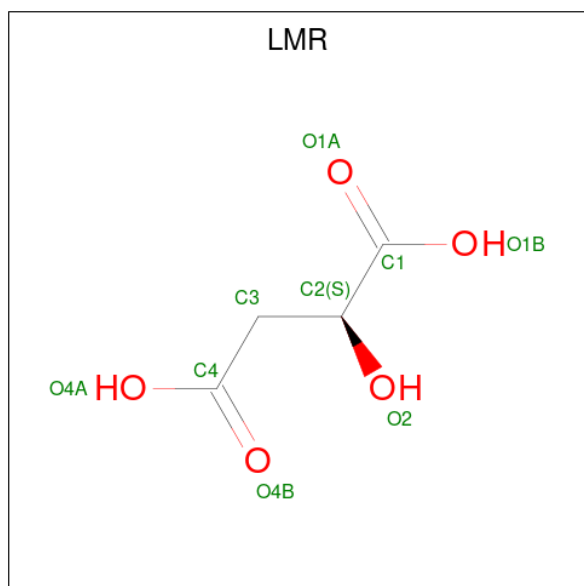
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9MAH0
C	-6	MET	-	initiating methionine	UNP Q9MAH0
C	-5	HIS	-	expression tag	UNP Q9MAH0
C	-4	HIS	-	expression tag	UNP Q9MAH0
C	-3	HIS	-	expression tag	UNP Q9MAH0
C	-2	HIS	-	expression tag	UNP Q9MAH0
C	-1	HIS	-	expression tag	UNP Q9MAH0
C	0	HIS	-	expression tag	UNP Q9MAH0
D	-6	MET	-	initiating methionine	UNP Q9MAH0
D	-5	HIS	-	expression tag	UNP Q9MAH0
D	-4	HIS	-	expression tag	UNP Q9MAH0
D	-3	HIS	-	expression tag	UNP Q9MAH0
D	-2	HIS	-	expression tag	UNP Q9MAH0
D	-1	HIS	-	expression tag	UNP Q9MAH0
D	0	HIS	-	expression tag	UNP Q9MAH0
E	-6	MET	-	initiating methionine	UNP Q9MAH0
E	-5	HIS	-	expression tag	UNP Q9MAH0
E	-4	HIS	-	expression tag	UNP Q9MAH0
E	-3	HIS	-	expression tag	UNP Q9MAH0
E	-2	HIS	-	expression tag	UNP Q9MAH0
E	-1	HIS	-	expression tag	UNP Q9MAH0
E	0	HIS	-	expression tag	UNP Q9MAH0
F	-6	MET	-	initiating methionine	UNP Q9MAH0
F	-5	HIS	-	expression tag	UNP Q9MAH0
F	-4	HIS	-	expression tag	UNP Q9MAH0
F	-3	HIS	-	expression tag	UNP Q9MAH0
F	-2	HIS	-	expression tag	UNP Q9MAH0
F	-1	HIS	-	expression tag	UNP Q9MAH0
F	0	HIS	-	expression tag	UNP Q9MAH0
G	-6	MET	-	initiating methionine	UNP Q9MAH0
G	-5	HIS	-	expression tag	UNP Q9MAH0
G	-4	HIS	-	expression tag	UNP Q9MAH0
G	-3	HIS	-	expression tag	UNP Q9MAH0
G	-2	HIS	-	expression tag	UNP Q9MAH0
G	-1	HIS	-	expression tag	UNP Q9MAH0
G	0	HIS	-	expression tag	UNP Q9MAH0
H	-6	MET	-	initiating methionine	UNP Q9MAH0
H	-5	HIS	-	expression tag	UNP Q9MAH0
H	-4	HIS	-	expression tag	UNP Q9MAH0
H	-3	HIS	-	expression tag	UNP Q9MAH0
H	-2	HIS	-	expression tag	UNP Q9MAH0
H	-1	HIS	-	expression tag	UNP Q9MAH0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP Q9MAH0

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: LMR) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		
2	C	1	Total	C	O	0	0
			9	4	5		
2	D	1	Total	C	O	0	0
			9	4	5		
2	E	1	Total	C	O	0	0
			9	4	5		
2	F	1	Total	C	O	0	0
			9	4	5		
2	G	1	Total	C	O	0	0
			9	4	5		
2	H	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 2 2	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C 2 2	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C 2 2	0	0
3	E	1	Total C O 6 4 2	0	0
3	E	1	Total C O 6 4 2	0	0
3	E	1	Total C 2 2	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C 2 2	0	0
3	F	1	Total C O 7 4 3	0	0
3	G	1	Total C O 7 4 3	0	0
3	G	1	Total C 2 2	0	0
3	G	1	Total C 2 2	0	0
3	G	1	Total C O 6 4 2	0	0
3	G	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C 2 2	0	0
3	G	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0
3	H	1	Total C 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	4	Total Cl 4 4	0	0
4	C	4	Total Cl 4 4	0	0
4	D	4	Total Cl 4 4	0	0
4	E	3	Total Cl 3 3	0	0
4	F	2	Total Cl 2 2	0	0
4	G	2	Total Cl 2 2	0	0
4	H	2	Total Cl 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	17	Total O 17 17	0	0
5	C	27	Total O 27 27	0	0
5	D	19	Total O 19 19	0	0

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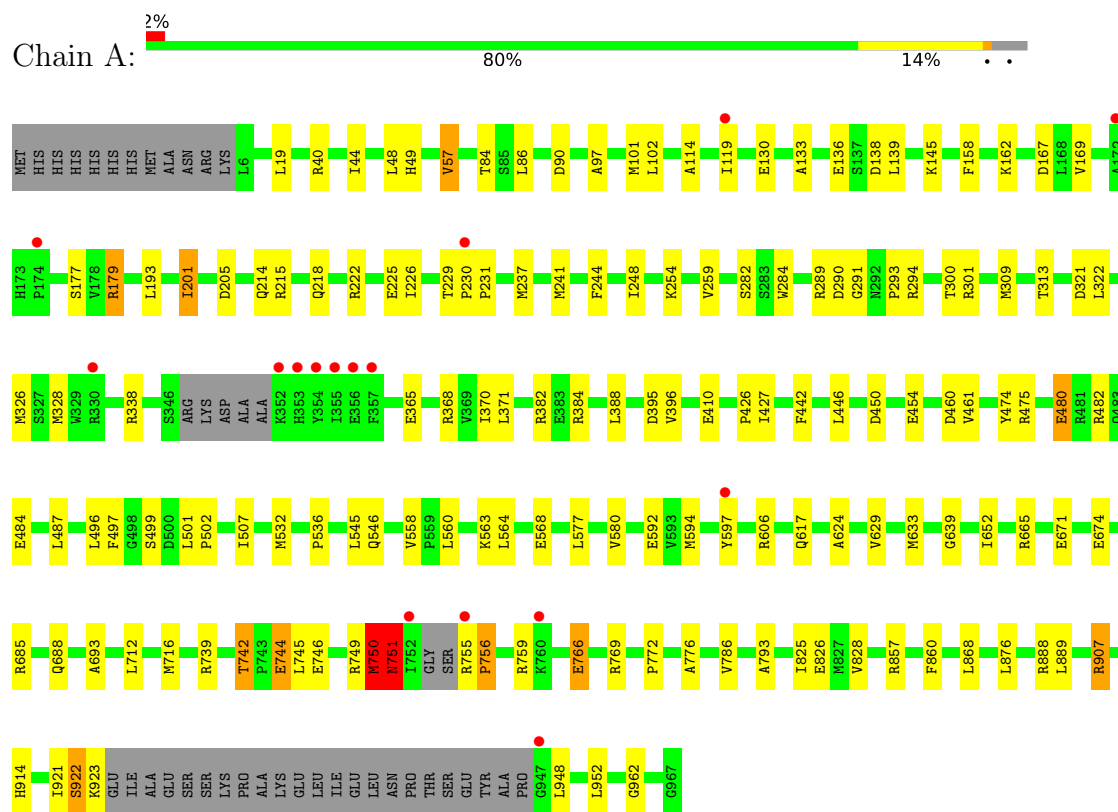
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	18	Total 18	O 18	0	0
5	F	18	Total 18	O 18	0	0
5	G	12	Total 12	O 12	0	0
5	H	17	Total 17	O 17	0	0

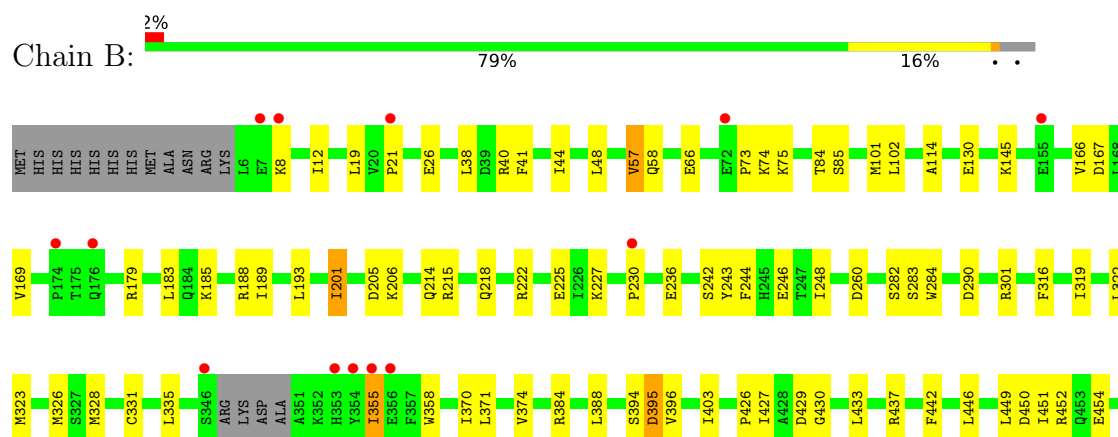
3 Residue-property plots [i](#)

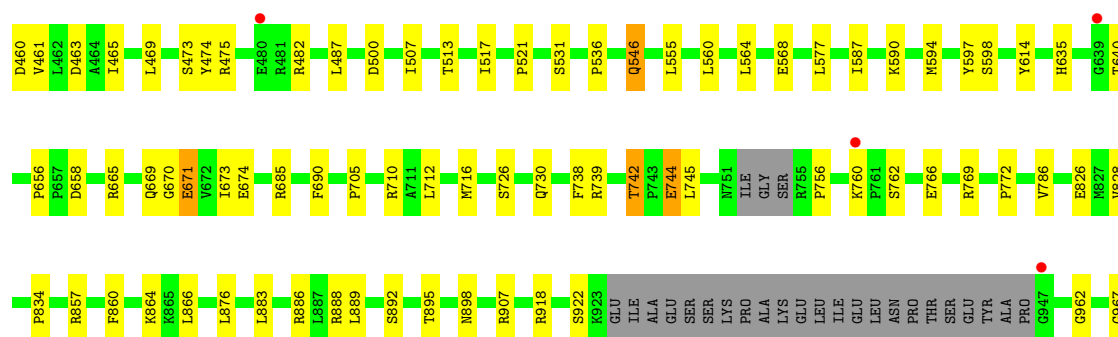
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

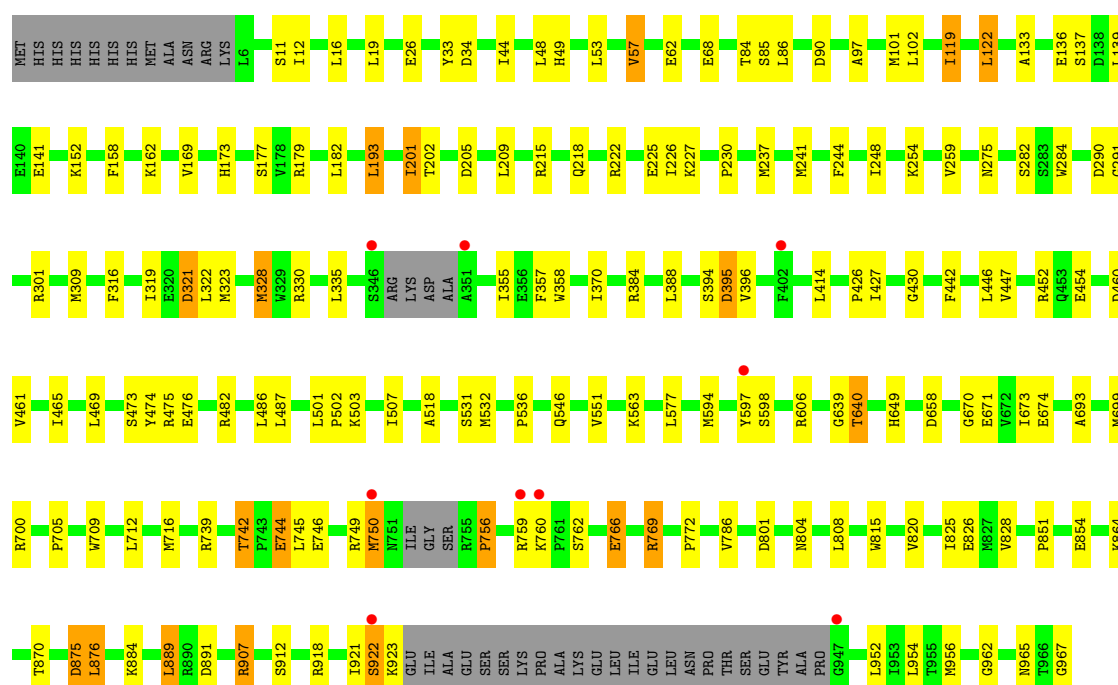
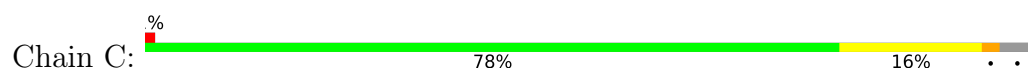


• Molecule 1: Phosphoenolpyruvate carboxylase 1

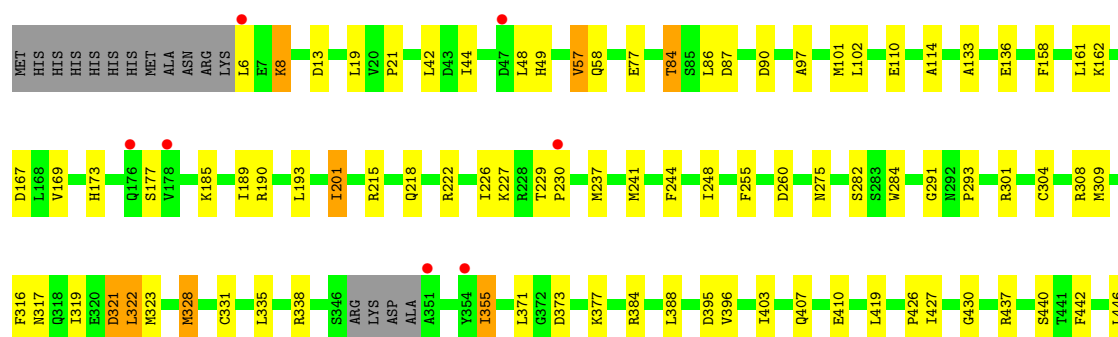
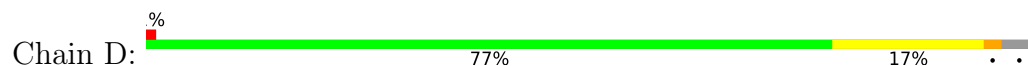


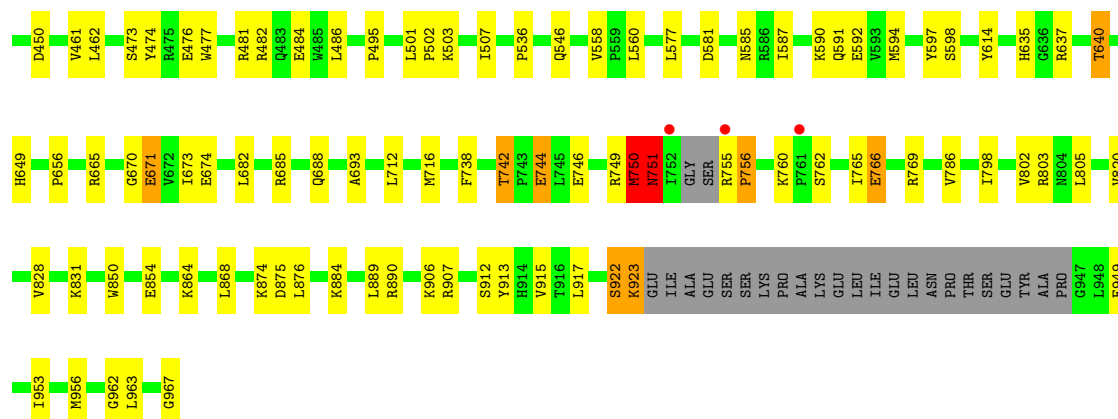


• Molecule 1: Phosphoenolpyruvate carboxylase 1

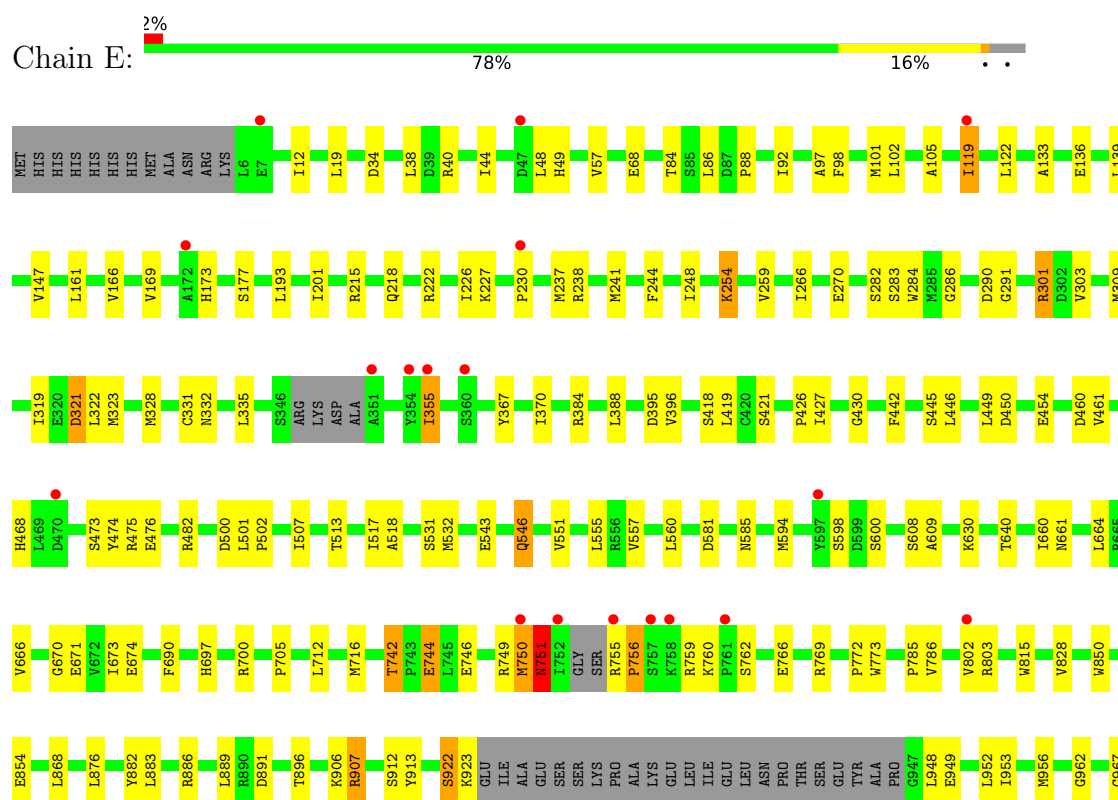


• Molecule 1: Phosphoenolpyruvate carboxylase 1

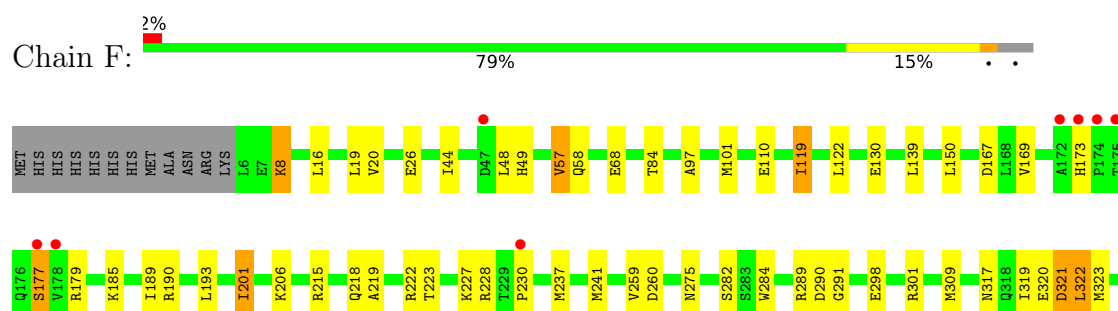


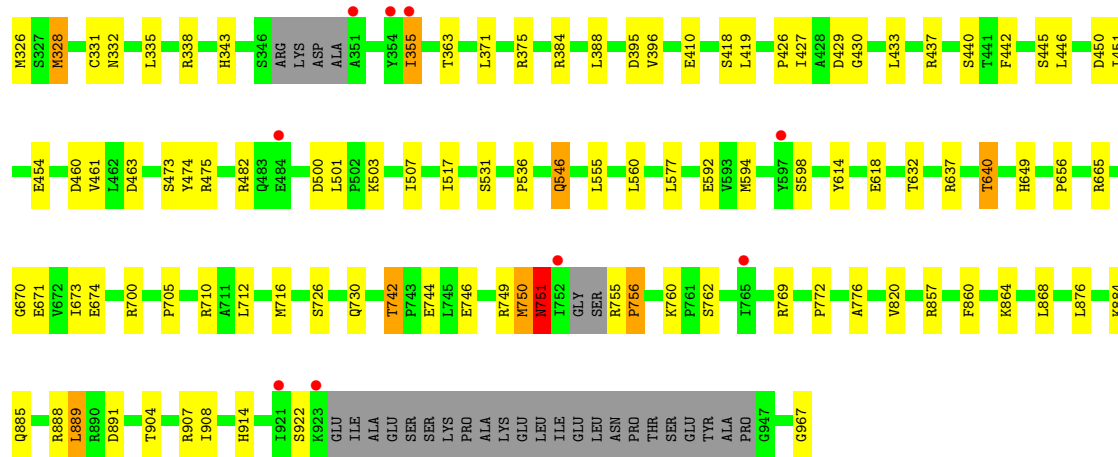


- Molecule 1: Phosphoenolpyruvate carboxylase 1

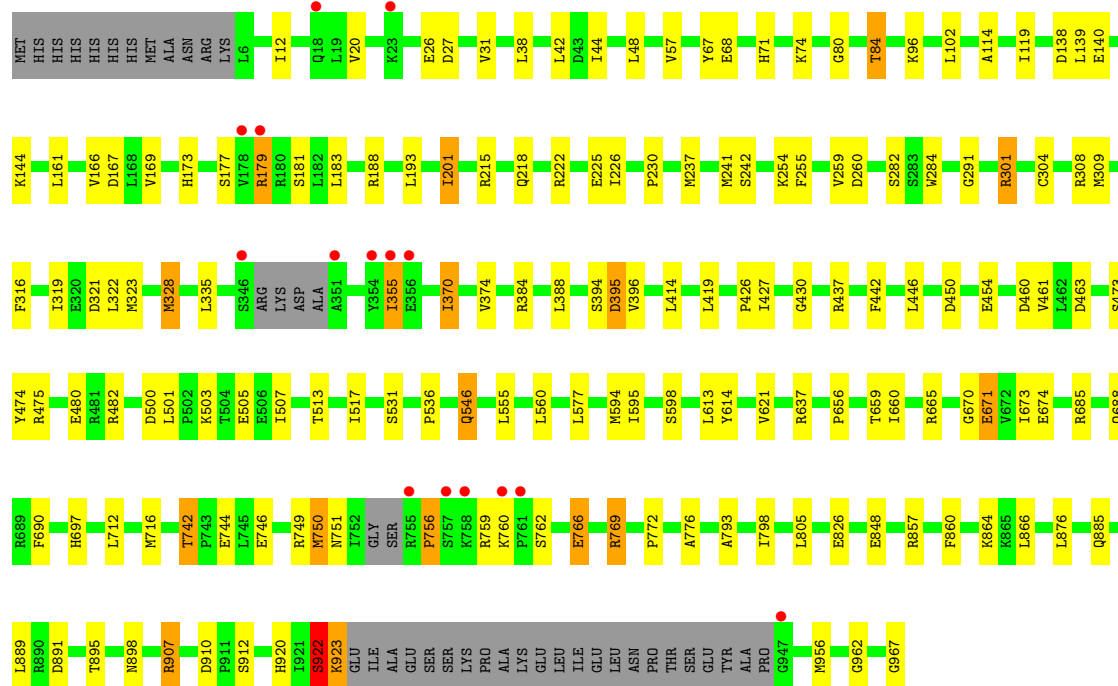
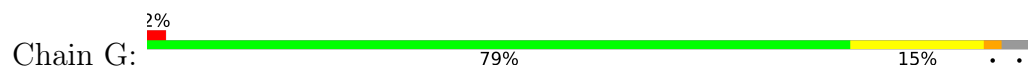


- Molecule 1: Phosphoenolpyruvate carboxylase 1

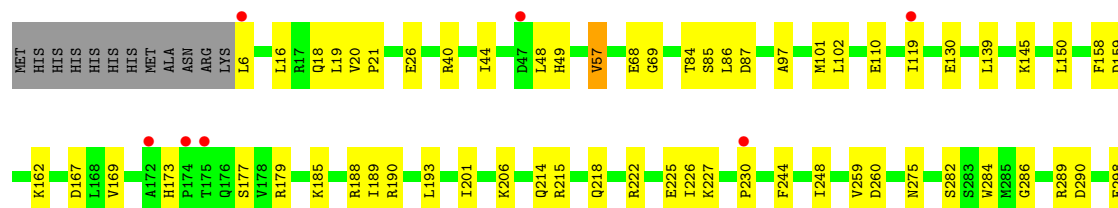
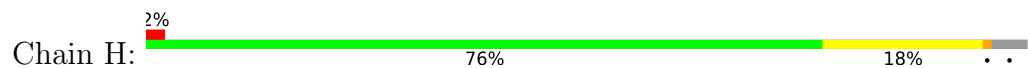


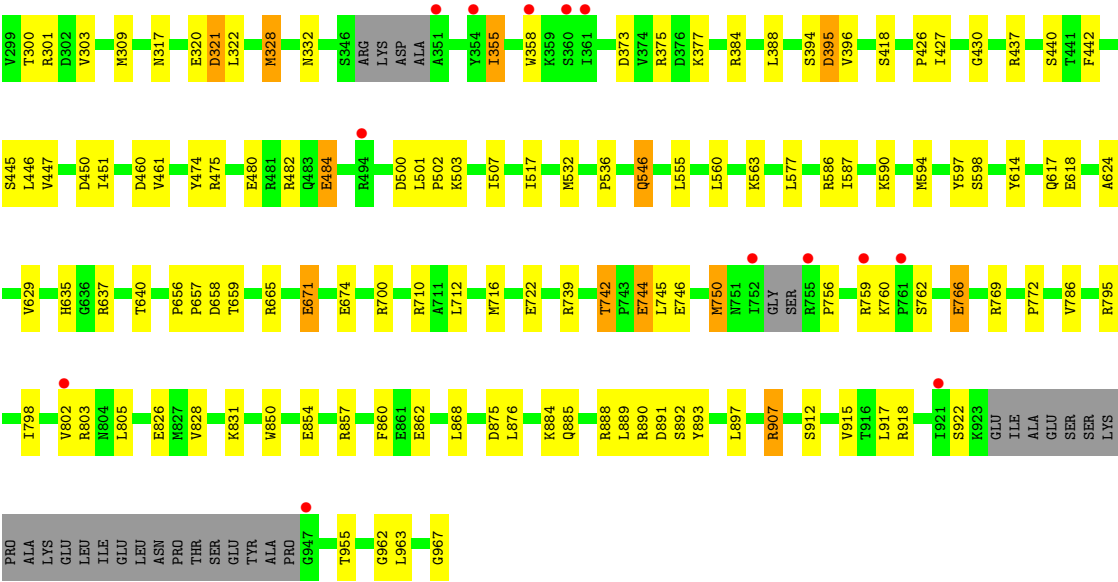


• Molecule 1: Phosphoenolpyruvate carboxylase 1



• Molecule 1: Phosphoenolpyruvate carboxylase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.08Å 352.20Å 176.04Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	48.93 – 3.14 48.93 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.93-3.14) 99.2 (48.93-3.14)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.202 , 0.240 0.212 , 0.248	Depositor DCC
R_{free} test set	11875 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	59093	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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 33.14 % 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 8.3954e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, PEG, 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	0.26	0/7426	0.47	0/10091
1	B	0.25	0/7391	0.47	0/10047
1	C	0.28	0/7563	0.50	0/10257
1	D	0.29	0/7586	0.51	0/10287
1	E	0.28	0/7494	0.50	1/10178 (0.0%)
1	F	0.27	0/7469	0.49	0/10148
1	G	0.27	0/7510	0.48	0/10195
1	H	0.26	0/7566	0.49	0/10265
All	All	0.27	0/60005	0.49	1/81468 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	266	ILE	N-CA-C	-5.67	107.22	112.43

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	750	MET	Peptide
1	D	750	MET	Peptide
1	E	750	MET	Peptide

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	7262	0	6975	91	0
1	B	7228	0	6951	92	0
1	C	7395	0	7240	105	0
1	D	7415	0	7261	113	0
1	E	7326	0	7095	103	0
1	F	7298	0	7044	92	0
1	G	7346	0	7136	102	0
1	H	7395	0	7200	111	0
2	A	9	0	4	0	0
2	B	9	0	4	0	0
2	C	9	0	4	1	0
2	D	9	0	4	1	0
2	E	9	0	4	0	0
2	F	9	0	4	0	0
2	G	9	0	4	0	0
2	H	9	0	4	1	0
3	A	33	0	35	0	0
3	B	16	0	18	1	0
3	C	26	0	26	0	0
3	D	23	0	27	1	0
3	E	30	0	32	0	0
3	F	23	0	27	2	0
3	G	33	0	35	0	0
3	H	16	0	18	2	0
4	A	2	0	0	0	0
4	B	4	0	0	1	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	3	0	0	1	0
4	F	2	0	0	0	0
4	G	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2	0	0	1	0
5	A	5	0	0	0	0
5	B	17	0	0	2	0
5	C	27	0	0	0	0
5	D	19	0	0	0	0
5	E	18	0	0	1	0
5	F	18	0	0	0	0
5	G	12	0	0	0	0
5	H	17	0	0	0	0
All	All	59093	0	57152	774	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 (774) 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:301[A]:ARG:NH2	1:B:388:LEU:O	2.11	0.84
1:F:169:VAL:HG22	1:F:282:SER:HB2	1.64	0.80
1:H:461:VAL:HG22	1:H:507:ILE:HG23	1.65	0.78
1:A:301:ARG:NH2	1:A:388:LEU:O	2.17	0.78
1:H:206:LYS:HE3	3:H:1003:PEG:H31	1.67	0.76
1:G:920:HIS:CE1	1:G:922:SER:HB2	2.19	0.76
1:F:884:LYS:HE2	1:F:888[B]:ARG:HH21	1.52	0.74
1:G:384:ARG:HG3	1:G:396:VAL:HB	1.69	0.74
1:A:751:ASN:ND2	1:A:755:ARG:O	2.21	0.73
1:G:746:GLU:O	1:G:750:MET:HG2	1.88	0.73
1:G:188:ARG:NH2	1:H:321[B]:ASP:OD2	2.22	0.73
1:D:751:ASN:ND2	1:D:755:ARG:O	2.22	0.72
1:G:920:HIS:HE1	1:G:922:SER:HB2	1.53	0.72
1:F:751:ASN:ND2	1:F:755:ARG:O	2.22	0.72
1:F:20:VAL:HG11	1:F:885:GLN:HG3	1.72	0.72
1:C:461:VAL:HG22	1:C:507:ILE:HG23	1.72	0.72
1:D:169:VAL:HG22	1:D:282:SER:HB2	1.70	0.72
1:B:460:ASP:OD1	1:B:475:ARG:NH2	2.22	0.72
1:D:317:ASN:HB3	3:D:1002:PEG:H41	1.72	0.71
1:E:751:ASN:ND2	1:E:755:ARG:O	2.24	0.71
1:G:48:LEU:HD13	1:G:222:ARG:HD3	1.73	0.71
1:H:460:ASP:OD1	1:H:475:ARG:NH2	2.23	0.71
1:F:460:ASP:OD1	1:F:475:ARG:NH2	2.25	0.70
1:E:598:SER:OG	1:E:967:GLY:OXT	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:MET:HE2	1:C:427:ILE:HD13	1.72	0.69
1:B:384:ARG:HG3	1:B:396:VAL:HB	1.74	0.69
1:F:301:ARG:NH2	1:F:388:LEU:O	2.26	0.69
1:G:169:VAL:HG22	1:G:282:SER:HB2	1.73	0.68
1:C:169:VAL:HG22	1:C:282:SER:HB2	1.73	0.68
1:H:44:ILE:HD13	1:H:218:GLN:HB2	1.76	0.68
1:C:48:LEU:HD13	1:C:222:ARG:HD3	1.75	0.68
1:H:169:VAL:HG22	1:H:282:SER:HB2	1.74	0.68
1:E:384:ARG:HG3	1:E:396:VAL:HB	1.76	0.67
1:H:746:GLU:O	1:H:750:MET:HG2	1.95	0.67
1:C:301:ARG:NH2	1:C:388:LEU:O	2.27	0.67
1:D:461:VAL:HG22	1:D:507:ILE:HG23	1.75	0.67
1:E:750:MET:O	1:E:751:ASN:HB2	1.95	0.67
1:A:750:MET:O	1:A:751:ASN:HB2	1.95	0.67
1:E:309:MET:HE1	1:F:355:ILE:HD13	1.75	0.67
1:H:373:ASP:OD2	1:H:377:LYS:NZ	2.28	0.66
1:A:328:MET:HE2	1:A:427:ILE:HD13	1.78	0.66
1:D:581:ASP:O	1:D:585:ASN:ND2	2.29	0.65
1:B:461:VAL:HG22	1:B:507:ILE:HG23	1.78	0.65
1:D:373:ASP:OD2	1:D:377:LYS:NZ	2.29	0.65
1:G:426:PRO:O	1:H:215:ARG:HD3	1.96	0.65
1:D:473:SER:OG	1:D:476:GLU:HG2	1.97	0.65
1:G:355:ILE:HD13	1:H:309:MET:HE1	1.79	0.65
1:C:598:SER:OG	1:C:967:GLY:OXT	2.15	0.65
1:F:750:MET:O	1:F:751:ASN:HB2	1.95	0.65
1:G:102:LEU:HD21	1:G:962:GLY:HA3	1.79	0.65
1:F:284:TRP:HH2	1:F:594:MET:HE1	1.63	0.64
1:G:460:ASP:OD1	1:G:475:ARG:NH2	2.31	0.64
1:C:44:ILE:HD13	1:C:218:GLN:HB2	1.78	0.64
1:F:44:ILE:HD13	1:F:218:GLN:HB2	1.79	0.64
1:C:454:GLU:HA	1:C:531:SER:HB2	1.80	0.64
1:F:48:LEU:HD13	1:F:222:ARG:HD3	1.80	0.64
1:F:598:SER:OG	1:F:967:GLY:OXT	2.14	0.64
1:C:746:GLU:O	1:C:750:MET:HG2	1.98	0.63
1:H:68:GLU:O	1:H:888:ARG:NH1	2.30	0.63
1:H:284:TRP:HH2	1:H:594:MET:HE1	1.62	0.63
1:A:461:VAL:HG22	1:A:507:ILE:HG23	1.80	0.63
1:D:750:MET:O	1:D:751:ASN:HB2	1.98	0.63
1:C:460:ASP:OD1	1:C:475:ARG:NH2	2.31	0.62
1:B:328:MET:HE2	1:B:427:ILE:HD13	1.81	0.62
1:G:284:TRP:HH2	1:G:594:MET:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:ASP:OD1	1:E:475:ARG:NH2	2.32	0.62
1:F:712:LEU:O	1:F:716:MET:HG3	2.00	0.62
1:A:480:GLU:O	1:A:484:GLU:HG2	1.99	0.62
1:G:68:GLU:CD	1:G:891:ASP:HB3	2.24	0.62
1:A:169:VAL:HG22	1:A:282:SER:HB2	1.80	0.62
1:G:474:TYR:CZ	1:G:482:ARG:HD3	2.34	0.62
1:E:238:ARG:NH2	4:E:1009:CL:CL	2.71	0.61
1:H:328:MET:HE2	1:H:427:ILE:HG21	1.82	0.61
1:E:802:VAL:HG23	1:E:803:ARG:HG3	1.81	0.61
1:G:712:LEU:O	1:G:716:MET:HG3	2.01	0.61
1:H:868:LEU:HD21	1:H:876:LEU:HD23	1.83	0.61
1:B:244:PHE:HA	1:B:248:ILE:HB	1.83	0.60
1:G:328:MET:SD	1:G:328:MET:N	2.74	0.60
1:D:284:TRP:HH2	1:D:594:MET:HE1	1.65	0.60
1:G:309:MET:HE1	1:H:355:ILE:HD13	1.83	0.60
1:D:301:ARG:NH2	1:D:388:LEU:O	2.34	0.60
1:E:426:PRO:O	1:F:215:ARG:HD3	2.01	0.60
1:E:355:ILE:HD13	1:F:309:MET:HE1	1.83	0.60
1:E:442:PHE:HB3	1:E:446:LEU:HD23	1.84	0.60
1:G:44:ILE:HD13	1:G:218:GLN:HB2	1.81	0.60
1:A:496:LEU:HB3	1:A:497:PHE:HD1	1.66	0.60
1:H:826:GLU:HG3	1:H:876:LEU:HD22	1.84	0.60
1:E:454:GLU:HA	1:E:531:SER:HB2	1.84	0.60
1:E:291:GLY:O	1:E:756:PRO:HD2	2.02	0.59
1:B:169:VAL:HG22	1:B:282:SER:HB2	1.85	0.59
1:C:532:MET:HG3	1:C:759:ARG:HH12	1.66	0.59
1:G:301:ARG:NH2	1:G:388:LEU:O	2.36	0.59
1:H:597[A]:TYR:OH	1:H:635:HIS:ND1	2.34	0.59
1:B:44:ILE:HD13	1:B:218:GLN:HB2	1.84	0.59
1:C:11:SER:OG	1:C:62:GLU:OE2	2.19	0.59
1:C:215:ARG:HD3	1:D:426:PRO:O	2.03	0.58
1:H:173:HIS:HB2	1:H:177:SER:HB3	1.85	0.58
1:H:301:ARG:NH2	1:H:388:LEU:O	2.36	0.58
1:D:637[B]:ARG:NH2	1:D:671:GLU:OE2	2.35	0.58
1:C:309:MET:HE1	1:D:355:ILE:HD13	1.86	0.58
1:F:167:ASP:HB3	1:F:665:ARG:HG3	1.84	0.57
1:H:49:HIS:O	1:H:922:SER:HB3	2.03	0.57
1:E:474:TYR:CZ	1:E:482:ARG:HD3	2.39	0.57
1:A:560:LEU:HD13	1:A:594:MET:HG2	1.87	0.57
1:C:291:GLY:O	1:C:756:PRO:HD2	2.04	0.57
1:D:384:ARG:HG3	1:D:396:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597[A]:TYR:OH	1:B:635:HIS:ND1	2.32	0.57
1:G:826:GLU:HG3	1:G:876:LEU:HD22	1.86	0.57
1:D:746:GLU:O	1:D:750:MET:HG2	2.05	0.57
1:F:384:ARG:HG3	1:F:396:VAL:HB	1.85	0.57
1:H:739:ARG:HB3	1:H:745:LEU:HD11	1.87	0.57
1:H:598:SER:OG	1:H:967:GLY:OXT	2.22	0.57
1:A:290:ASP:CG	1:A:769:ARG:HH12	2.13	0.57
1:B:74:LYS:HG3	5:B:1112:HOH:O	2.04	0.57
1:E:49:HIS:O	1:E:922:SER:HB3	2.05	0.57
1:E:907:ARG:HB3	1:E:948:LEU:HD13	1.86	0.57
1:F:110:GLU:OE1	1:F:190:ARG:NH1	2.37	0.56
1:H:328:MET:SD	1:H:328:MET:N	2.78	0.56
1:E:546:GLN:OE1	1:E:555:LEU:N	2.37	0.56
1:D:328:MET:HE2	1:D:427:ILE:HD13	1.87	0.56
1:H:159:ASP:HA	1:H:162:LYS:HD3	1.87	0.56
1:E:48:LEU:HD13	1:E:222:ARG:HD3	1.88	0.56
1:E:906:LYS:HE3	1:E:913:TYR:CD1	2.40	0.56
1:H:798:ILE:HD11	1:H:805:LEU:HD13	1.87	0.56
1:E:746:GLU:HG3	1:E:749:ARG:HH21	1.71	0.56
1:A:215:ARG:HD3	1:B:426:PRO:O	2.05	0.55
1:B:12:ILE:HD13	1:B:38:LEU:HD23	1.87	0.55
1:C:742:THR:HG23	1:C:744:GLU:H	1.71	0.55
1:B:8:LYS:HB3	1:B:58:GLN:HE22	1.71	0.55
1:A:321[B]:ASP:OD2	1:B:188:ARG:NH2	2.39	0.55
1:B:319:ILE:O	1:B:323:MET:HG3	2.06	0.55
1:C:426:PRO:O	1:D:215:ARG:HD3	2.06	0.55
1:E:290:ASP:CG	1:E:769:ARG:HH12	2.15	0.55
1:D:291:GLY:O	1:D:756:PRO:HD2	2.07	0.55
1:D:328:MET:SD	1:D:328:MET:N	2.80	0.55
1:F:442:PHE:HB3	1:F:446:LEU:HA	1.89	0.55
1:G:215:ARG:HD2	1:H:430:GLY:HA3	1.88	0.55
1:H:394:SER:OG	1:H:395:ASP:N	2.37	0.55
1:C:474:TYR:CZ	1:C:482:ARG:HD3	2.41	0.55
1:D:712:LEU:O	1:D:716:MET:HG3	2.06	0.55
1:F:150:LEU:HD11	1:F:700:ARG:HG3	1.89	0.55
1:D:746:GLU:HG3	1:D:749:ARG:HH21	1.71	0.55
1:A:750:MET:HE3	1:A:952:LEU:HD23	1.89	0.55
1:E:133:ALA:HA	1:E:136:GLU:HG2	1.89	0.55
1:G:114:ALA:O	1:G:685:ARG:NH2	2.39	0.54
1:A:284:TRP:HH2	1:A:594:MET:HE1	1.71	0.54
1:A:426:PRO:O	1:B:215:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PRO:HB3	1:A:577:LEU:HG	1.88	0.54
1:C:766:GLU:CD	1:C:766:GLU:H	2.14	0.54
1:D:167:ASP:HB3	1:D:665:ARG:HG3	1.88	0.54
1:D:536:PRO:HB3	1:D:577:LEU:HG	1.88	0.54
1:E:301:ARG:NH2	1:E:388:LEU:O	2.40	0.54
1:H:130:GLU:OE2	1:H:145:LYS:NZ	2.40	0.54
1:B:284:TRP:HH2	1:B:594:MET:HE1	1.72	0.54
1:G:442:PHE:HB3	1:G:446:LEU:HA	1.89	0.54
1:A:384:ARG:HG3	1:A:396:VAL:HB	1.90	0.54
1:H:442:PHE:HB3	1:H:446:LEU:HA	1.90	0.54
1:B:726:SER:HA	1:B:730:GLN:HB2	1.90	0.54
1:C:384:ARG:HG3	1:C:396:VAL:HB	1.88	0.54
1:B:826:GLU:HG3	1:B:876:LEU:HD22	1.90	0.54
1:C:173:HIS:HB2	1:C:177:SER:HB3	1.89	0.54
1:C:712:LEU:O	1:C:716:MET:HG3	2.06	0.54
1:D:322:LEU:HD13	1:D:371:LEU:HD13	1.89	0.54
1:D:442:PHE:HB3	1:D:446:LEU:HA	1.89	0.54
1:D:798:ILE:HD11	1:D:805:LEU:HD13	1.90	0.54
1:F:461:VAL:HG22	1:F:507:ILE:HG23	1.88	0.54
1:H:637[B]:ARG:NH2	1:H:671:GLU:OE2	2.36	0.54
1:B:206:LYS:HE3	3:B:1003:PEG:H31	1.90	0.54
1:C:875:ASP:O	1:C:876:LEU:HB2	2.08	0.54
1:D:173:HIS:HB2	1:D:177:SER:HB3	1.88	0.54
1:D:284:TRP:CD1	1:D:450:ASP:HB2	2.42	0.54
1:H:384:ARG:HG3	1:H:396:VAL:HB	1.90	0.54
1:D:338:ARG:NH2	1:D:410:GLU:OE1	2.26	0.53
1:D:560:LEU:HD13	1:D:594:MET:HG2	1.89	0.53
1:E:331:CYS:HB2	1:E:335:LEU:HD23	1.91	0.53
1:H:48:LEU:HD13	1:H:222:ARG:HD3	1.89	0.53
1:D:501:LEU:HD12	1:D:502:PRO:HD2	1.91	0.53
1:E:284:TRP:CD1	1:E:450:ASP:HB2	2.43	0.53
1:E:244:PHE:HA	1:E:248:ILE:HB	1.91	0.53
1:D:442:PHE:HB3	1:D:446:LEU:HD23	1.90	0.53
1:F:317:ASN:HB3	3:F:1002:PEG:H41	1.91	0.53
1:B:454:GLU:HA	1:B:531:SER:HB2	1.91	0.53
1:D:766:GLU:H	1:D:766:GLU:CD	2.16	0.53
1:B:201:ILE:HG13	1:B:205:ASP:HB2	1.91	0.53
1:E:786:VAL:HG11	1:E:828:VAL:HG21	1.89	0.53
1:H:284:TRP:CD1	1:H:450:ASP:HB2	2.44	0.53
1:D:786:VAL:HG11	1:D:828:VAL:HG21	1.91	0.53
1:A:40:ARG:HD2	1:A:214:GLN:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:618:GLU:OE1	1:F:710:ARG:NH2	2.41	0.53
1:A:532:MET:HG3	1:A:759:ARG:HH12	1.73	0.52
1:G:461:VAL:HG22	1:G:507:ILE:HG23	1.90	0.52
1:H:532:MET:HG3	1:H:759:ARG:HH12	1.74	0.52
1:B:712:LEU:O	1:B:716:MET:HG3	2.09	0.52
1:D:746:GLU:HG3	1:D:749:ARG:NH2	2.23	0.52
1:G:536:PRO:HB3	1:G:577:LEU:HG	1.92	0.52
1:A:922:SER:OG	1:A:923:LYS:N	2.42	0.52
1:D:328:MET:HE2	1:D:427:ILE:HG21	1.91	0.52
1:E:119:ILE:HG13	1:E:122:LEU:HD22	1.92	0.52
1:D:864:LYS:HE2	1:D:876:LEU:HD11	1.91	0.52
1:D:244:PHE:HA	1:D:248:ILE:HB	1.91	0.52
1:D:890:ARG:NH2	2:D:1001:LMR:O4B	2.36	0.52
1:F:322:LEU:HD13	1:F:371:LEU:HD13	1.92	0.52
1:F:546:GLN:OE1	1:F:555:LEU:N	2.40	0.52
1:H:284:TRP:CH2	1:H:594:MET:HE1	2.44	0.52
1:H:480:GLU:O	1:H:484:GLU:HG2	2.10	0.52
1:A:86:LEU:O	1:A:907:ARG:NH2	2.43	0.52
1:A:102:LEU:HD21	1:A:962:GLY:HA3	1.91	0.52
1:B:451:ILE:HG13	1:B:517:ILE:HD11	1.91	0.52
1:G:760:LYS:C	1:G:762:SER:H	2.17	0.52
1:B:742:THR:HG23	1:B:744:GLU:H	1.74	0.52
1:E:44:ILE:HD13	1:E:218:GLN:HB2	1.92	0.52
1:F:331:CYS:HB2	1:F:335:LEU:HD23	1.92	0.52
1:E:102:LEU:HD21	1:E:962:GLY:HA3	1.92	0.52
1:F:451:ILE:HG13	1:F:517:ILE:HD11	1.91	0.52
1:E:461:VAL:HG22	1:E:507:ILE:HG23	1.92	0.51
1:H:150:LEU:HD21	1:H:700:ARG:HG3	1.92	0.51
1:H:451:ILE:HG13	1:H:517:ILE:HD11	1.91	0.51
1:B:48:LEU:HD22	1:B:222:ARG:NH1	2.25	0.51
1:B:331:CYS:HB2	1:B:335:LEU:HD23	1.91	0.51
1:C:760:LYS:C	1:C:762:SER:H	2.19	0.51
1:E:442:PHE:HB3	1:E:446:LEU:HA	1.92	0.51
1:F:139:LEU:HD21	1:F:259:VAL:HG22	1.92	0.51
1:G:746:GLU:HG3	1:G:749:ARG:HH21	1.76	0.51
1:H:875:ASP:HB3	1:H:884:LYS:NZ	2.25	0.51
1:G:84:THR:O	1:G:907:ARG:NH2	2.40	0.51
1:A:44:ILE:HD13	1:A:218:GLN:HB2	1.93	0.51
1:H:712:LEU:O	1:H:716:MET:HG3	2.11	0.51
1:A:532:MET:HE1	1:A:563:LYS:HD2	1.92	0.51
1:C:750:MET:HE3	1:C:952:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:HD13	1:D:222:ARG:HD3	1.93	0.51
1:E:97:ALA:C	1:E:101:MET:HE3	2.36	0.51
1:E:742:THR:HG23	1:E:744:GLU:H	1.76	0.51
1:F:328:MET:SD	1:F:328:MET:N	2.84	0.51
1:F:429:ASP:HA	1:F:433:LEU:HB2	1.92	0.51
1:F:474:TYR:CZ	1:F:482:ARG:HD3	2.46	0.51
1:F:284:TRP:CH2	1:F:594:MET:HE1	2.46	0.51
1:A:742:THR:CG2	1:A:776:ALA:HB1	2.41	0.51
1:A:746:GLU:HG3	1:A:749:ARG:HH21	1.75	0.51
1:F:284:TRP:CD1	1:F:450:ASP:HB2	2.45	0.51
1:F:501:LEU:O	1:F:503:LYS:HG3	2.11	0.51
1:F:746:GLU:O	1:F:750:MET:HG2	2.10	0.51
1:A:48:LEU:HD13	1:A:222:ARG:HD3	1.92	0.51
1:G:173:HIS:HB2	1:G:177:SER:HB3	1.93	0.51
1:H:802:VAL:HG23	1:H:803:ARG:HG3	1.92	0.50
1:A:309:MET:HE1	1:B:355:ILE:HD13	1.93	0.50
1:B:598:SER:OG	1:B:967:GLY:OXT	2.23	0.50
1:C:746:GLU:HG3	1:C:749:ARG:HH21	1.75	0.50
1:D:133:ALA:HA	1:D:136:GLU:HG2	1.93	0.50
1:F:328:MET:HE2	1:F:427:ILE:HD13	1.93	0.50
1:G:560:LEU:HD13	1:G:594:MET:HG2	1.93	0.50
1:C:875:ASP:HB3	1:C:884:LYS:NZ	2.27	0.50
1:E:169:VAL:HG22	1:E:282:SER:HB2	1.93	0.50
1:A:442:PHE:HB3	1:A:446:LEU:HD23	1.94	0.50
1:E:501:LEU:HD12	1:E:502:PRO:HD2	1.94	0.50
1:G:291:GLY:O	1:G:756:PRO:HD2	2.11	0.50
1:A:742:THR:HG22	1:A:744:GLU:H	1.75	0.50
1:D:598:SER:OG	1:D:967:GLY:OXT	2.28	0.50
1:G:321:ASP:OD1	1:H:188:ARG:NH2	2.44	0.50
1:C:965:ASN:OD1	2:C:1001:LMR:O2	2.29	0.50
1:E:215:ARG:HD2	1:F:430:GLY:HA3	1.92	0.50
1:E:760:LYS:C	1:E:762:SER:H	2.20	0.50
1:A:712:LEU:O	1:A:716:MET:HG3	2.12	0.50
1:C:328:MET:SD	1:C:328:MET:N	2.85	0.50
1:E:473:SER:OG	1:E:476:GLU:HG2	2.11	0.50
1:F:8:LYS:HB3	1:F:58:GLN:HE22	1.76	0.50
1:G:864:LYS:HE2	1:G:876:LEU:HD11	1.94	0.50
1:B:48:LEU:HD13	1:B:222:ARG:HD3	1.94	0.50
1:D:49:HIS:O	1:D:922:SER:HB3	2.12	0.50
1:G:140:GLU:HG2	1:G:144:LYS:HE3	1.94	0.50
1:B:739:ARG:HB3	1:B:745:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ARG:HD3	1:F:426:PRO:O	2.12	0.49
1:G:284:TRP:CH2	1:G:594:MET:HE1	2.45	0.49
1:G:500:ASP:OD1	1:G:500:ASP:N	2.44	0.49
1:B:167:ASP:HB3	1:B:665:ARG:HG3	1.94	0.49
1:E:882:TYR:O	1:E:886:ARG:HG3	2.12	0.49
1:H:289:ARG:NH2	1:H:300:THR:OG1	2.40	0.49
1:G:215:ARG:HD3	1:H:426:PRO:O	2.12	0.49
1:C:786:VAL:HG11	1:C:828:VAL:HG21	1.94	0.49
1:D:44:ILE:HD13	1:D:218:GLN:HB2	1.95	0.49
1:E:332:ASN:HB2	1:E:418:SER:HA	1.92	0.49
1:G:237:MET:O	1:G:241:MET:HG2	2.12	0.49
1:G:394:SER:OG	1:G:395:ASP:N	2.45	0.49
1:C:284:TRP:HH2	1:C:594:MET:HE1	1.77	0.49
1:B:834:PRO:HD2	1:G:74:LYS:HE2	1.95	0.49
1:C:536:PRO:HB3	1:C:577:LEU:HG	1.94	0.49
1:H:532:MET:HE1	1:H:563:LYS:HD2	1.94	0.49
1:H:857:ARG:O	1:H:860:PHE:HB3	2.13	0.49
1:F:319:ILE:O	1:F:323:MET:HG3	2.13	0.49
1:F:670:GLY:O	1:F:673:ILE:HG22	2.13	0.49
1:A:606:ARG:HD3	1:A:825:ILE:HD11	1.95	0.49
1:D:169:VAL:HA	1:D:282:SER:O	2.13	0.49
1:D:293:PRO:HD3	1:D:756:PRO:HG3	1.95	0.49
1:H:760:LYS:C	1:H:762:SER:H	2.20	0.49
1:A:133:ALA:HA	1:A:136:GLU:HG2	1.94	0.49
1:G:546:GLN:OE1	1:G:555:LEU:N	2.45	0.49
1:H:68:GLU:CD	1:H:891:ASP:HB3	2.38	0.49
1:A:244:PHE:HA	1:A:248:ILE:HB	1.95	0.48
1:B:614:TYR:CD2	1:B:656:PRO:HG3	2.48	0.48
1:C:864:LYS:HE2	1:C:876:LEU:HD11	1.95	0.48
1:D:922:SER:OG	1:D:923:LYS:N	2.38	0.48
1:E:430:GLY:HA3	1:F:215:ARG:HD2	1.95	0.48
1:H:320:GLU:HB3	1:H:375:ARG:NH1	2.28	0.48
1:H:332:ASN:HB2	1:H:418:SER:HA	1.95	0.48
1:B:760:LYS:C	1:B:762:SER:H	2.21	0.48
1:G:501:LEU:O	1:G:503:LYS:HG3	2.13	0.48
1:C:133:ALA:HA	1:C:136:GLU:HG2	1.95	0.48
1:A:291:GLY:O	1:A:756:PRO:HD2	2.13	0.48
1:H:560:LEU:HD13	1:H:594:MET:HG2	1.96	0.48
1:D:319:ILE:O	1:D:323:MET:HG3	2.14	0.48
1:D:331:CYS:HB2	1:D:335:LEU:HD23	1.95	0.48
1:E:173:HIS:HB2	1:E:177:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:MET:HG3	1:E:759:ARG:HH12	1.79	0.48
1:F:904:THR:O	1:F:908:ILE:HG13	2.13	0.48
1:C:597[B]:TYR:CD2	1:C:639:GLY:HA2	2.48	0.48
1:G:454:GLU:HA	1:G:531:SER:HB2	1.96	0.48
1:E:215:ARG:HD2	1:F:430:GLY:CA	2.44	0.48
1:H:890:ARG:NH2	2:H:1001:LMR:O4A	2.31	0.48
1:A:293:PRO:HD3	1:A:756:PRO:HG3	1.95	0.48
1:A:474:TYR:CZ	1:A:482:ARG:HD3	2.49	0.48
1:B:864:LYS:HE2	1:B:876:LEU:HD11	1.95	0.48
1:D:614:TYR:CD2	1:D:656:PRO:HG3	2.49	0.48
1:D:850:TRP:O	1:D:854:GLU:HG3	2.14	0.48
1:E:12:ILE:HD13	1:E:38:LEU:HD23	1.95	0.48
1:F:260:ASP:CG	1:F:437:ARG:HH22	2.21	0.48
1:H:532:MET:CG	1:H:759:ARG:HH12	2.26	0.48
1:F:463:ASP:OD1	1:F:473:SER:HB2	2.13	0.48
1:H:260:ASP:OD2	1:H:437:ARG:NH2	2.28	0.48
1:A:284:TRP:CH2	1:A:594:MET:HE1	2.48	0.47
1:D:316:PHE:O	1:D:319:ILE:HG22	2.13	0.47
1:F:173:HIS:CG	1:F:177:SER:HB3	2.49	0.47
1:F:332:ASN:HB2	1:F:418:SER:HA	1.96	0.47
1:F:614:TYR:CD2	1:F:656:PRO:HG3	2.49	0.47
1:C:158:PHE:CE2	1:C:162:LYS:HD2	2.50	0.47
1:C:473:SER:OG	1:C:476:GLU:HG2	2.14	0.47
1:F:640:THR:HG21	1:F:820:VAL:HG23	1.97	0.47
1:F:864:LYS:HE2	1:F:876:LEU:HD11	1.96	0.47
1:H:57:VAL:CG1	1:H:101:MET:HE1	2.44	0.47
1:H:110:GLU:OE1	1:H:190:ARG:NH1	2.45	0.47
1:A:215:ARG:HD2	1:B:430:GLY:HA3	1.95	0.47
1:C:808:LEU:HB3	1:C:870:THR:HG23	1.95	0.47
1:D:760:LYS:C	1:D:762:SER:H	2.20	0.47
1:E:543:GLU:HG2	1:E:557:VAL:HG21	1.97	0.47
1:C:97:ALA:C	1:C:101:MET:HE3	2.39	0.47
1:C:430:GLY:HA3	1:D:215:ARG:HD2	1.96	0.47
1:C:501:LEU:O	1:C:503:LYS:HG3	2.15	0.47
1:B:316:PHE:O	1:B:319:ILE:HG22	2.15	0.47
1:B:328:MET:SD	1:B:328:MET:N	2.87	0.47
1:C:215:ARG:HD2	1:D:430:GLY:HA3	1.96	0.47
1:D:8:LYS:HB3	1:D:58:GLN:HE22	1.78	0.47
1:F:560:LEU:HD13	1:F:594:MET:HG2	1.97	0.47
1:C:244:PHE:HA	1:C:248:ILE:HB	1.96	0.47
1:E:746:GLU:HG3	1:E:749:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:ILE:HD13	1:G:38:LEU:HD23	1.97	0.47
1:G:255:PHE:O	1:G:259:VAL:HG23	2.14	0.47
1:A:857:ARG:O	1:A:860:PHE:HB3	2.14	0.47
1:B:474:TYR:CZ	1:B:482:ARG:HD3	2.49	0.47
1:D:158:PHE:CE2	1:D:162:LYS:HD2	2.50	0.47
1:E:147:VAL:HG13	1:H:18:GLN:HE21	1.80	0.47
1:G:670:GLY:O	1:G:673:ILE:HG22	2.15	0.47
1:A:746:GLU:HG3	1:A:749:ARG:NH2	2.29	0.47
1:F:237:MET:O	1:F:241:MET:HG2	2.14	0.47
1:G:96:LYS:HE3	1:G:225:GLU:OE2	2.15	0.47
1:C:355:ILE:HD11	1:D:309:MET:HE1	1.97	0.47
1:D:474:TYR:CZ	1:D:482:ARG:HD3	2.50	0.47
1:D:501:LEU:O	1:D:503:LYS:HG3	2.14	0.47
1:E:323:MET:HE2	1:E:323:MET:HB3	1.80	0.47
1:G:102:LEU:HD21	1:G:962:GLY:CA	2.44	0.47
1:B:857:ARG:O	1:B:860:PHE:HB3	2.14	0.46
1:C:394:SER:OG	1:C:395:ASP:N	2.48	0.46
1:C:465:ILE:O	1:C:469:LEU:HG	2.15	0.46
1:F:705:PRO:HG2	1:F:710:ARG:NH1	2.30	0.46
1:G:370:ILE:O	1:G:374:VAL:HG23	2.15	0.46
1:B:185:LYS:O	1:B:189:ILE:HG13	2.15	0.46
1:E:468:HIS:NE2	1:E:500:ASP:O	2.48	0.46
1:G:20:VAL:HG11	1:G:885:GLN:HG3	1.97	0.46
1:G:766:GLU:H	1:G:766:GLU:CD	2.23	0.46
1:C:739:ARG:HB3	1:C:745:LEU:HD11	1.96	0.46
1:C:851:PRO:HA	1:C:854:GLU:HB2	1.96	0.46
1:D:750:MET:HG3	1:D:956:MET:HE1	1.97	0.46
1:A:284:TRP:CD1	1:A:450:ASP:HB2	2.50	0.46
1:B:66:GLU:OE1	1:B:75:LYS:NZ	2.33	0.46
1:B:442:PHE:HB3	1:B:446:LEU:HD23	1.98	0.46
1:B:536:PRO:HB3	1:B:577:LEU:HG	1.97	0.46
1:B:658:ASP:HA	4:B:1005:CL:CL	2.51	0.46
1:D:201:ILE:HA	1:D:201:ILE:HD12	1.77	0.46
1:E:912:SER:O	1:E:912:SER:OG	2.34	0.46
1:G:621:VAL:HG21	1:G:659:THR:HG22	1.96	0.46
1:G:284:TRP:CD1	1:G:450:ASP:HB2	2.51	0.46
1:G:697:HIS:CE1	4:G:1009:CL:CL	3.05	0.46
1:D:260:ASP:CG	1:D:437:ARG:HH22	2.22	0.46
1:D:640:THR:HG21	1:D:820:VAL:HG23	1.97	0.46
1:G:167:ASP:HB3	1:G:665:ARG:HG3	1.97	0.46
1:G:614:TYR:CD2	1:G:656:PRO:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:769:ARG:C	1:G:772:PRO:HD2	2.41	0.46
1:H:298:GLU:OE2	1:H:301:ARG:NH1	2.48	0.46
1:E:86:LEU:O	1:E:907:ARG:NH2	2.49	0.46
1:G:463:ASP:OD1	1:G:473:SER:HB2	2.15	0.46
1:H:139:LEU:HD21	1:H:259:VAL:HG22	1.97	0.46
1:H:158:PHE:CE2	1:H:162:LYS:HD2	2.51	0.46
1:H:501:LEU:O	1:H:503:LYS:HG3	2.16	0.46
1:B:284:TRP:CH2	1:B:594:MET:HE1	2.50	0.46
1:B:560:LEU:HD13	1:B:594:MET:HG2	1.97	0.46
1:C:532:MET:CG	1:C:759:ARG:HH12	2.27	0.46
1:G:183:LEU:HD12	1:G:242:SER:HB2	1.97	0.46
1:H:474:TYR:CZ	1:H:482:ARG:HD3	2.50	0.46
1:C:316:PHE:O	1:C:319:ILE:HG22	2.16	0.46
1:F:454:GLU:HA	1:F:531:SER:HB2	1.97	0.46
1:F:857:ARG:O	1:F:860:PHE:HB3	2.15	0.46
1:A:179:ARG:HH22	1:B:358:TRP:HE1	1.64	0.46
1:C:769:ARG:HB2	1:C:772:PRO:HD2	1.98	0.46
1:G:769:ARG:HE	1:G:769:ARG:HB3	1.40	0.46
1:H:618:GLU:OE1	1:H:710:ARG:NH2	2.45	0.46
1:B:669:GLN:HB3	1:B:671:GLU:OE2	2.15	0.45
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.76	0.45
1:E:102:LEU:HD21	1:E:962:GLY:CA	2.46	0.45
1:A:90:ASP:OD2	1:A:921:ILE:HG13	2.17	0.45
1:B:463:ASP:OD1	1:B:473:SER:HB2	2.15	0.45
1:B:670:GLY:O	1:B:673:ILE:HG22	2.16	0.45
1:D:769:ARG:HE	1:D:769:ARG:HB3	1.63	0.45
1:E:68:GLU:CD	1:E:891:ASP:HB3	2.41	0.45
1:E:660:ILE:HD12	1:E:697:HIS:ND1	2.31	0.45
1:F:298:GLU:OE2	1:F:301:ARG:NH1	2.49	0.45
1:G:598:SER:OG	1:G:967:GLY:OXT	2.29	0.45
1:A:487:LEU:HD22	1:A:580:VAL:HG11	1.97	0.45
1:C:284:TRP:CH2	1:C:594:MET:HE1	2.51	0.45
1:C:670:GLY:O	1:C:673:ILE:HG22	2.15	0.45
1:E:166:VAL:HG11	1:E:690:PHE:HB3	1.99	0.45
1:E:922:SER:OG	1:E:923:LYS:N	2.47	0.45
1:F:130:GLU:O	1:F:649:HIS:HB3	2.17	0.45
1:G:161:LEU:HD23	1:G:161:LEU:HA	1.86	0.45
1:A:624:ALA:HB1	1:A:629:VAL:O	2.16	0.45
1:B:429:ASP:HA	1:B:433:LEU:HB2	1.98	0.45
1:E:949:GLU:O	1:E:953:ILE:HG13	2.17	0.45
1:F:760:LYS:C	1:F:762:SER:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:759:ARG:HG3	1:G:769:ARG:HD2	1.99	0.45
1:H:69:GLY:HA2	1:H:888:ARG:HH22	1.81	0.45
1:A:49:HIS:O	1:A:922:SER:HB3	2.16	0.45
1:D:97:ALA:O	1:D:101:MET:HG3	2.16	0.45
1:F:445:SER:O	1:F:446:LEU:HB2	2.17	0.45
1:G:201:ILE:HD12	1:G:201:ILE:HA	1.89	0.45
1:H:87:ASP:HB3	1:H:917:LEU:HD13	1.99	0.45
1:E:161:LEU:HA	1:E:161:LEU:HD23	1.79	0.45
1:C:49:HIS:O	1:C:922:SER:HB3	2.16	0.45
1:E:98:PHE:CE2	1:E:896:THR:HG21	2.52	0.45
1:A:826:GLU:HG3	1:A:876:LEU:HD22	1.99	0.45
1:D:477:TRP:HB3	1:D:481:ARG:HB3	1.98	0.45
1:D:802:VAL:HG23	1:D:803:ARG:HG3	1.99	0.45
1:E:532:MET:CG	1:E:759:ARG:HH12	2.28	0.45
1:E:769:ARG:HB2	1:E:772:PRO:HD2	1.99	0.45
1:H:260:ASP:CG	1:H:437:ARG:HH22	2.19	0.45
1:A:201:ILE:HD12	1:A:201:ILE:HA	1.86	0.45
1:C:86:LEU:O	1:C:907:ARG:NH2	2.49	0.45
1:C:330:ARG:NH1	1:D:222:ARG:HD2	2.32	0.45
1:E:705:PRO:HB3	1:E:815:TRP:CZ2	2.52	0.45
1:F:338:ARG:NH2	1:F:410:GLU:OE1	2.38	0.45
1:H:766:GLU:CD	1:H:766:GLU:H	2.24	0.45
1:A:558:VAL:HG22	1:A:592:GLU:HB3	1.99	0.45
1:B:201:ILE:HD12	1:B:201:ILE:HA	1.82	0.45
1:B:403:ILE:HD11	1:B:521:PRO:HG3	1.99	0.45
1:C:658:ASP:HA	4:C:1008:CL:CL	2.53	0.45
1:G:910:ASP:OD1	1:G:912:SER:HB3	2.17	0.45
1:A:237:MET:O	1:A:241:MET:HG2	2.17	0.44
1:A:427:ILE:HD11	1:B:218:GLN:HG2	1.99	0.44
1:B:465:ILE:O	1:B:469:LEU:HG	2.17	0.44
1:B:769:ARG:O	1:B:772:PRO:HD2	2.18	0.44
1:C:90:ASP:OD2	1:C:921:ILE:HG13	2.17	0.44
1:G:798:ILE:HD11	1:G:805:LEU:HD13	1.99	0.44
1:H:286:GLY:HA3	1:H:303:VAL:HG21	1.99	0.44
1:A:40:ARG:O	1:A:44:ILE:HG13	2.18	0.44
1:F:57:VAL:HG13	1:F:101:MET:HE1	1.98	0.44
1:F:97:ALA:O	1:F:101:MET:HG3	2.17	0.44
1:F:746:GLU:HG3	1:F:749:ARG:HH21	1.82	0.44
1:H:167:ASP:HB3	1:H:665:ARG:HG3	1.98	0.44
1:B:284:TRP:CD1	1:B:450:ASP:HB2	2.53	0.44
1:B:895:THR:O	1:B:898:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597[A]:TYR:OH	1:D:635:HIS:ND1	2.43	0.44
1:G:260:ASP:CG	1:G:437:ARG:HH22	2.26	0.44
1:H:290:ASP:C	1:H:769:ARG:HH12	2.22	0.44
1:A:167:ASP:HB3	1:A:665:ARG:HG3	1.98	0.44
1:C:201:ILE:HG13	1:C:205:ASP:HB2	1.99	0.44
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.80	0.44
1:H:97:ALA:C	1:H:101:MET:HE3	2.42	0.44
1:A:326:MET:HG3	1:A:371:LEU:HD11	2.00	0.44
1:A:742:THR:HG23	1:A:776:ALA:HB1	1.99	0.44
1:C:290:ASP:HB3	1:C:452:ARG:HH21	1.82	0.44
1:C:606:ARG:HD3	1:C:825:ILE:HD11	1.99	0.44
1:C:750:MET:HG3	1:C:956:MET:HE1	2.00	0.44
1:F:206:LYS:HE3	3:F:1003:PEG:H31	1.98	0.44
1:H:769:ARG:HB2	1:H:772:PRO:HD2	2.00	0.44
1:A:617:GLN:HG2	1:A:633:MET:HE2	2.00	0.44
1:C:34:ASP:CG	1:C:889:LEU:HD11	2.43	0.44
1:E:630:LYS:NZ	1:E:661:ASN:O	2.48	0.44
1:E:670:GLY:O	1:E:673:ILE:HG22	2.17	0.44
1:F:275:ASN:HA	1:F:440:SER:OG	2.18	0.44
1:A:868:LEU:HD21	1:A:876:LEU:HD23	1.99	0.44
1:B:883:LEU:HD13	1:B:886:ARG:NH2	2.33	0.44
1:D:403:ILE:HG22	1:D:407:GLN:OE1	2.18	0.44
1:D:462:LEU:HD13	1:D:486:LEU:HD21	1.99	0.44
1:E:34:ASP:OD1	1:E:105:ALA:HA	2.17	0.44
1:E:419:LEU:HD23	1:E:419:LEU:HA	1.85	0.44
1:E:518:ALA:HB2	1:E:551:VAL:HG22	1.99	0.44
1:F:201:ILE:HD12	1:F:201:ILE:HA	1.84	0.44
1:G:304:CYS:O	1:G:308:ARG:HG3	2.17	0.44
1:H:102:LEU:HD21	1:H:962:GLY:HA3	1.99	0.44
1:H:536:PRO:HB3	1:H:577:LEU:HG	1.99	0.44
1:A:130:GLU:OE2	1:A:145:LYS:NZ	2.48	0.44
1:A:564:LEU:O	1:A:568:GLU:HG3	2.18	0.44
1:C:357:PHE:HB2	1:C:358:TRP:CE3	2.53	0.44
1:C:501:LEU:HD12	1:C:502:PRO:HD2	1.99	0.44
1:D:57:VAL:HG13	1:D:101:MET:HE1	2.00	0.44
1:D:875:ASP:HB3	1:D:884:LYS:NZ	2.33	0.44
1:G:750:MET:HG3	1:G:956:MET:HE1	1.98	0.44
1:G:857:ARG:O	1:G:860:PHE:HB3	2.17	0.44
1:C:237:MET:O	1:C:241:MET:HG2	2.18	0.44
1:C:954:LEU:HD23	1:C:954:LEU:HA	1.86	0.44
1:D:874:LYS:HA	1:D:874:LYS:HD3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:HIS:CE1	1:F:363:THR:HG23	2.53	0.44
1:G:637[A]:ARG:HH22	1:G:671:GLU:CD	2.26	0.44
1:H:101:MET:HB3	1:H:893:TYR:CE1	2.53	0.44
1:H:826:GLU:HG3	1:H:876:LEU:CD2	2.47	0.44
1:A:97:ALA:C	1:A:101:MET:HE3	2.43	0.43
1:A:460:ASP:OD1	1:A:475:ARG:NH2	2.51	0.43
1:D:185:LYS:O	1:D:189:ILE:HG13	2.18	0.43
1:G:912:SER:O	1:G:912:SER:OG	2.34	0.43
1:H:275:ASN:HA	1:H:440:SER:OG	2.18	0.43
1:C:85:SER:HB2	1:C:918:ARG:HG3	1.99	0.43
1:C:119:ILE:HG13	1:C:122:LEU:HD22	1.99	0.43
1:G:179[A]:ARG:NH2	1:H:358:TRP:HE1	2.16	0.43
1:A:328:MET:SD	1:A:328:MET:N	2.92	0.43
1:E:660:ILE:HD12	1:E:697:HIS:CG	2.53	0.43
1:G:769:ARG:O	1:G:772:PRO:HD2	2.18	0.43
1:H:20:VAL:CG1	1:H:885:GLN:HG3	2.48	0.43
1:B:786:VAL:HG11	1:B:828:VAL:HG21	1.99	0.43
1:E:430:GLY:CA	1:F:215:ARG:HD2	2.48	0.43
1:E:883:LEU:HD13	1:E:886:ARG:NH2	2.33	0.43
1:G:750:MET:O	1:G:751:ASN:HB2	2.17	0.43
1:H:624:ALA:HB1	1:H:629:VAL:O	2.17	0.43
1:B:564:LEU:O	1:B:568:GLU:HG3	2.18	0.43
1:C:209:LEU:HD23	1:C:209:LEU:HA	1.81	0.43
1:C:241:MET:HE1	1:C:447:VAL:HG13	1.99	0.43
1:C:826:GLU:HG3	1:C:876:LEU:HD23	2.00	0.43
1:E:286:GLY:HA3	1:E:303:VAL:HG21	2.01	0.43
1:G:742:THR:CG2	1:G:776:ALA:HB1	2.48	0.43
1:H:290:ASP:O	1:H:769:ARG:NH1	2.40	0.43
1:H:328:MET:HE2	1:H:427:ILE:HD13	2.00	0.43
1:C:442:PHE:HB3	1:C:446:LEU:HA	2.01	0.43
1:F:49:HIS:O	1:F:922:SER:HB3	2.18	0.43
1:G:67:TYR:O	1:G:71:HIS:N	2.47	0.43
1:B:290:ASP:HB3	1:B:452:ARG:HH21	1.84	0.43
1:B:326:MET:HG3	1:B:371:LEU:CD1	2.49	0.43
1:B:394:SER:OG	1:B:395:ASP:N	2.51	0.43
1:B:487:LEU:HD23	1:B:487:LEU:HA	1.78	0.43
1:C:649:HIS:CD2	1:C:693:ALA:HB2	2.54	0.43
1:D:649:HIS:CD2	1:D:693:ALA:HB2	2.54	0.43
1:D:868:LEU:HD21	1:D:876:LEU:HD23	1.99	0.43
1:H:19:LEU:HD21	1:H:892:SER:HB3	2.01	0.43
1:H:445:SER:O	1:H:447:VAL:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:500:ASP:OD1	1:H:500:ASP:N	2.49	0.43
1:H:831:LYS:HB3	1:H:963:LEU:HD22	2.01	0.43
1:A:766:GLU:CD	1:A:766:GLU:H	2.26	0.43
1:C:532:MET:HE1	1:C:563:LYS:HG3	2.00	0.43
1:D:110:GLU:OE1	1:D:190:ARG:HD3	2.19	0.43
1:D:474:TYR:OH	1:D:486:LEU:HD11	2.18	0.43
1:E:88:PRO:O	1:E:92:ILE:HG13	2.18	0.43
1:G:716:MET:HB3	1:G:793:ALA:HB1	2.01	0.43
1:H:309:MET:HE2	1:H:309:MET:HB3	1.84	0.43
1:H:614:TYR:CD2	1:H:656:PRO:HG3	2.54	0.43
1:A:501:LEU:HD12	1:A:502:PRO:HD2	1.99	0.43
1:B:57:VAL:HG13	1:B:101:MET:HE1	2.01	0.43
1:D:906:LYS:HE3	1:D:913:TYR:CD1	2.53	0.43
1:E:328:MET:HE2	1:E:427:ILE:HD13	2.01	0.43
1:E:581:ASP:O	1:E:585:ASN:ND2	2.40	0.43
1:F:290:ASP:OD1	1:F:454:GLU:HG3	2.18	0.43
1:F:442:PHE:HB3	1:F:446:LEU:HD23	2.01	0.43
1:F:500:ASP:OD1	1:F:500:ASP:N	2.50	0.43
1:G:419:LEU:HD23	1:G:419:LEU:HA	1.89	0.43
1:G:826:GLU:HG3	1:G:876:LEU:CD2	2.48	0.43
1:C:33:TYR:HB3	1:C:193:LEU:HD11	2.01	0.42
1:D:97:ALA:C	1:D:101:MET:HE3	2.44	0.42
1:E:367:TYR:CE1	1:E:419:LEU:HG	2.54	0.42
1:C:801:ASP:O	1:C:804:ASN:HB2	2.19	0.42
1:C:922:SER:OG	1:C:923:LYS:N	2.43	0.42
1:F:16:LEU:HD23	1:F:16:LEU:HA	1.88	0.42
1:F:322:LEU:HD22	1:F:326:MET:HG2	2.01	0.42
1:G:335:LEU:HD12	1:G:414:LEU:HG	2.00	0.42
1:G:595:ILE:HB	1:G:613:LEU:HD22	2.01	0.42
1:A:769:ARG:HB2	1:A:772:PRO:HD2	2.00	0.42
1:B:183:LEU:HD12	1:B:242:SER:HB2	2.01	0.42
1:D:275:ASN:HA	1:D:440:SER:OG	2.18	0.42
1:D:591:GLN:NE2	1:D:592:GLU:O	2.53	0.42
1:F:119:ILE:HG13	1:F:122:LEU:HD22	2.01	0.42
1:F:726:SER:HA	1:F:730:GLN:HB2	2.01	0.42
1:G:922:SER:HB3	1:G:923:LYS:H	1.48	0.42
1:H:897:LEU:HD22	1:H:955:THR:HA	2.01	0.42
1:A:545:LEU:HD23	1:A:545:LEU:HA	1.90	0.42
1:C:152:LYS:HE3	1:C:699:MET:HB3	2.00	0.42
1:A:532:MET:CG	1:A:759:ARG:HH12	2.30	0.42
1:A:597[B]:TYR:CD2	1:A:639:GLY:HA2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:ILE:HB	1:A:693:ALA:HB1	2.01	0.42
1:E:750:MET:HG3	1:E:956:MET:HE1	2.02	0.42
1:H:185:LYS:O	1:H:189:ILE:HG13	2.19	0.42
1:A:139:LEU:CD2	1:A:259:VAL:HG22	2.50	0.42
1:A:716:MET:HB3	1:A:793:ALA:HB1	2.01	0.42
1:B:260:ASP:CG	1:B:437:ARG:HH22	2.27	0.42
1:C:215:ARG:HD2	1:D:430:GLY:CA	2.49	0.42
1:E:283:SER:O	1:E:449:LEU:HD12	2.19	0.42
1:E:850:TRP:O	1:E:854:GLU:HG3	2.19	0.42
1:F:185:LYS:O	1:F:189:ILE:HG13	2.20	0.42
1:G:42:LEU:HD23	1:G:42:LEU:HA	1.85	0.42
1:G:328:MET:HE2	1:G:427:ILE:HG21	2.01	0.42
1:H:85:SER:HB2	1:H:918:ARG:HG3	2.00	0.42
1:H:850:TRP:O	1:H:854:GLU:HG3	2.20	0.42
1:A:769:ARG:HE	1:A:769:ARG:HB3	1.71	0.42
1:D:587:ILE:HB	1:D:590:LYS:O	2.20	0.42
1:E:319:ILE:O	1:E:323:MET:HG3	2.19	0.42
1:B:130:GLU:OE2	1:B:145:LYS:NZ	2.52	0.42
1:D:102:LEU:HD21	1:D:962:GLY:HA3	2.00	0.42
1:D:738:PHE:CE1	1:D:742:THR:HG21	2.55	0.42
1:E:97:ALA:O	1:E:101:MET:HG3	2.19	0.42
1:F:68:GLU:CD	1:F:891:ASP:HB3	2.43	0.42
1:G:637[A]:ARG:NH2	1:G:671:GLU:OE1	2.48	0.42
1:G:769:ARG:HB2	1:G:772:PRO:CD	2.50	0.42
1:H:501:LEU:HD12	1:H:502:PRO:HD2	2.02	0.42
1:C:139:LEU:HD21	1:C:259:VAL:HG22	2.00	0.42
1:D:255:PHE:CE1	1:D:688:GLN:HA	2.54	0.42
1:D:484[A]:GLU:OE1	1:D:484[A]:GLU:HA	2.20	0.42
1:E:712:LEU:O	1:E:716:MET:HG3	2.19	0.42
1:F:320:GLU:HB3	1:F:375:ARG:NH1	2.33	0.42
1:F:419:LEU:HD23	1:F:419:LEU:HA	1.91	0.42
1:F:742:THR:CG2	1:F:776:ALA:HB1	2.50	0.42
1:C:705:PRO:HB3	1:C:815:TRP:CE2	2.55	0.42
1:C:912:SER:O	1:C:912:SER:OG	2.34	0.42
1:D:84:THR:CG2	1:D:915:VAL:HG11	2.50	0.42
1:E:600:SER:HB2	1:E:609:ALA:HB1	2.02	0.42
1:A:158:PHE:O	1:A:162:LYS:HG3	2.20	0.41
1:B:442:PHE:HB3	1:B:446:LEU:HA	2.02	0.41
1:B:866:LEU:HD23	1:B:866:LEU:HA	1.89	0.41
1:C:102:LEU:HD21	1:C:962:GLY:HA3	2.02	0.41
1:D:19:LEU:HD12	1:D:19:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:750:MET:HE3	1:E:952:LEU:HD23	2.02	0.41
1:F:19:LEU:HD23	1:F:889:LEU:HD23	2.02	0.41
1:G:80:GLY:O	1:G:84:THR:OG1	2.36	0.41
1:G:166:VAL:HG11	1:G:690:PHE:HB3	2.01	0.41
1:A:102:LEU:HD21	1:A:962:GLY:CA	2.50	0.41
1:A:138:ASP:HB2	1:A:688:GLN:OE1	2.20	0.41
1:A:496:LEU:HA	1:A:496:LEU:HD12	1.78	0.41
1:C:275:ASN:OD1	1:C:275:ASN:N	2.53	0.41
1:C:742:THR:CG2	1:C:744:GLU:H	2.33	0.41
1:C:769:ARG:HE	1:C:769:ARG:HB3	1.36	0.41
1:D:161:LEU:HD23	1:D:161:LEU:HA	1.82	0.41
1:G:138:ASP:HB2	1:G:688:GLN:OE1	2.19	0.41
1:G:660:ILE:HD12	1:G:697:HIS:ND1	2.35	0.41
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.84	0.41
1:A:289:ARG:NH2	1:A:300:THR:OG1	2.49	0.41
1:A:338:ARG:NH2	1:A:410:GLU:OE1	2.34	0.41
1:B:73:PRO:HD2	5:B:1112:HOH:O	2.20	0.41
1:B:546:GLN:OE1	1:B:555:LEU:N	2.52	0.41
1:C:57:VAL:HG13	1:C:101:MET:HE1	2.02	0.41
1:E:254:LYS:NZ	5:E:1101:HOH:O	2.52	0.41
1:E:769:ARG:HB2	1:E:772:PRO:CD	2.49	0.41
1:F:769:ARG:O	1:F:772:PRO:HD2	2.20	0.41
1:G:742:THR:HG21	1:G:776:ALA:HB1	2.03	0.41
1:A:201:ILE:HG13	1:A:205:ASP:HB2	2.02	0.41
1:A:313:THR:OG1	1:A:382:ARG:HD3	2.20	0.41
1:B:19:LEU:HD21	1:B:892:SER:HB3	2.01	0.41
1:B:738:PHE:O	1:B:742:THR:HG22	2.20	0.41
1:C:518:ALA:HB2	1:C:551:VAL:HG22	2.03	0.41
1:E:40:ARG:O	1:E:44:ILE:HG13	2.20	0.41
1:G:27:ASP:OD1	1:G:27:ASP:N	2.54	0.41
1:G:430:GLY:CA	1:H:215:ARG:HD2	2.50	0.41
1:A:57:VAL:CG1	1:A:101:MET:HE1	2.51	0.41
1:B:114:ALA:O	1:B:685:ARG:NH2	2.53	0.41
1:D:237:MET:O	1:D:241:MET:HG2	2.20	0.41
1:D:760:LYS:O	1:D:762:SER:N	2.46	0.41
1:E:560:LEU:HD13	1:E:594:MET:HG2	2.03	0.41
1:H:786:VAL:HG11	1:H:828:VAL:HG21	2.02	0.41
1:A:229:THR:HG23	1:A:231:PRO:HA	2.03	0.41
1:B:513:THR:O	1:B:517:ILE:HG13	2.21	0.41
1:C:709:TRP:CZ3	1:C:815:TRP:HB2	2.56	0.41
1:C:769:ARG:HB2	1:C:772:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:831:LYS:HB3	1:D:963:LEU:HD22	2.02	0.41
1:H:40:ARG:HD2	1:H:214:GLN:HG2	2.02	0.41
1:H:244:PHE:HA	1:H:248:ILE:HB	2.01	0.41
1:B:370:ILE:O	1:B:374:VAL:HG23	2.20	0.41
1:C:68:GLU:CD	1:C:891:ASP:HB3	2.45	0.41
1:D:419:LEU:HD23	1:D:419:LEU:HA	1.91	0.41
1:E:119:ILE:H	1:E:119:ILE:HG12	1.55	0.41
1:E:139:LEU:CD2	1:E:259:VAL:HG22	2.51	0.41
1:E:237:MET:O	1:E:241:MET:HG2	2.21	0.41
1:E:355:ILE:H	1:E:355:ILE:HG13	1.63	0.41
1:E:868:LEU:HD21	1:E:876:LEU:HD23	2.02	0.41
1:G:513:THR:O	1:G:517:ILE:HG13	2.21	0.41
1:H:57:VAL:HG13	1:H:101:MET:HE1	2.02	0.41
1:H:442:PHE:HB3	1:H:446:LEU:HD23	2.02	0.41
1:A:907:ARG:HB3	1:A:948:LEU:HD13	2.03	0.41
1:B:57:VAL:CG1	1:B:101:MET:HE1	2.51	0.41
1:B:102:LEU:HD21	1:B:962:GLY:CA	2.51	0.41
1:C:487:LEU:HD23	1:C:487:LEU:HA	1.79	0.41
1:D:304:CYS:O	1:D:308:ARG:HG3	2.20	0.41
1:E:335:LEU:HD11	1:E:370:ILE:HG13	2.01	0.41
1:E:773:TRP:NE1	1:E:785:PRO:HB3	2.35	0.41
1:F:592:GLU:HA	1:F:632:THR:O	2.20	0.41
1:H:86:LEU:O	1:H:907:ARG:NH2	2.54	0.41
1:H:546:GLN:OE1	1:H:555:LEU:N	2.53	0.41
1:H:795:ARG:NE	1:H:862:GLU:OE2	2.53	0.41
1:A:114:ALA:O	1:A:685:ARG:NH2	2.54	0.41
1:A:290:ASP:OD1	1:A:454:GLU:HG3	2.20	0.41
1:A:365:GLU:CD	1:A:368:ARG:HH21	2.29	0.41
1:B:40:ARG:HD2	1:B:214:GLN:HG2	2.03	0.41
1:B:166:VAL:HG11	1:B:690:PHE:HB3	2.02	0.41
1:B:587:ILE:HB	1:B:590:LYS:O	2.20	0.41
1:C:319:ILE:O	1:C:323:MET:HG3	2.20	0.41
1:C:482:ARG:O	1:C:486:LEU:HG	2.20	0.41
1:D:309:MET:HE2	1:D:309:MET:HB3	1.80	0.41
1:D:474:TYR:CE1	1:D:482:ARG:HD3	2.56	0.41
1:D:670:GLY:O	1:D:673:ILE:HG22	2.21	0.41
1:E:760:LYS:O	1:E:762:SER:N	2.51	0.41
1:F:536:PRO:HB3	1:F:577:LEU:HG	2.02	0.41
1:F:868:LEU:HD21	1:F:876:LEU:HD23	2.02	0.41
1:G:139:LEU:CD2	1:G:259:VAL:HG22	2.51	0.41
1:G:179[A]:ARG:HH12	1:G:181:SER:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:866:LEU:HD23	1:G:866:LEU:HA	1.92	0.41
1:H:317:ASN:HB3	3:H:1002:PEG:H32	2.03	0.41
1:H:587:ILE:HB	1:H:590:LYS:O	2.21	0.41
1:H:656:PRO:HA	1:H:657:PRO:HD3	1.97	0.41
1:H:658:ASP:HA	4:H:1005:CL:CL	2.58	0.41
1:H:742:THR:HG23	1:H:744:GLU:H	1.85	0.41
1:B:102:LEU:HD21	1:B:962:GLY:HA3	2.02	0.41
1:B:243:TYR:HA	1:B:246:GLU:HB2	2.03	0.41
1:B:500:ASP:OD1	1:B:500:ASP:N	2.53	0.41
1:B:705:PRO:HG2	1:B:710:ARG:NH1	2.36	0.41
1:C:16:LEU:HA	1:C:16:LEU:HD23	1.77	0.41
1:C:330:ARG:HD3	1:D:222:ARG:CZ	2.50	0.41
1:C:640:THR:HG21	1:C:820:VAL:HG23	2.03	0.41
1:D:949:GLU:O	1:D:953:ILE:HG13	2.21	0.41
1:F:219:ALA:O	1:F:223:THR:HG23	2.20	0.41
1:G:316:PHE:O	1:G:319:ILE:HG22	2.20	0.41
1:A:739:ARG:HB3	1:A:745:LEU:HD11	2.02	0.40
1:A:876:LEU:HD23	1:A:876:LEU:HA	1.91	0.40
1:B:41:PHE:HE2	1:B:101:MET:HE2	1.86	0.40
1:B:283:SER:O	1:B:449:LEU:HD12	2.20	0.40
1:C:193:LEU:HD23	1:C:193:LEU:HA	1.89	0.40
1:A:786:VAL:HG11	1:A:828:VAL:HG21	2.03	0.40
1:D:86:LEU:HB3	1:D:90:ASP:HB2	2.03	0.40
1:D:87:ASP:HB3	1:D:917:LEU:HD13	2.02	0.40
1:E:513:THR:O	1:E:517:ILE:HG13	2.21	0.40
1:G:140:GLU:O	1:G:144:LYS:HG3	2.21	0.40
1:G:319:ILE:O	1:G:323:MET:HG3	2.21	0.40
1:G:895:THR:O	1:G:898:ASN:HB2	2.21	0.40
1:H:16:LEU:HD23	1:H:16:LEU:HA	1.89	0.40
1:B:85:SER:OG	1:B:918:ARG:HD3	2.22	0.40
1:C:137:SER:HA	1:C:141:GLU:OE1	2.21	0.40
1:C:760:LYS:O	1:C:762:SER:N	2.49	0.40
1:D:558:VAL:HG22	1:D:592:GLU:HB3	2.03	0.40
1:D:765:ILE:H	1:D:765:ILE:HD12	1.85	0.40
1:F:289:ARG:NH1	1:F:451:ILE:HG23	2.36	0.40
1:H:20:VAL:HG13	1:H:885:GLN:HG3	2.04	0.40
1:C:335:LEU:HD12	1:C:414:LEU:HG	2.03	0.40
1:D:114:ALA:O	1:D:685:ARG:NH2	2.53	0.40
1:E:664:LEU:HG	1:E:666:VAL:HG23	2.04	0.40
1:F:769:ARG:C	1:F:772:PRO:HD2	2.47	0.40
1:H:617:GLN:HB3	1:H:659:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD12	1:C:19:LEU:HA	1.88	0.40
1:C:182:LEU:HD12	1:C:182:LEU:HA	1.96	0.40
1:D:110:GLU:OE1	1:D:190:ARG:NH1	2.52	0.40
1:D:275:ASN:OD1	1:D:275:ASN:N	2.55	0.40
1:D:742:THR:HG23	1:D:744:GLU:H	1.86	0.40
1:E:445:SER:O	1:E:446:LEU:HB2	2.22	0.40
1:F:291:GLY:O	1:F:756:PRO:HD2	2.22	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	926/974 (95%)	885 (96%)	34 (4%)	7 (1%)	16	44
1	B	926/974 (95%)	882 (95%)	38 (4%)	6 (1%)	21	50
1	C	927/974 (95%)	882 (95%)	37 (4%)	8 (1%)	14	41
1	D	929/974 (95%)	882 (95%)	38 (4%)	9 (1%)	12	38
1	E	928/974 (95%)	882 (95%)	39 (4%)	7 (1%)	16	44
1	F	929/974 (95%)	884 (95%)	38 (4%)	7 (1%)	16	44
1	G	927/974 (95%)	882 (95%)	40 (4%)	5 (0%)	24	54
1	H	929/974 (95%)	884 (95%)	40 (4%)	5 (0%)	24	54
All	All	7421/7792 (95%)	7063 (95%)	304 (4%)	54 (1%)	18	47

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	395	ASP
1	B	227	LYS
1	B	395	ASP

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Mol	Chain	Res	Type
1	B	922	SER
1	C	395	ASP
1	C	750	MET
1	C	876	LEU
1	D	227	LYS
1	D	395	ASP
1	D	922	SER
1	E	395	ASP
1	E	751	ASN
1	F	227	LYS
1	F	395	ASP
1	G	395	ASP
1	H	227	LYS
1	H	395	ASP
1	A	751	ASN
1	A	922	SER
1	D	751	ASN
1	E	922	SER
1	F	750	MET
1	G	922	SER
1	A	750	MET
1	C	922	SER
1	D	750	MET
1	E	756	PRO
1	F	751	ASN
1	F	756	PRO
1	H	756	PRO
1	A	756	PRO
1	B	756	PRO
1	C	756	PRO
1	G	756	PRO
1	C	230	PRO
1	D	230	PRO
1	D	756	PRO
1	F	228	ARG
1	A	230	PRO
1	C	227	LYS
1	E	227	LYS
1	E	230	PRO
1	A	226	ILE
1	B	230	PRO
1	C	226	ILE

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Mol	Chain	Res	Type
1	E	226	ILE
1	F	230	PRO
1	G	230	PRO
1	H	21	PRO
1	D	21	PRO
1	G	226	ILE
1	H	230	PRO
1	B	21	PRO
1	D	495	PRO

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	743/849 (88%)	718 (97%)	25 (3%)	32	58
1	B	738/849 (87%)	718 (97%)	20 (3%)	39	63
1	C	784/849 (92%)	754 (96%)	30 (4%)	29	56
1	D	787/849 (93%)	759 (96%)	28 (4%)	31	58
1	E	767/849 (90%)	742 (97%)	25 (3%)	33	59
1	F	757/849 (89%)	732 (97%)	25 (3%)	33	59
1	G	769/849 (91%)	739 (96%)	30 (4%)	28	56
1	H	780/849 (92%)	750 (96%)	30 (4%)	29	56
All	All	6125/6792 (90%)	5912 (96%)	213 (4%)	32	58

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	84	THR
1	A	119	ILE
1	A	177	SER
1	A	179	ARG
1	A	193	LEU

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Mol	Chain	Res	Type
1	A	201	ILE
1	A	225	GLU
1	A	254	LYS
1	A	294	ARG
1	A	322	LEU
1	A	370	ILE
1	A	480	GLU
1	A	499	SER
1	A	546	GLN
1	A	671	GLU
1	A	674	GLU
1	A	742	THR
1	A	744	GLU
1	A	751	ASN
1	A	766	GLU
1	A	888	ARG
1	A	889	LEU
1	A	907	ARG
1	A	914	HIS
1	B	26	GLU
1	B	57	VAL
1	B	84	THR
1	B	179	ARG
1	B	193	LEU
1	B	201	ILE
1	B	225	GLU
1	B	236	GLU
1	B	322	LEU
1	B	355	ILE
1	B	546	GLN
1	B	640	THR
1	B	671	GLU
1	B	674	GLU
1	B	742	THR
1	B	744	GLU
1	B	766	GLU
1	B	888	ARG
1	B	889	LEU
1	B	907	ARG
1	C	12	ILE
1	C	26	GLU
1	C	53	LEU

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Mol	Chain	Res	Type
1	C	57	VAL
1	C	84	THR
1	C	119	ILE
1	C	122	LEU
1	C	179	ARG
1	C	193	LEU
1	C	201	ILE
1	C	202	THR
1	C	225	GLU
1	C	254	LYS
1	C	321[A]	ASP
1	C	321[B]	ASP
1	C	322	LEU
1	C	328	MET
1	C	370	ILE
1	C	546	GLN
1	C	640	THR
1	C	671	GLU
1	C	674	GLU
1	C	700	ARG
1	C	742	THR
1	C	744	GLU
1	C	766	GLU
1	C	769	ARG
1	C	875	ASP
1	C	889	LEU
1	C	907	ARG
1	D	6	LEU
1	D	8	LYS
1	D	13	ASP
1	D	57	VAL
1	D	77	GLU
1	D	84	THR
1	D	193	LEU
1	D	201	ILE
1	D	226	ILE
1	D	229	THR
1	D	321[A]	ASP
1	D	321[B]	ASP
1	D	322	LEU
1	D	328	MET
1	D	355	ILE

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Mol	Chain	Res	Type
1	D	546	GLN
1	D	640	THR
1	D	671	GLU
1	D	674	GLU
1	D	682	LEU
1	D	742	THR
1	D	744	GLU
1	D	751	ASN
1	D	766	GLU
1	D	889	LEU
1	D	907	ARG
1	D	912	SER
1	D	923	LYS
1	E	57	VAL
1	E	84	THR
1	E	119	ILE
1	E	193	LEU
1	E	201	ILE
1	E	254	LYS
1	E	270	GLU
1	E	301	ARG
1	E	321[A]	ASP
1	E	321[B]	ASP
1	E	322	LEU
1	E	355	ILE
1	E	421	SER
1	E	546	GLN
1	E	608	SER
1	E	640	THR
1	E	671	GLU
1	E	674	GLU
1	E	700	ARG
1	E	742	THR
1	E	744	GLU
1	E	751	ASN
1	E	766	GLU
1	E	889	LEU
1	E	907	ARG
1	F	8	LYS
1	F	26	GLU
1	F	57	VAL
1	F	84	THR

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Mol	Chain	Res	Type
1	F	119	ILE
1	F	177	SER
1	F	179	ARG
1	F	193	LEU
1	F	201	ILE
1	F	321[A]	ASP
1	F	321[B]	ASP
1	F	322	LEU
1	F	328	MET
1	F	355	ILE
1	F	546	GLN
1	F	637	ARG
1	F	640	THR
1	F	671	GLU
1	F	674	GLU
1	F	742	THR
1	F	744	GLU
1	F	751	ASN
1	F	889	LEU
1	F	907	ARG
1	F	914	HIS
1	G	26	GLU
1	G	31	VAL
1	G	57	VAL
1	G	84	THR
1	G	119	ILE
1	G	179[A]	ARG
1	G	179[B]	ARG
1	G	193	LEU
1	G	201	ILE
1	G	254	LYS
1	G	301	ARG
1	G	322	LEU
1	G	328	MET
1	G	355	ILE
1	G	370	ILE
1	G	480	GLU
1	G	505	GLU
1	G	546	GLN
1	G	671	GLU
1	G	674	GLU
1	G	742	THR

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Mol	Chain	Res	Type
1	G	744	GLU
1	G	750	MET
1	G	766	GLU
1	G	769	ARG
1	G	848	GLU
1	G	889	LEU
1	G	907	ARG
1	G	922	SER
1	G	923	LYS
1	H	6	LEU
1	H	26	GLU
1	H	57	VAL
1	H	84	THR
1	H	119	ILE
1	H	179	ARG
1	H	193	LEU
1	H	201	ILE
1	H	225	GLU
1	H	226	ILE
1	H	321[A]	ASP
1	H	321[B]	ASP
1	H	322	LEU
1	H	328	MET
1	H	355	ILE
1	H	484	GLU
1	H	546	GLN
1	H	586	ARG
1	H	640	THR
1	H	671	GLU
1	H	674	GLU
1	H	722	GLU
1	H	742	THR
1	H	744	GLU
1	H	750	MET
1	H	766	GLU
1	H	889	LEU
1	H	907	ARG
1	H	912	SER
1	H	915	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	100	HIS
1	A	195	GLN
1	A	591	GLN
1	A	751	ASN
1	B	151	ASN
1	B	173	HIS
1	B	964	GLN
1	C	49	HIS
1	C	63	HIS
1	C	106	ASN
1	C	617	GLN
1	C	885	GLN
1	D	353	HIS
1	D	585	ASN
1	D	751	ASN
1	D	869	GLN
1	E	391	ASN
1	E	438	GLN
1	E	751	ASN
1	E	806	HIS
1	E	869	GLN
1	F	49	HIS
1	F	71	HIS
1	F	106	ASN
1	F	245	HIS
1	F	591	GLN
1	F	751	ASN
1	F	869	GLN
1	F	964	GLN
1	G	71	HIS
1	G	675	GLN
1	G	783	HIS
1	G	869	GLN
1	H	391	ASN
1	H	438	GLN
1	H	669	GLN
1	H	964	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 71 ligands modelled in this entry, 23 are monoatomic - leaving 48 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	$\# Z > 2$
3	PEG	B	1002	3	6,6,6	0.49	0	5,5,5	0.45	0
3	PEG	A	1004	3	1,1,6	0.33	0	-		
3	PEG	D	1004	3	1,1,6	0.37	0	-		
3	PEG	F	1005	3	6,6,6	0.50	0	5,5,5	0.41	0
3	PEG	E	1004	3	5,5,6	0.33	0	4,4,5	2.61	1 (25%)
2	LMR	G	1001	-	8,8,8	1.50	1 (12%)	10,10,10	1.62	1 (10%)
2	LMR	C	1001	-	8,8,8	1.44	1 (12%)	10,10,10	1.66	1 (10%)
2	LMR	F	1001	-	8,8,8	1.62	1 (12%)	10,10,10	1.61	2 (20%)
3	PEG	D	1002	3	6,6,6	0.48	0	5,5,5	0.40	0
3	PEG	A	1002	3	6,6,6	0.51	0	5,5,5	0.51	0
3	PEG	H	1002	3	6,6,6	0.48	0	5,5,5	0.42	0
3	PEG	E	1002	3	6,6,6	0.52	0	5,5,5	0.41	0
3	PEG	E	1007	-	6,6,6	0.47	0	5,5,5	0.28	0
3	PEG	A	1007	3	1,1,6	0.38	0	-		
3	PEG	G	1007	3	1,1,6	0.40	0	-		
3	PEG	G	1006	3	6,6,6	0.51	0	5,5,5	0.45	0
3	PEG	C	1004	3	1,1,6	0.37	0	-		
3	PEG	C	1002	3	6,6,6	0.49	0	5,5,5	0.37	0
3	PEG	A	1008	-	6,6,6	0.50	0	5,5,5	0.36	0
3	PEG	F	1002	3	6,6,6	0.49	0	5,5,5	0.43	0
3	PEG	C	1007	-	6,6,6	0.50	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	H	1003	3	6,6,6	0.46	0	5,5,5	0.51	0
3	PEG	A	1005	-	5,5,6	0.58	0	4,4,5	0.43	0
3	PEG	H	1004	3	1,1,6	0.33	0	-		
2	LMR	E	1001	-	8,8,8	1.50	1 (12%)	10,10,10	1.59	2 (20%)
3	PEG	E	1005	3	5,5,6	0.72	0	4,4,5	1.26	0
3	PEG	C	1005	-	5,5,6	0.56	0	4,4,5	0.58	0
3	PEG	E	1006	3	1,1,6	0.54	0	-		
3	PEG	C	1006	3	1,1,6	0.43	0	-		
3	PEG	G	1004	3	1,1,6	0.29	0	-		
3	PEG	A	1003	3	1,1,6	0.35	0	-		
3	PEG	D	1003	3	6,6,6	0.47	0	5,5,5	0.63	0
3	PEG	F	1004	3	1,1,6	0.33	0	-		
3	PEG	G	1003	3	1,1,6	0.40	0	-		
3	PEG	A	1006	3	6,6,6	0.49	0	5,5,5	0.31	0
2	LMR	B	1001	-	8,8,8	1.53	1 (12%)	10,10,10	1.43	1 (10%)
2	LMR	H	1001	-	8,8,8	1.51	1 (12%)	10,10,10	1.62	1 (10%)
2	LMR	D	1001	-	8,8,8	1.44	1 (12%)	10,10,10	1.53	1 (10%)
3	PEG	G	1002	3	6,6,6	0.51	0	5,5,5	0.64	0
3	PEG	B	1004	3	1,1,6	0.39	0	-		
3	PEG	E	1003	3	1,1,6	0.39	0	-		
3	PEG	C	1003	3	1,1,6	0.46	0	-		
3	PEG	D	1005	3	6,6,6	0.51	0	5,5,5	0.42	0
3	PEG	F	1003	3	6,6,6	0.48	0	5,5,5	0.51	0
3	PEG	G	1005	-	5,5,6	0.56	0	4,4,5	0.48	0
3	PEG	G	1008	-	6,6,6	0.51	0	5,5,5	0.50	0
3	PEG	B	1003	3	6,6,6	0.48	0	5,5,5	0.49	0
2	LMR	A	1001	-	8,8,8	1.45	1 (12%)	10,10,10	1.51	1 (10%)

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
3	PEG	B	1002	3	-	0/4/4/4	-
3	PEG	F	1005	3	-	2/4/4/4	-
3	PEG	E	1004	3	-	3/3/3/4	-
2	LMR	G	1001	-	-	0/8/8/8	-
2	LMR	C	1001	-	-	3/8/8/8	-
2	LMR	F	1001	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	1002	3	-	2/4/4/4	-
3	PEG	A	1002	3	-	3/4/4/4	-
3	PEG	B	1003	3	-	3/4/4/4	-
3	PEG	H	1002	3	-	0/4/4/4	-
3	PEG	E	1002	3	-	2/4/4/4	-
3	PEG	E	1007	-	-	2/4/4/4	-
3	PEG	G	1006	3	-	3/4/4/4	-
3	PEG	C	1002	3	-	2/4/4/4	-
3	PEG	A	1008	-	-	2/4/4/4	-
3	PEG	F	1002	3	-	1/4/4/4	-
3	PEG	C	1007	-	-	3/4/4/4	-
3	PEG	H	1003	3	-	3/4/4/4	-
3	PEG	A	1005	-	-	2/3/3/4	-
2	LMR	E	1001	-	-	1/8/8/8	-
3	PEG	E	1005	3	-	3/3/3/4	-
3	PEG	D	1003	3	-	4/4/4/4	-
3	PEG	A	1006	3	-	2/4/4/4	-
2	LMR	B	1001	-	-	1/8/8/8	-
2	LMR	H	1001	-	-	1/8/8/8	-
2	LMR	D	1001	-	-	2/8/8/8	-
3	PEG	G	1002	3	-	2/4/4/4	-
3	PEG	D	1005	3	-	2/4/4/4	-
3	PEG	F	1003	3	-	3/4/4/4	-
3	PEG	G	1005	-	-	2/3/3/4	-
3	PEG	G	1008	-	-	2/4/4/4	-
3	PEG	C	1005	-	-	2/3/3/4	-
2	LMR	A	1001	-	-	3/8/8/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	LMR	C2-C1	-3.29	1.47	1.52
2	E	1001	LMR	C2-C1	-3.13	1.47	1.52
2	G	1001	LMR	C2-C1	-2.96	1.48	1.52
2	C	1001	LMR	C2-C1	-2.94	1.48	1.52
2	H	1001	LMR	C2-C1	-2.91	1.48	1.52
2	A	1001	LMR	C2-C1	-2.84	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	LMR	C2-C1	-2.77	1.48	1.52
2	D	1001	LMR	C2-C1	-2.74	1.48	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1004	PEG	C2-O2-C3	4.95	130.44	113.06
2	G	1001	LMR	O1B-C1-C2	3.65	120.46	112.74
2	H	1001	LMR	O1B-C1-C2	3.58	120.31	112.74
2	C	1001	LMR	O1B-C1-C2	3.51	120.16	112.74
2	D	1001	LMR	O1B-C1-C2	3.36	119.84	112.74
2	A	1001	LMR	O1B-C1-C2	3.29	119.70	112.74
2	F	1001	LMR	O1B-C1-C2	3.16	119.43	112.74
2	E	1001	LMR	O1B-C1-C2	3.06	119.20	112.74
2	B	1001	LMR	O1B-C1-C2	3.02	119.14	112.74
2	F	1001	LMR	O4A-C4-C3	2.21	120.87	114.00
2	E	1001	LMR	C2-C3-C4	-2.11	106.56	112.08

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1001	LMR	O1A-C1-C2-O2
2	F	1001	LMR	O1B-C1-C2-O2
3	E	1004	PEG	O2-C3-C4-O4
3	E	1007	PEG	O1-C1-C2-O2
3	A	1008	PEG	O2-C3-C4-O4
3	E	1007	PEG	O2-C3-C4-O4
3	F	1003	PEG	O2-C3-C4-O4
3	F	1005	PEG	O2-C3-C4-O4
3	G	1006	PEG	O1-C1-C2-O2
3	D	1002	PEG	O2-C3-C4-O4
3	D	1003	PEG	O2-C3-C4-O4
3	E	1005	PEG	O2-C3-C4-O4
3	H	1003	PEG	O2-C3-C4-O4
3	B	1003	PEG	O2-C3-C4-O4
3	C	1007	PEG	O2-C3-C4-O4
3	F	1003	PEG	O1-C1-C2-O2
3	D	1003	PEG	O1-C1-C2-O2
3	H	1003	PEG	O1-C1-C2-O2
2	F	1001	LMR	O2-C2-C3-C4
3	B	1003	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	F	1001	LMR	O1A-C1-C2-C3
2	F	1001	LMR	O1B-C1-C2-C3
3	E	1005	PEG	C1-C2-O2-C3
3	C	1007	PEG	O1-C1-C2-O2
3	G	1005	PEG	C1-C2-O2-C3
2	F	1001	LMR	C1-C2-C3-C4
3	G	1008	PEG	O2-C3-C4-O4
3	D	1005	PEG	C4-C3-O2-C2
3	G	1006	PEG	C1-C2-O2-C3
3	G	1006	PEG	C4-C3-O2-C2
3	A	1005	PEG	C1-C2-O2-C3
3	A	1002	PEG	C1-C2-O2-C3
3	H	1003	PEG	C1-C2-O2-C3
3	A	1005	PEG	C4-C3-O2-C2
3	E	1002	PEG	C1-C2-O2-C3
3	C	1002	PEG	C1-C2-O2-C3
3	D	1003	PEG	C1-C2-O2-C3
3	C	1005	PEG	C4-C3-O2-C2
3	A	1006	PEG	C4-C3-O2-C2
3	G	1002	PEG	C1-C2-O2-C3
3	F	1003	PEG	C1-C2-O2-C3
3	E	1002	PEG	C4-C3-O2-C2
2	D	1001	LMR	O1A-C1-C2-O2
2	D	1001	LMR	O1B-C1-C2-O2
3	F	1002	PEG	O2-C3-C4-O4
3	B	1003	PEG	C1-C2-O2-C3
2	H	1001	LMR	O1B-C1-C2-C3
3	A	1002	PEG	O1-C1-C2-O2
3	G	1008	PEG	C4-C3-O2-C2
3	D	1002	PEG	O1-C1-C2-O2
3	E	1005	PEG	C4-C3-O2-C2
3	G	1005	PEG	C4-C3-O2-C2
3	E	1004	PEG	C1-C2-O2-C3
3	C	1002	PEG	C4-C3-O2-C2
3	D	1003	PEG	C4-C3-O2-C2
2	A	1001	LMR	C1-C2-C3-C4
3	C	1007	PEG	C4-C3-O2-C2
2	C	1001	LMR	O1B-C1-C2-O2
3	A	1008	PEG	C1-C2-O2-C3
3	D	1005	PEG	C1-C2-O2-C3
2	B	1001	LMR	O1A-C1-C2-C3
2	C	1001	LMR	O1A-C1-C2-C3

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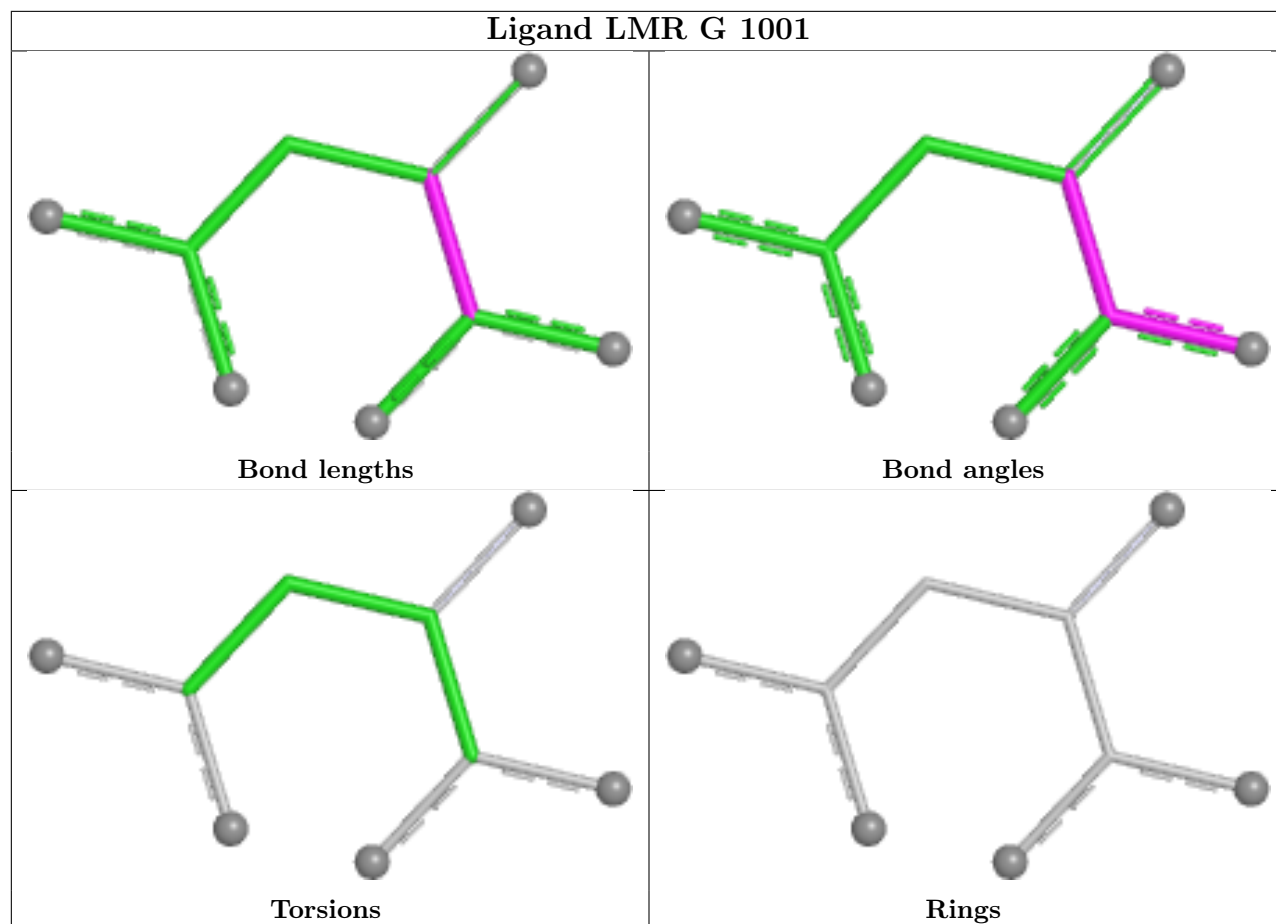
Mol	Chain	Res	Type	Atoms
3	G	1002	PEG	C4-C3-O2-C2
2	A	1001	LMR	O2-C2-C3-C4
3	E	1004	PEG	C4-C3-O2-C2
3	A	1006	PEG	O2-C3-C4-O4
3	F	1005	PEG	O1-C1-C2-O2
2	A	1001	LMR	O1B-C1-C2-O2
2	C	1001	LMR	O1A-C1-C2-O2
2	E	1001	LMR	O1B-C1-C2-O2
3	C	1005	PEG	O2-C3-C4-O4
3	A	1002	PEG	C4-C3-O2-C2

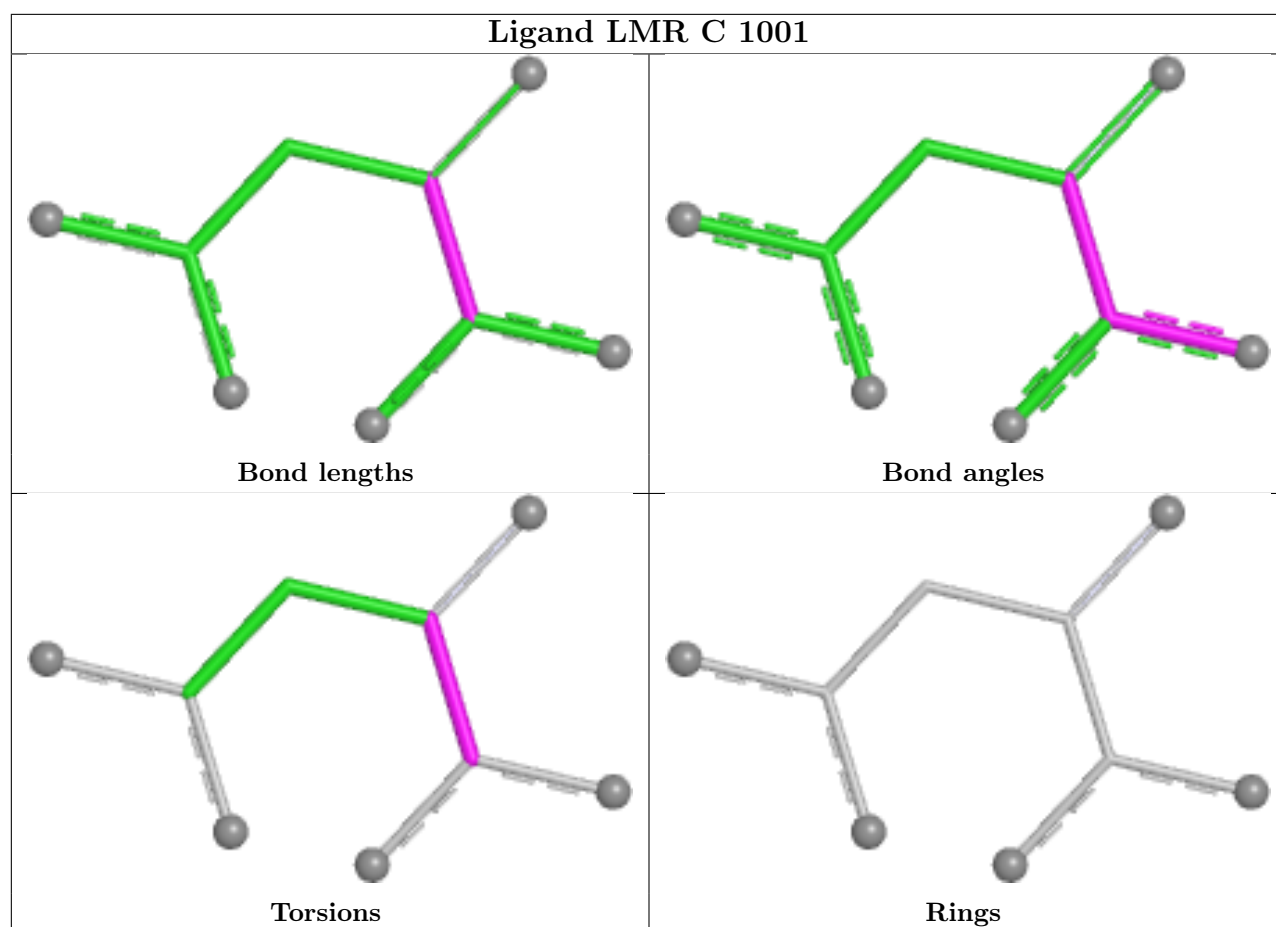
There are no ring outliers.

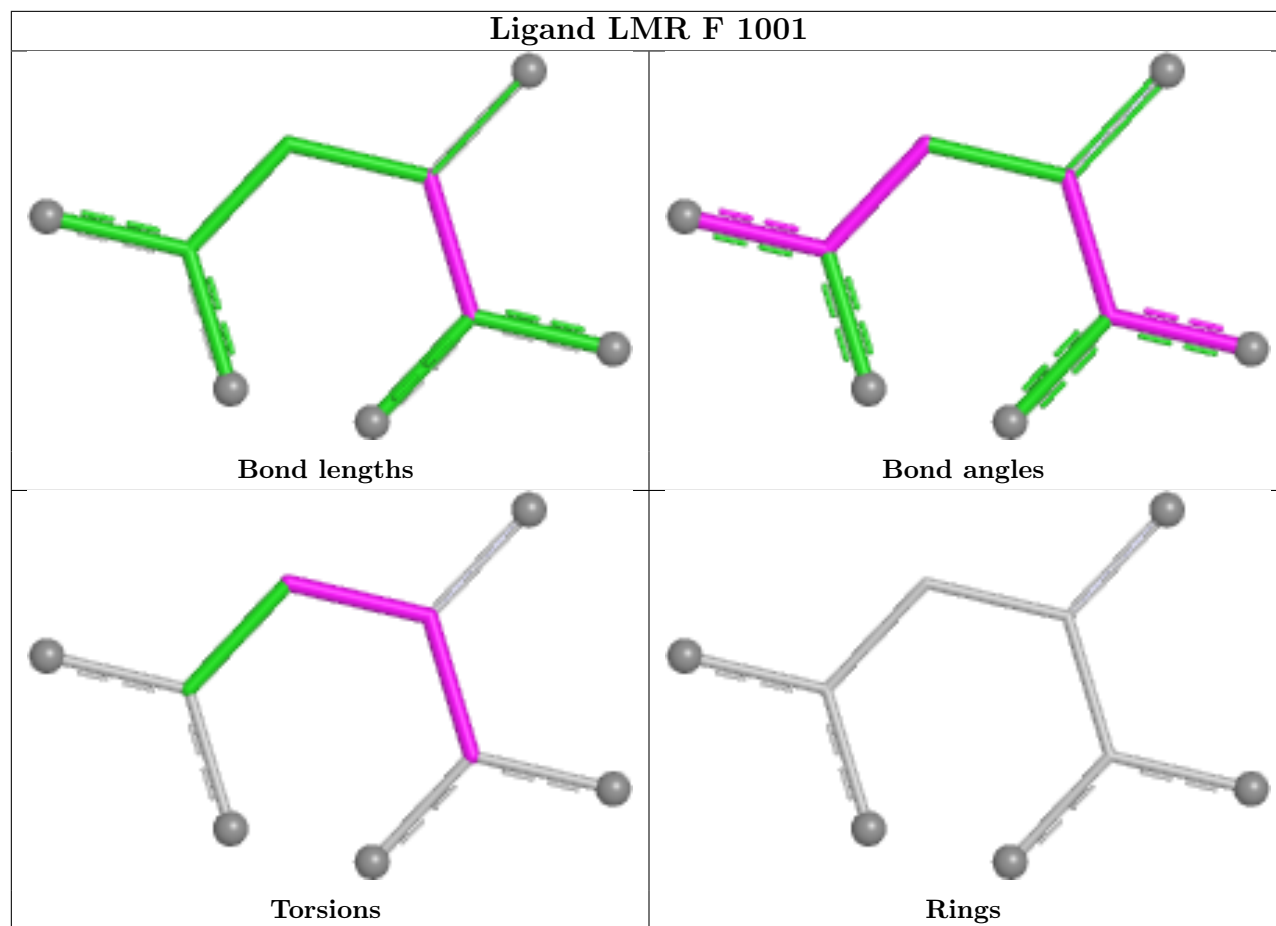
9 monomers are involved in 9 short contacts:

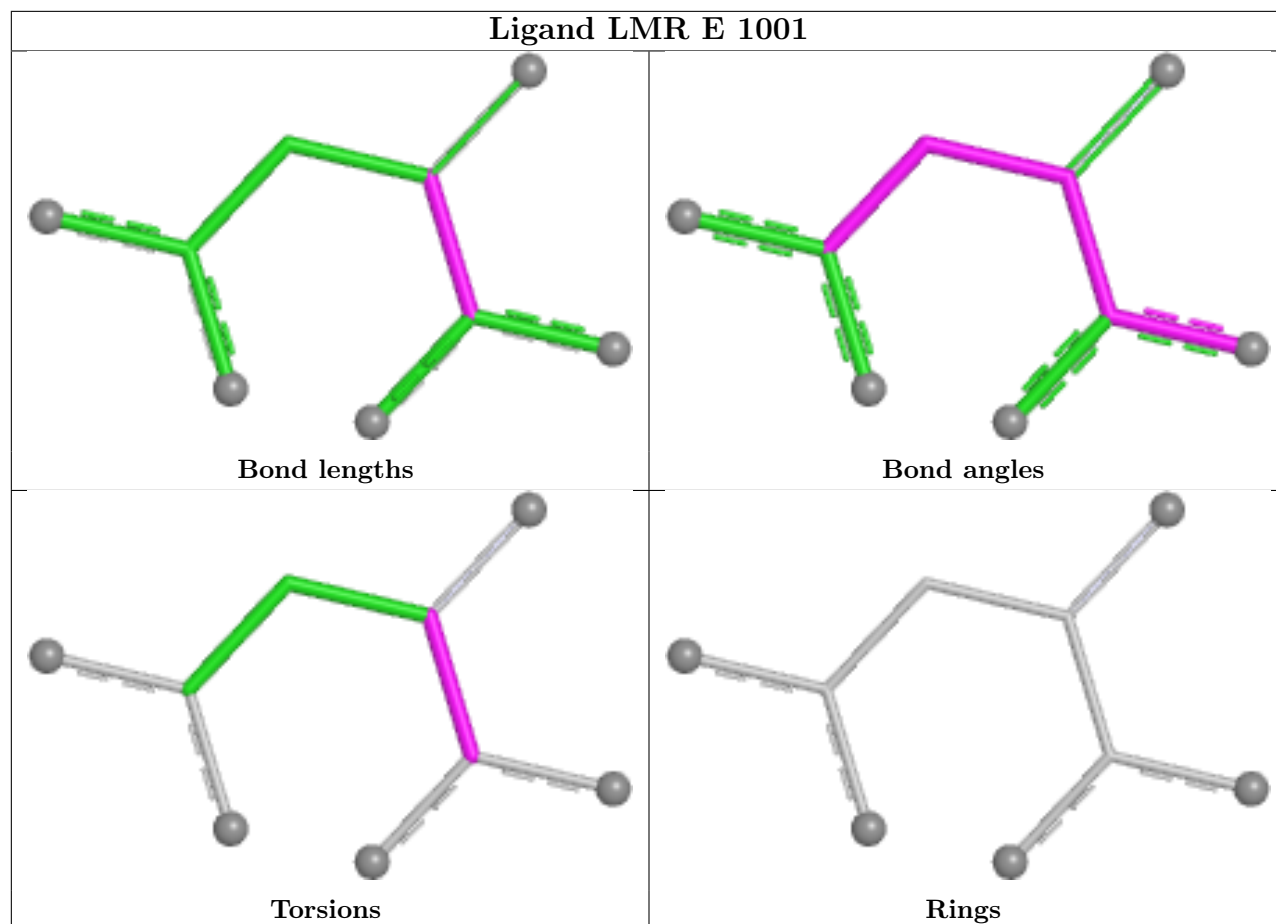
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	LMR	1	0
3	D	1002	PEG	1	0
3	H	1002	PEG	1	0
3	F	1002	PEG	1	0
3	H	1003	PEG	1	0
2	H	1001	LMR	1	0
2	D	1001	LMR	1	0
3	F	1003	PEG	1	0
3	B	1003	PEG	1	0

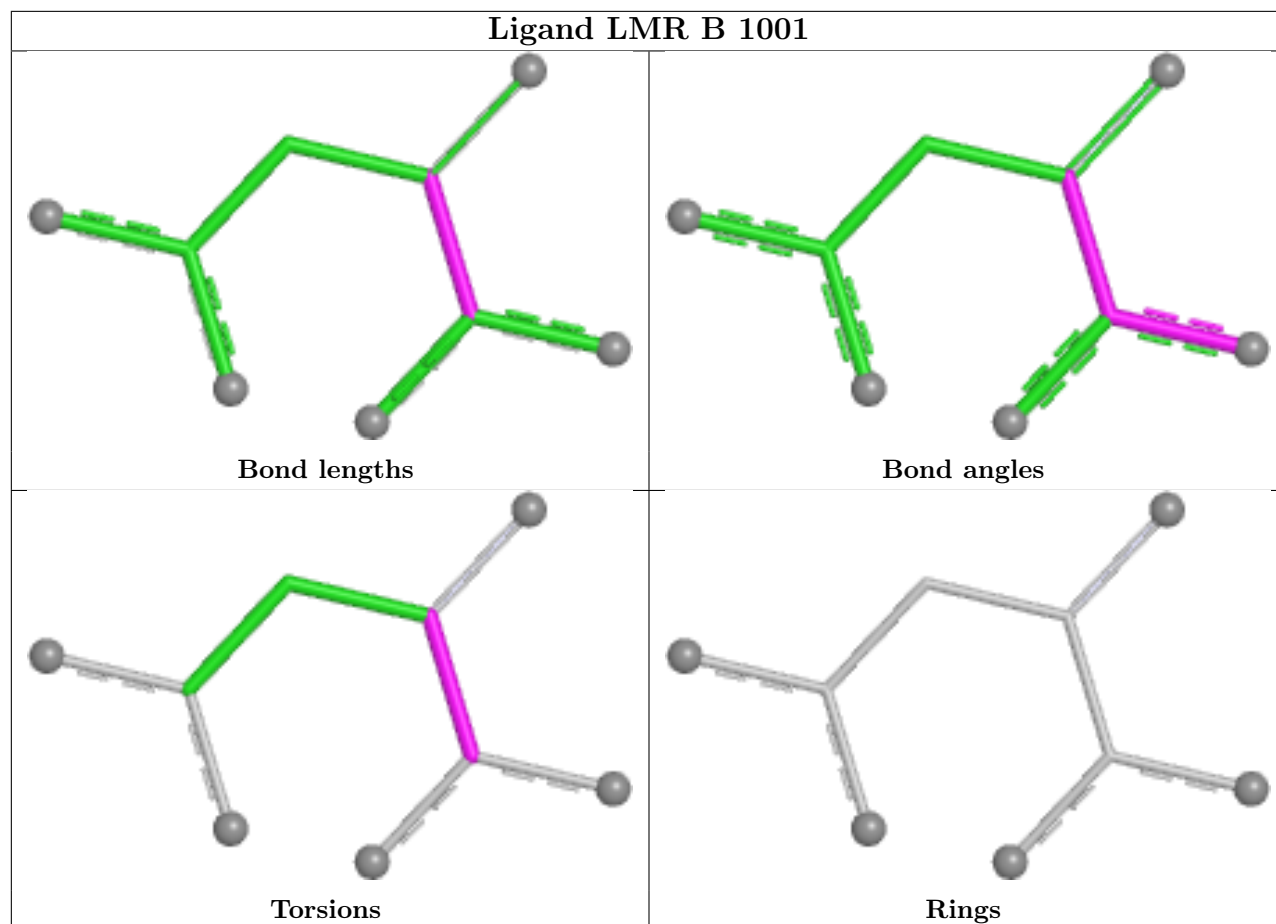
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

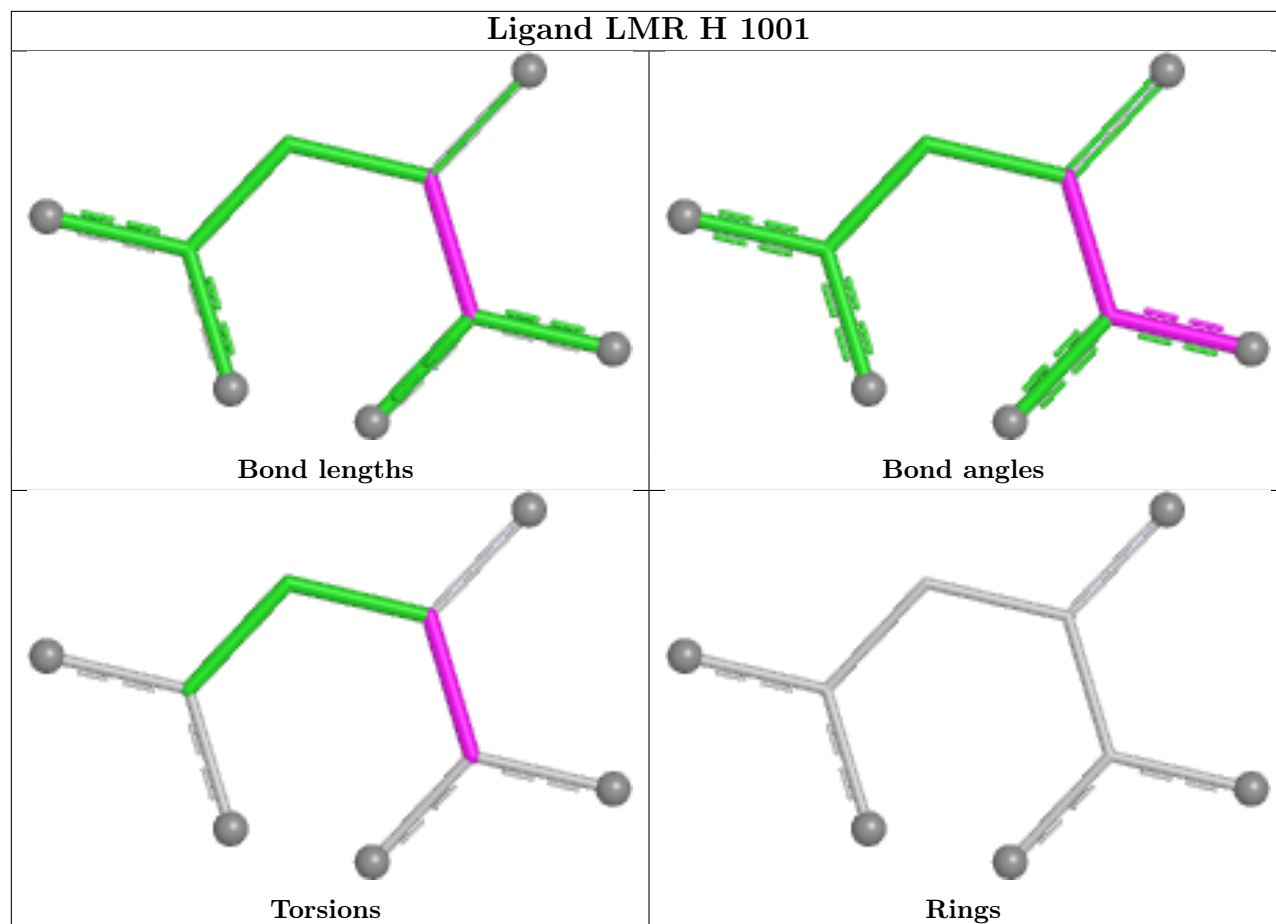


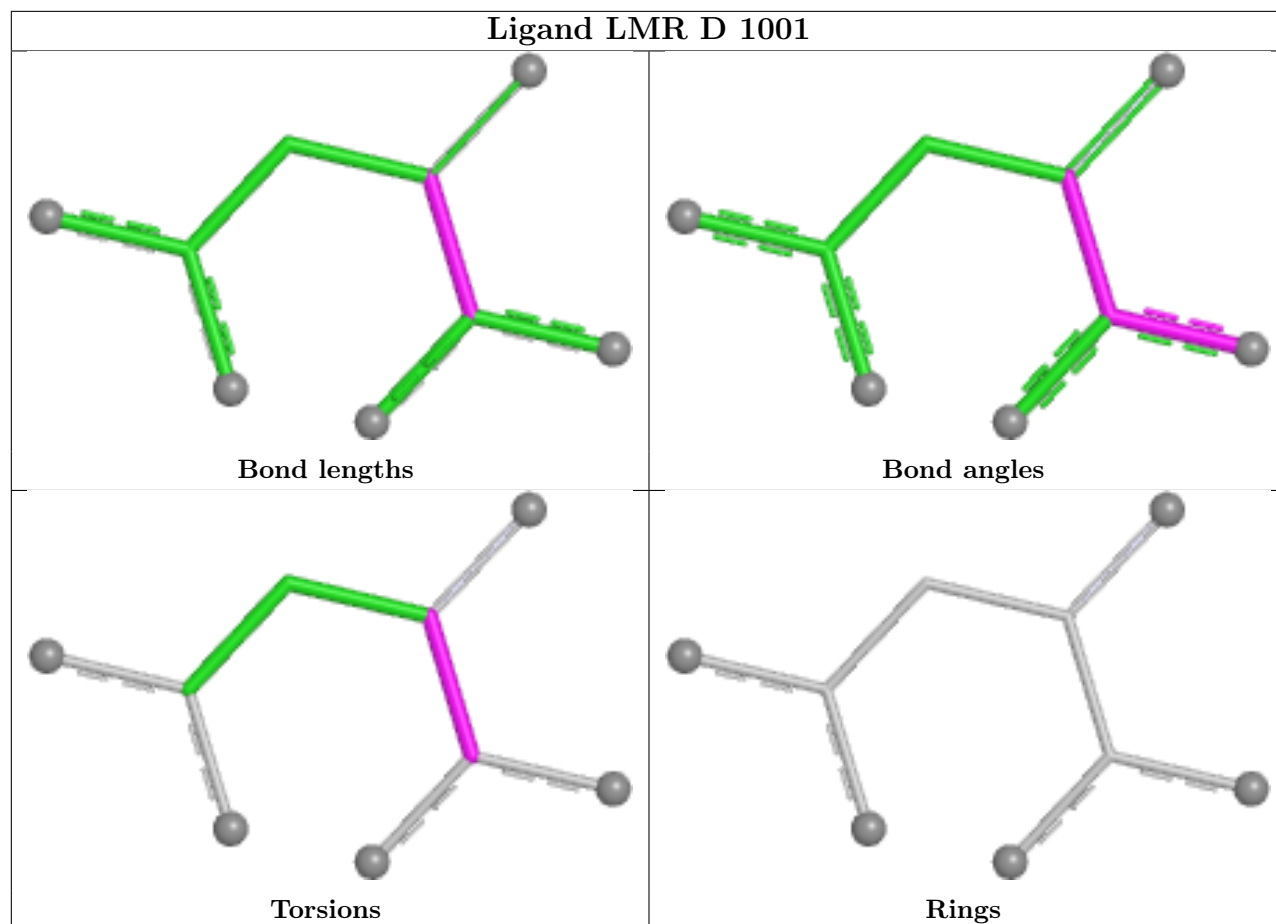


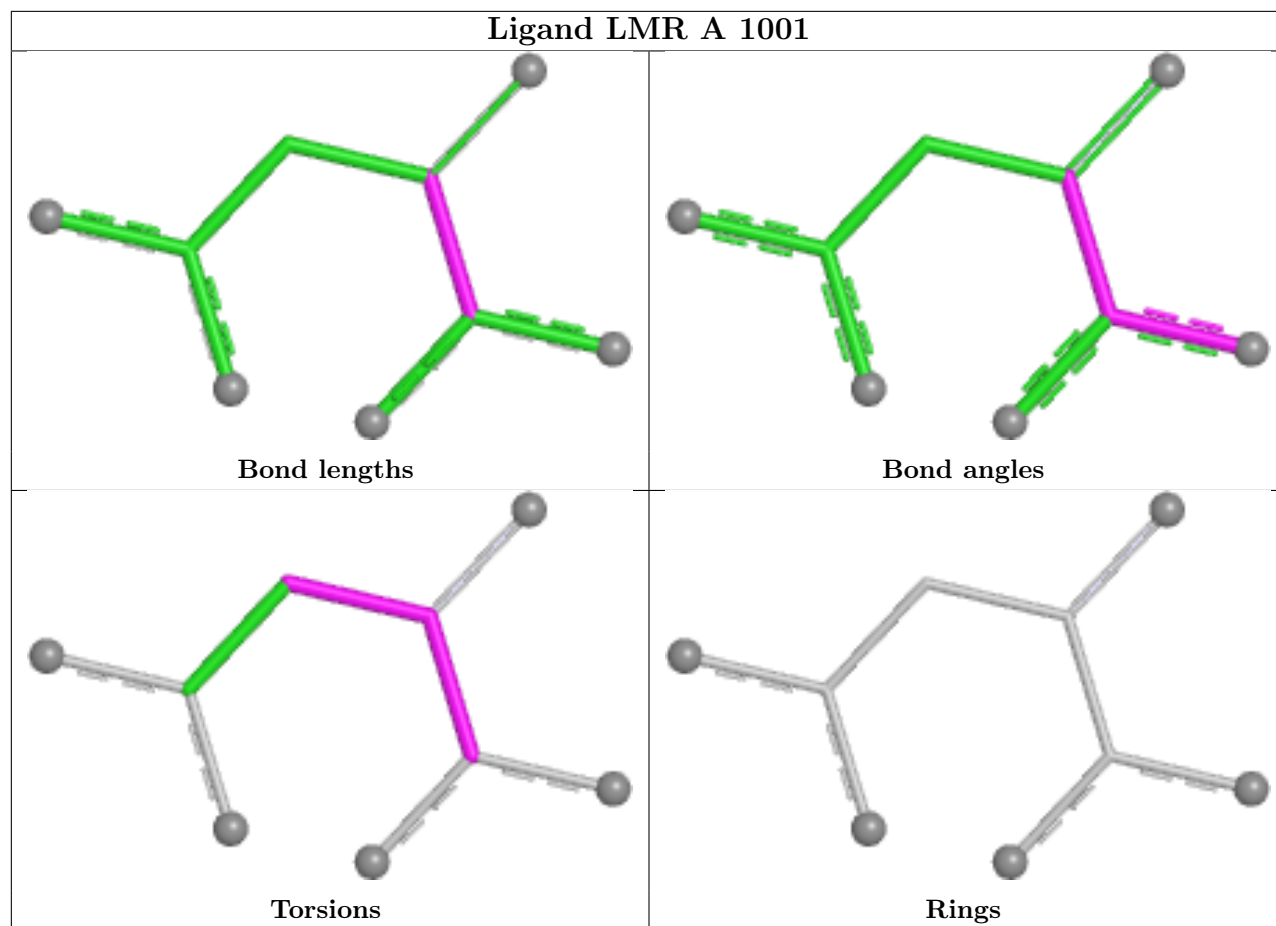












5.7 Other polymers [i](#)

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	932/974 (95%)	-0.13	16 (1%) 69 48	36, 75, 125, 207	2 (0%)
1	B	932/974 (95%)	-0.12	17 (1%) 67 46	39, 78, 133, 226	2 (0%)
1	C	932/974 (95%)	-0.25	9 (0%) 79 61	33, 65, 116, 227	3 (0%)
1	D	933/974 (95%)	-0.29	10 (1%) 78 59	30, 64, 115, 209	4 (0%)
1	E	933/974 (95%)	-0.22	18 (1%) 66 45	32, 64, 119, 223	3 (0%)
1	F	933/974 (95%)	-0.17	17 (1%) 67 46	34, 68, 124, 217	4 (0%)
1	G	933/974 (95%)	-0.14	15 (1%) 70 49	44, 74, 130, 269	2 (0%)
1	H	933/974 (95%)	-0.15	20 (2%) 63 42	32, 73, 128, 227	4 (0%)
All	All	7461/7792 (95%)	-0.18	122 (1%) 70 49	30, 71, 124, 269	24 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	GLU	6.0
1	B	355	ILE	5.3
1	D	351	ALA	4.3
1	E	172	ALA	4.3
1	D	755	ARG	4.1
1	A	353	HIS	4.0
1	F	351	ALA	4.0
1	E	351	ALA	3.9
1	C	597[A]	TYR	3.8
1	B	947	GLY	3.7
1	A	230	PRO	3.5
1	G	354	TYR	3.5
1	H	351	ALA	3.3
1	E	755	ARG	3.3
1	E	7	GLU	3.3
1	A	597[A]	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	752	ILE	3.3
1	E	230	PRO	3.2
1	E	354	TYR	3.2
1	H	752	ILE	3.1
1	F	173	HIS	3.1
1	F	177	SER	3.1
1	E	597[A]	TYR	3.1
1	H	230	PRO	3.1
1	H	6	LEU	3.0
1	B	353	HIS	3.0
1	E	355	ILE	3.0
1	G	179[A]	ARG	2.9
1	A	172	ALA	2.9
1	E	757	SER	2.9
1	G	351	ALA	2.9
1	D	230	PRO	2.8
1	F	752	ILE	2.8
1	H	119	ILE	2.8
1	A	355	ILE	2.8
1	G	355	ILE	2.8
1	B	354	TYR	2.8
1	E	758	LYS	2.8
1	F	178	VAL	2.8
1	H	921	ILE	2.8
1	F	172	ALA	2.7
1	C	922	SER	2.7
1	A	755	ARG	2.7
1	G	755	ARG	2.7
1	D	6	LEU	2.7
1	B	346	SER	2.7
1	H	761	PRO	2.7
1	F	354	TYR	2.7
1	H	175	THR	2.6
1	A	752	ILE	2.6
1	B	21	PRO	2.6
1	H	755	ARG	2.6
1	A	760	LYS	2.6
1	A	174	PRO	2.6
1	A	947	GLY	2.6
1	E	752	ILE	2.5
1	F	921	ILE	2.5
1	G	758	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	360	SER	2.5
1	B	760	LYS	2.5
1	C	351	ALA	2.4
1	B	7	GLU	2.4
1	A	352	LYS	2.4
1	H	354	TYR	2.4
1	C	947	GLY	2.4
1	G	23	LYS	2.4
1	A	357	PHE	2.4
1	B	174	PRO	2.4
1	G	760	LYS	2.4
1	G	178	VAL	2.4
1	F	47	ASP	2.4
1	H	494	ARG	2.4
1	B	480	GLU	2.4
1	G	18	GLN	2.3
1	F	484	GLU	2.3
1	H	174	PRO	2.3
1	C	760	LYS	2.3
1	G	947	GLY	2.3
1	B	155	GLU	2.3
1	A	356	GLU	2.3
1	C	346	SER	2.3
1	F	230	PRO	2.3
1	A	330	ARG	2.3
1	C	759	ARG	2.3
1	D	47	ASP	2.3
1	E	470	ASP	2.3
1	E	119	ILE	2.2
1	B	639	GLY	2.2
1	H	947	GLY	2.2
1	B	72	GLU	2.2
1	H	172	ALA	2.2
1	G	757	SER	2.2
1	A	354	TYR	2.2
1	B	176	GLN	2.2
1	F	174	PRO	2.2
1	E	47	ASP	2.2
1	H	358	TRP	2.2
1	F	597[A]	TYR	2.1
1	F	355	ILE	2.1
1	C	750	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	402	PHE	2.1
1	H	802	VAL	2.1
1	E	750	MET	2.1
1	A	119	ILE	2.1
1	F	765	ILE	2.1
1	F	175	THR	2.1
1	D	176	GLN	2.1
1	E	761	PRO	2.1
1	G	356	GLU	2.1
1	G	346	SER	2.1
1	H	47	ASP	2.1
1	G	761	PRO	2.1
1	B	8	LYS	2.0
1	E	802	VAL	2.0
1	H	759	ARG	2.0
1	B	230	PRO	2.0
1	D	761	PRO	2.0
1	F	923	LYS	2.0
1	H	360	SER	2.0
1	D	354	TYR	2.0
1	D	178	VAL	2.0
1	H	361	ILE	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(Å ²)	Q<0.9
3	PEG	C	1003	2/7	0.15	0.49	49,49,49,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	G	1003	2/7	0.21	0.59	62,62,62,78	0
4	CL	C	1009	1/1	0.38	0.54	233,233,233,233	0
3	PEG	A	1003	2/7	0.43	0.62	75,75,75,85	0
3	PEG	E	1003	2/7	0.52	0.43	56,56,56,69	0
3	PEG	C	1004	2/7	0.60	0.29	49,49,49,72	0
3	PEG	F	1004	2/7	0.70	0.23	46,46,46,69	0
3	PEG	B	1004	2/7	0.72	0.39	87,87,87,98	0
3	PEG	A	1005	6/7	0.74	0.26	77,88,90,92	0
3	PEG	G	1004	2/7	0.74	0.29	63,63,63,75	0
3	PEG	A	1004	2/7	0.74	0.30	64,64,64,77	0
3	PEG	C	1005	6/7	0.77	0.24	46,78,84,93	0
3	PEG	D	1004	2/7	0.79	0.19	56,56,56,79	0
4	CL	B	1006	1/1	0.80	0.30	125,125,125,125	0
3	PEG	E	1004	6/7	0.82	0.15	80,83,89,90	0
3	PEG	A	1006	7/7	0.83	0.29	66,80,102,102	0
3	PEG	G	1005	6/7	0.83	0.23	75,89,90,98	0
3	PEG	F	1005	7/7	0.83	0.24	56,58,66,73	0
3	PEG	E	1006	2/7	0.83	0.41	52,52,52,54	0
3	PEG	H	1002	7/7	0.85	0.18	77,83,95,98	0
3	PEG	E	1005	6/7	0.85	0.23	85,88,96,97	0
3	PEG	G	1007	2/7	0.85	0.32	58,58,58,65	0
3	PEG	B	1002	7/7	0.86	0.15	80,92,101,103	0
3	PEG	D	1002	7/7	0.87	0.14	66,74,84,85	0
3	PEG	G	1006	7/7	0.87	0.26	71,73,87,90	0
3	PEG	E	1002	7/7	0.87	0.17	60,68,77,77	0
3	PEG	F	1002	7/7	0.88	0.15	76,81,95,96	0
3	PEG	H	1004	2/7	0.88	0.20	48,48,48,64	0
3	PEG	A	1002	7/7	0.88	0.22	70,74,83,84	0
3	PEG	G	1008	7/7	0.88	0.15	72,75,82,85	0
4	CL	H	1006	1/1	0.88	0.16	83,83,83,83	0
4	CL	B	1008	1/1	0.89	0.14	67,67,67,67	0
3	PEG	C	1006	2/7	0.89	0.23	39,39,39,53	0
2	LMR	B	1001	9/9	0.89	0.12	89,93,97,101	0
3	PEG	G	1002	7/7	0.90	0.17	58,70,82,86	0
3	PEG	B	1003	7/7	0.91	0.18	79,82,84,86	0
4	CL	A	1010	1/1	0.91	0.09	81,81,81,81	0
4	CL	E	1010	1/1	0.91	0.07	76,76,76,76	0
3	PEG	C	1002	7/7	0.91	0.14	33,53,68,86	0
4	CL	C	1011	1/1	0.92	0.09	71,71,71,71	0
4	CL	E	1009	1/1	0.92	0.24	114,114,114,114	0
4	CL	D	1008	1/1	0.93	0.17	66,66,66,66	0
4	CL	D	1009	1/1	0.93	0.16	64,64,64,64	0

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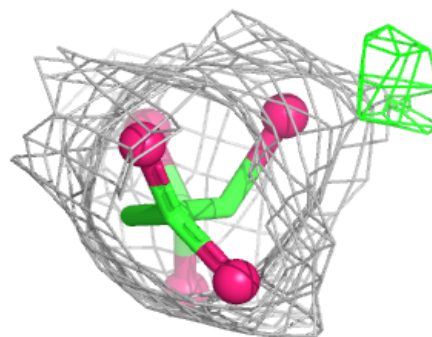
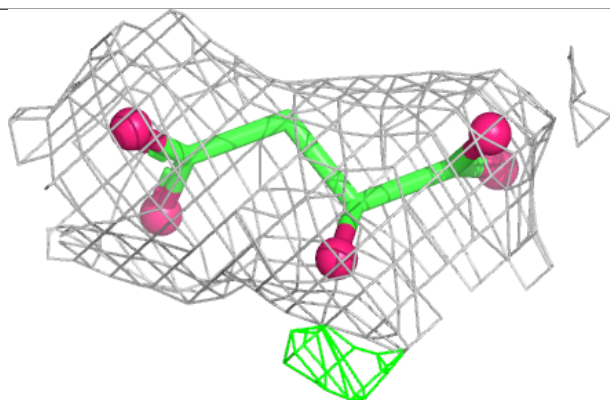
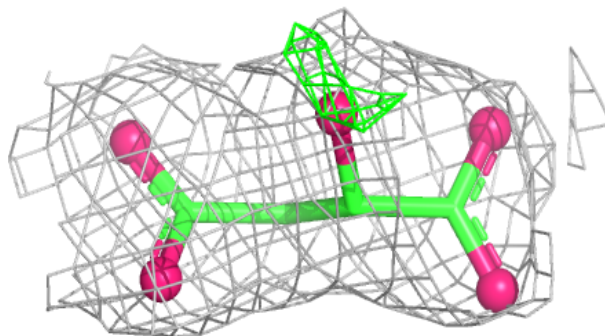
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	1007	2/7	0.93	0.28	43,43,43,56	0
3	PEG	D	1005	7/7	0.93	0.15	61,66,71,75	0
4	CL	F	1006	1/1	0.93	0.15	56,56,56,56	0
3	PEG	H	1003	7/7	0.93	0.10	63,64,75,84	0
2	LMR	D	1001	9/9	0.94	0.18	63,65,68,71	0
2	LMR	F	1001	9/9	0.94	0.09	64,71,76,79	0
2	LMR	A	1001	9/9	0.94	0.13	68,70,79,79	0
4	CL	G	1009	1/1	0.94	0.08	65,65,65,65	0
3	PEG	E	1007	7/7	0.94	0.08	56,58,66,75	0
4	CL	B	1007	1/1	0.95	0.16	71,71,71,71	0
4	CL	E	1008	1/1	0.95	0.21	64,64,64,64	0
3	PEG	D	1003	7/7	0.95	0.10	59,70,89,95	0
2	LMR	G	1001	9/9	0.95	0.11	71,76,80,81	0
3	PEG	C	1007	7/7	0.95	0.12	55,64,85,92	0
4	CL	D	1006	1/1	0.95	0.21	70,70,70,70	0
2	LMR	E	1001	9/9	0.95	0.10	57,61,69,69	0
2	LMR	C	1001	9/9	0.96	0.09	64,67,73,74	0
4	CL	B	1005	1/1	0.96	0.06	63,63,63,63	0
2	LMR	H	1001	9/9	0.96	0.11	74,79,84,84	0
4	CL	G	1010	1/1	0.96	0.05	57,57,57,57	0
3	PEG	F	1003	7/7	0.96	0.09	64,68,88,94	0
4	CL	C	1010	1/1	0.97	0.07	64,64,64,64	0
4	CL	D	1007	1/1	0.97	0.06	62,62,62,62	0
4	CL	H	1005	1/1	0.97	0.15	68,68,68,68	0
4	CL	F	1007	1/1	0.97	0.08	66,66,66,66	0
3	PEG	A	1008	7/7	0.98	0.07	70,70,72,79	0
4	CL	C	1008	1/1	0.98	0.13	53,53,53,53	0
4	CL	A	1009	1/1	0.98	0.16	66,66,66,66	0

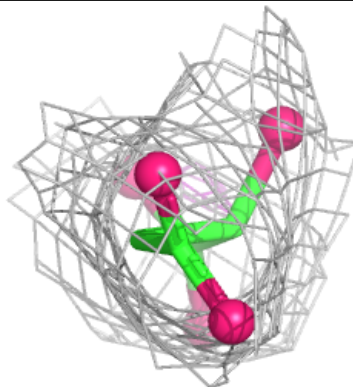
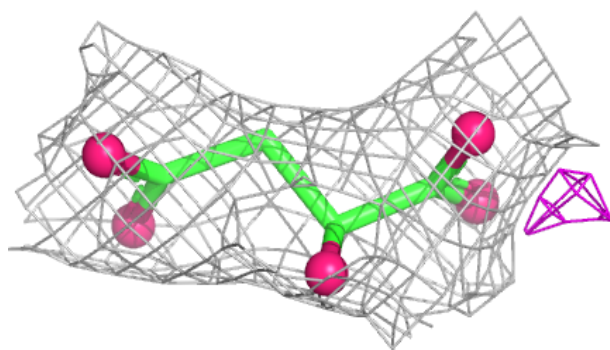
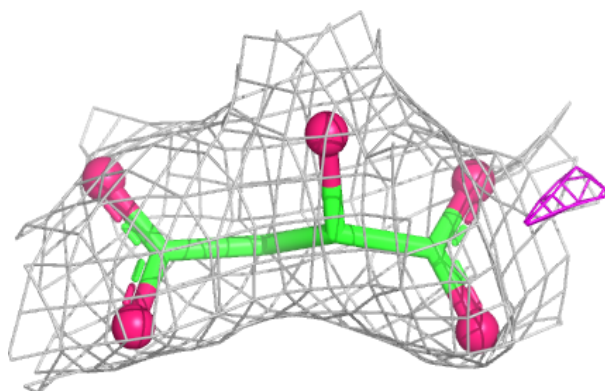
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMR 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)

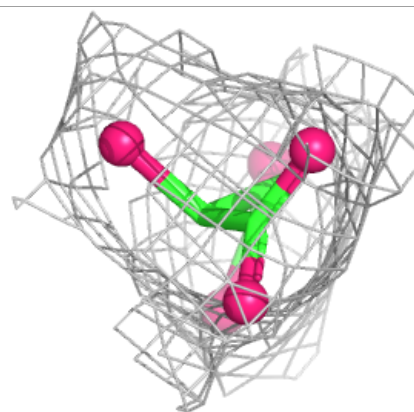
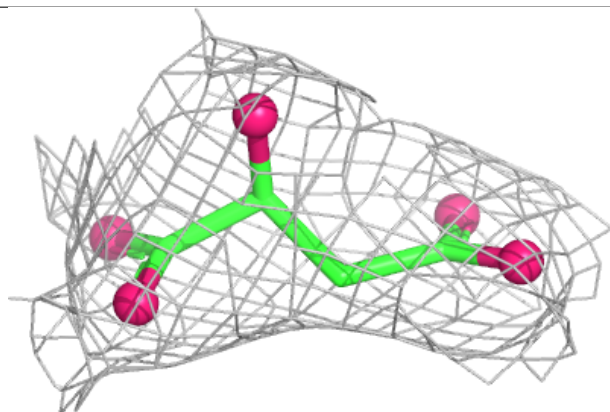
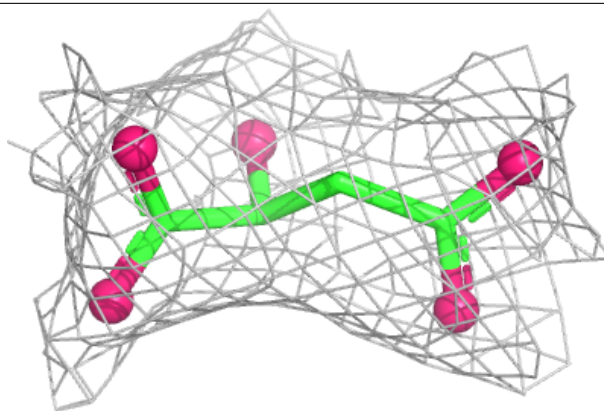
**Electron density around LMR D 1001:**

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

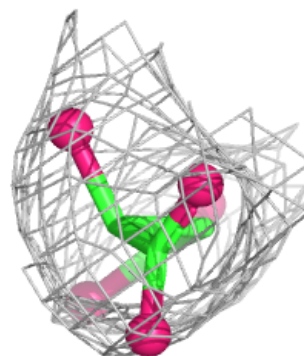
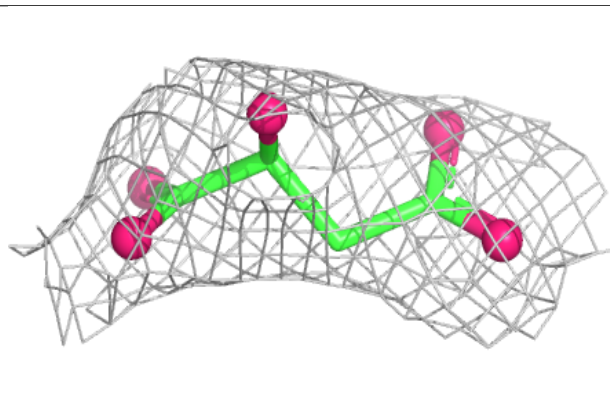
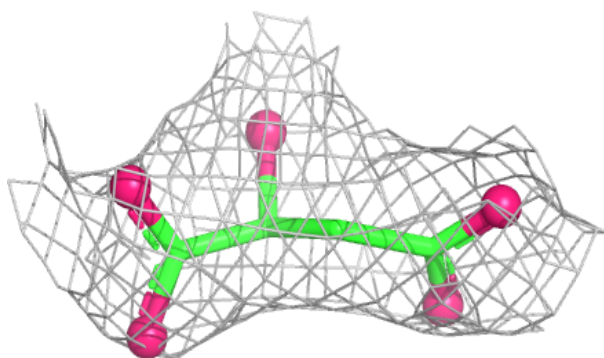


Electron density around LMR F 1001:

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

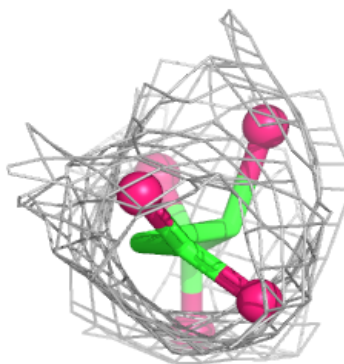
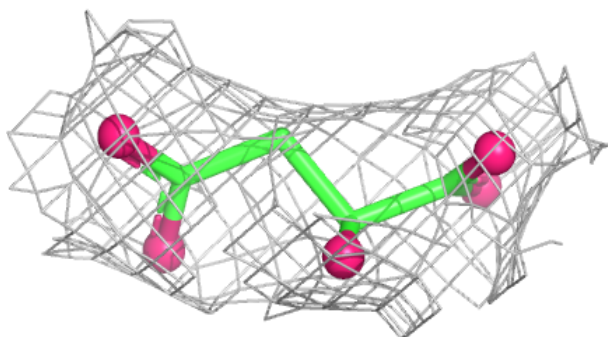
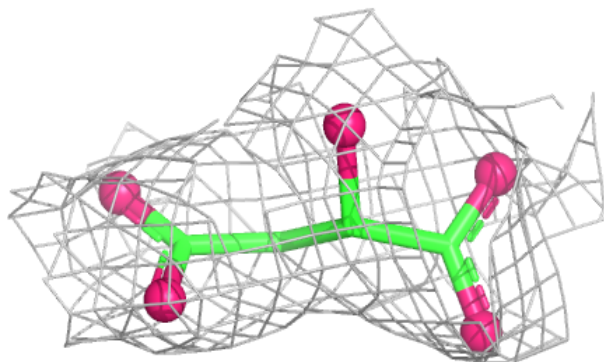
**Electron density around LMR A 1001:**

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

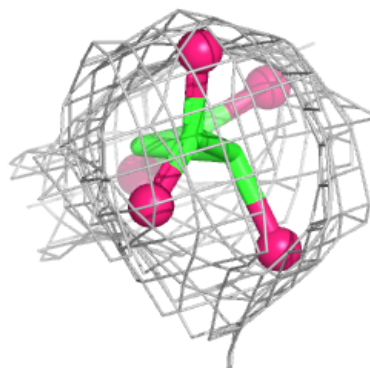
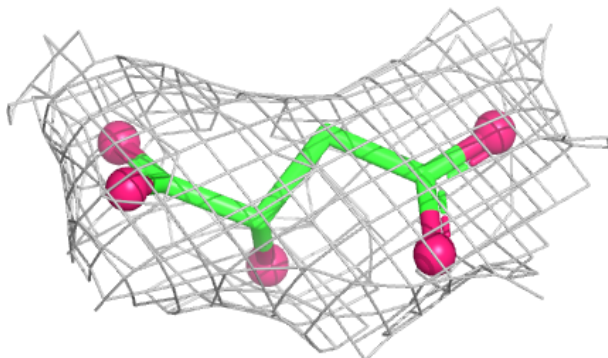
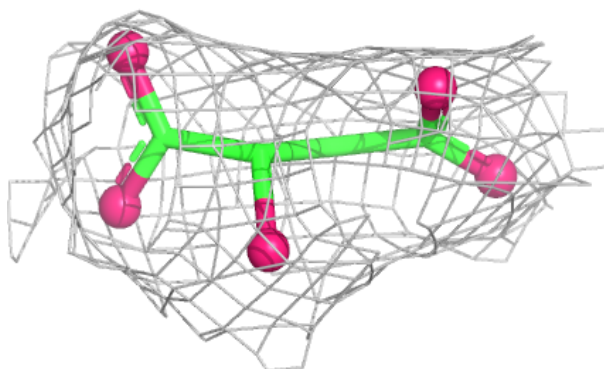


Electron density around LMR G 1001:

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

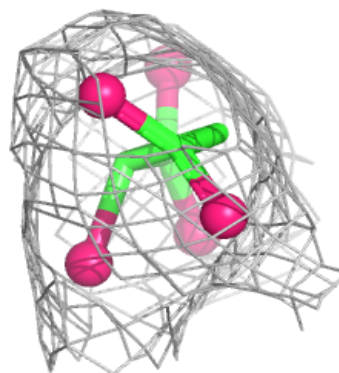
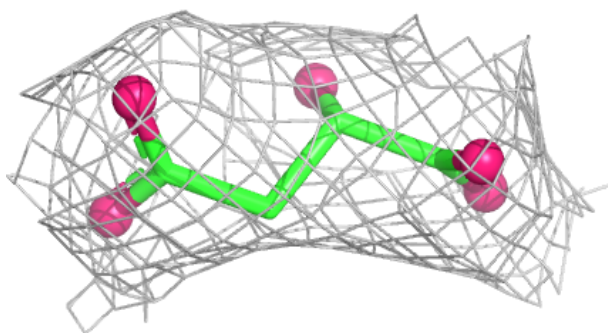
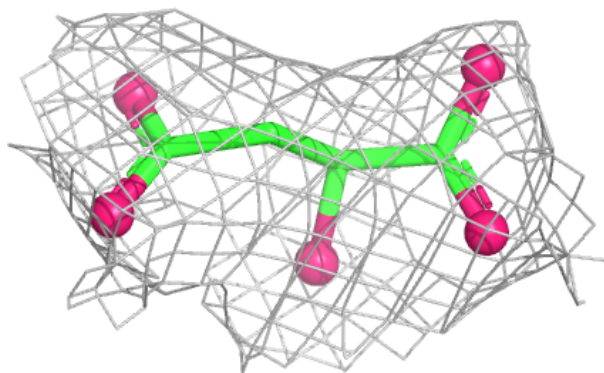
**Electron density around LMR E 1001:**

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

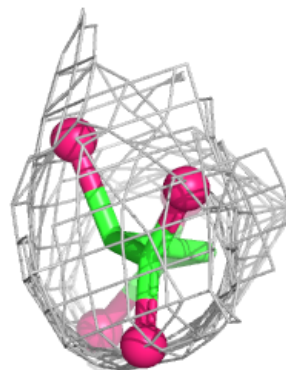
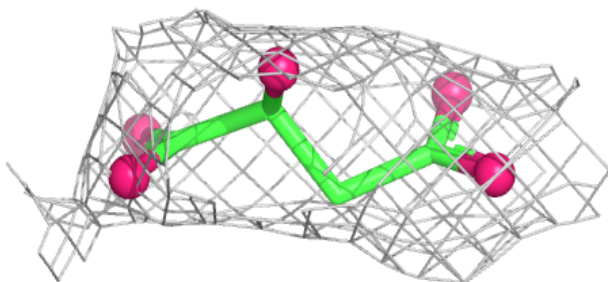
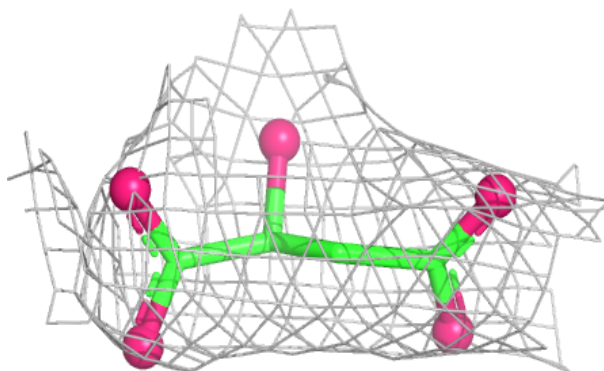


Electron density around LMR C 1001:

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

**Electron density around LMR H 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 ⓘ

There are no such residues in this entry.